



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2021 – 06:48 am BST

PDB ID : 7OK2
Title : Crystal structure of Pseudomonas aeruginosa LpxA in complex with compound 3
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 : 2.89 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

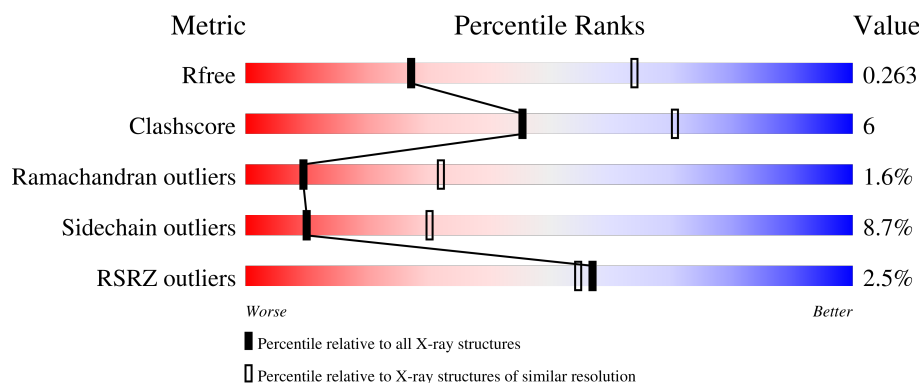
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	1	261	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>..</div> </div> </div>
1	2	261	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>..</div> </div> </div>
1	3	261	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>..</div> </div> </div>
1	4	261	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>..</div> </div> </div>
1	A	261	<div> <div></div> <div> <div></div> <div>78%</div> <div>19%</div> <div>..</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	B	261	
1	C	261	
1	D	261	
1	E	261	
1	F	261	
1	G	261	
1	H	261	
1	I	261	
1	J	261	
1	K	261	
1	L	261	
1	M	261	
1	N	261	
1	O	261	
1	P	261	
1	Q	261	
1	R	261	
1	S	261	
1	T	261	
1	U	261	
1	V	261	
1	W	261	
1	X	261	
1	Y	261	
1	Z	261	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 60216 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	1	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	2	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	3	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	4	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	A	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	B	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	C	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	D	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	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	0	0
			1974	1235	364	368	7			
1	G	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	H	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	I	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	J	258	Total	C	N	O	S	0	0	0
			1974	1235	364	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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	N	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	O	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	P	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	Q	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	R	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
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	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	W	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	X	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	Y	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	Z	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-2	GLY	-	expression tag	UNP A6V1E4
1	-1	SER	-	expression tag	UNP A6V1E4
1	0	HIS	-	expression tag	UNP A6V1E4
2	-2	GLY	-	expression tag	UNP A6V1E4
2	-1	SER	-	expression tag	UNP A6V1E4
2	0	HIS	-	expression tag	UNP A6V1E4
3	-2	GLY	-	expression tag	UNP A6V1E4
3	-1	SER	-	expression tag	UNP A6V1E4
3	0	HIS	-	expression tag	UNP A6V1E4
4	-2	GLY	-	expression tag	UNP A6V1E4
4	-1	SER	-	expression tag	UNP A6V1E4

Continued on next page...

Continued from previous page...

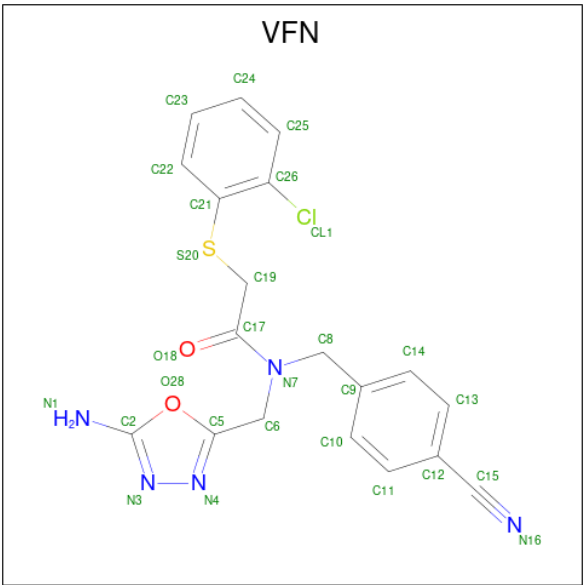
Chain	Residue	Modelled	Actual	Comment	Reference
4	0	HIS	-	expression tag	UNP A6V1E4
A	-2	GLY	-	expression tag	UNP A6V1E4
A	-1	SER	-	expression tag	UNP A6V1E4
A	0	HIS	-	expression tag	UNP A6V1E4
B	-2	GLY	-	expression tag	UNP A6V1E4
B	-1	SER	-	expression tag	UNP A6V1E4
B	0	HIS	-	expression tag	UNP A6V1E4
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- Molecule 2 is {N}-[(5-azanyl-1,3,4-oxadiazol-2-yl)methyl]-2-(2-chlorophenyl)sulfanyl- {N}-[(4-cyanophenyl)methyl]ethanamide (three-letter code: VFN) (formula: C₁₉H₁₆ClN₅O₂S) (labeled as "Ligand of Interest" by depositor).



Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	J	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	K	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	L	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	N	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	O	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	O	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	P	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	P	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	R	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	S	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	S	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	T	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	V	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	W	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	W	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	Z	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1	1	Total	O	S	0	0
			5	4	1		
3	2	1	Total	O	S	0	0
			5	4	1		
3	3	1	Total	O	S	0	0
			5	4	1		
3	4	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		
3	S	1	Total	O	S	0	0
			5	4	1		
3	T	1	Total	O	S	0	0
			5	4	1		
3	U	1	Total	O	S	0	0
			5	4	1		
3	V	1	Total	O	S	0	0
			5	4	1		
3	W	1	Total	O	S	0	0
			5	4	1		
3	X	1	Total	O	S	0	0
			5	4	1		
3	Y	1	Total	O	S	0	0
			5	4	1		
3	Z	1	Total	O	S	0	0
			5	4	1		

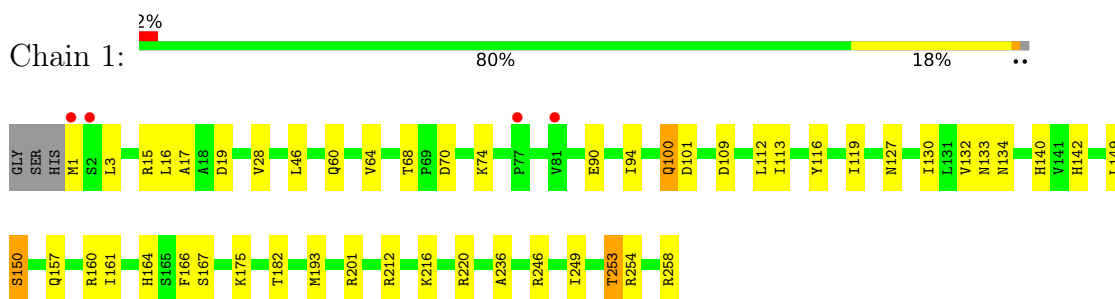
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		

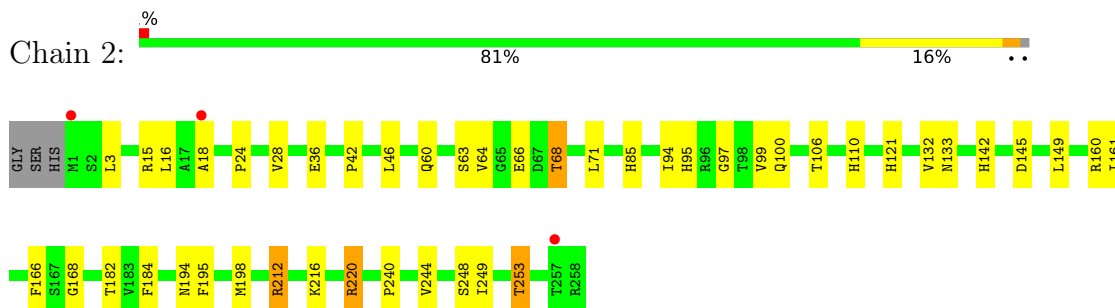
3 Residue-property plots

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.

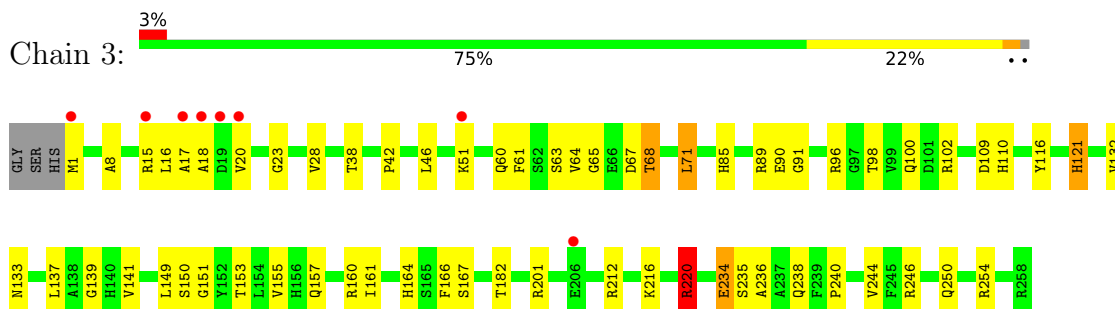
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



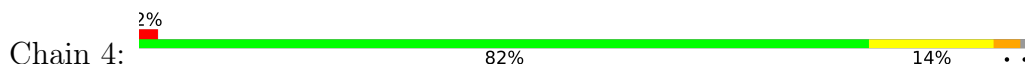
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

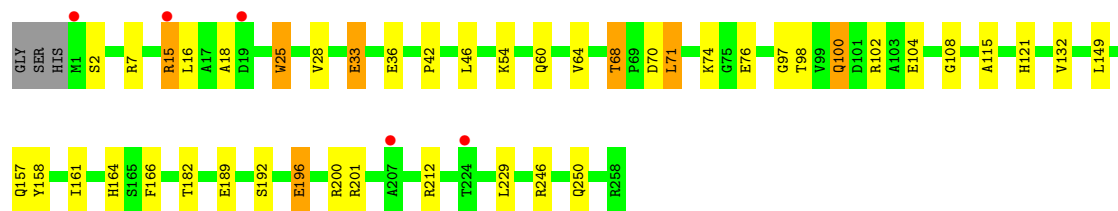


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



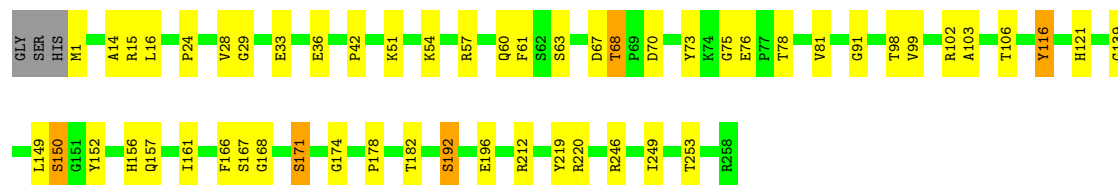
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase





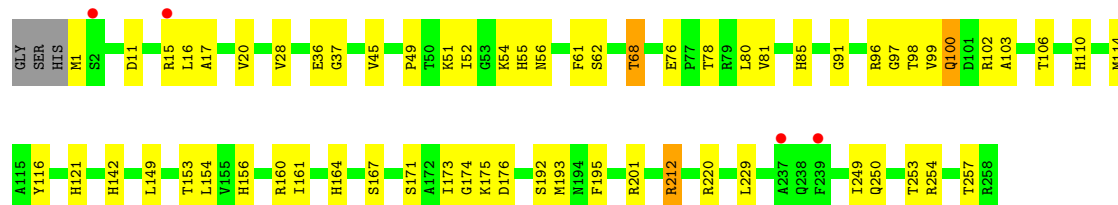
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain A: 78% 19% ..



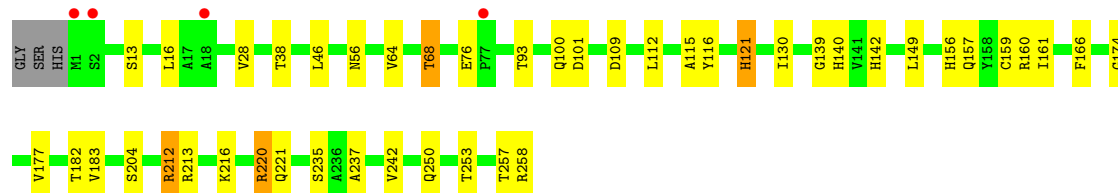
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain B: 75% 23% ..



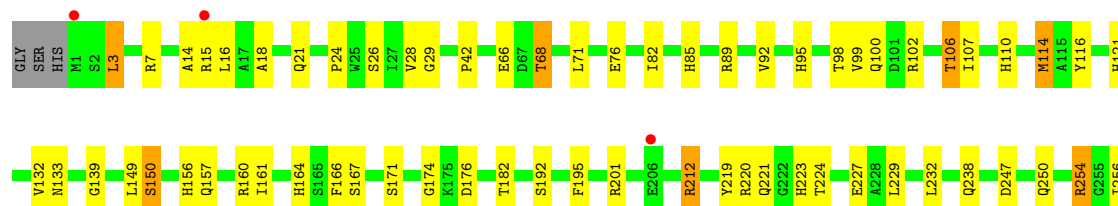
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain C: 82% 16% ..




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

Chain D: 74% 22% ..



T257
R258


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

Chain E: 

GLY SER HIS M1 S2 L3 S13 A14 R15 V28 Q29 A30 G35 L46 Y51 D67 T68 P69 K72 R79 L80 Y81 R89 V92 T98 Y99 Q100 D101 R102 A103 E104 T105 T106 D109 M114 A115 Y116 H121 N133 H142 L149 S150

H156 Q157 R160 I161 H164 S165 F166 S167 G174 T182 M193 S204 S205 A207 R213 A214 Y215 K216 R220 R253


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

Chain F: 

GLY SER HIS M1 S2 L3 I4 R15 L16 A17 V20 Q21 V22 V28 F61 D67 T68 P69 D70 L71 K72 Y73 V81 R89 E90 G91 V99 Q100 D101 R102 T106 M114 A115 Y116 H121 N127 V132 N133 H142 D145 G151 H156 Q157

Y158 G159 R160 H164 S165 F166 G174 K175 D176 T182 M193 R201 R212 Y215 K216 V217 Y218 Y219 R220 Q221 H222 T224 V225 E226 F239 V242 F245 R246 I249 Q250 T253 R258


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

Chain G: 

GLY SER HIS M1 S2 I9 R15 L16 Q21 I27 V28 E33 I34 G35 E36 L46 K47 K54 T58 G65 T68 P69 D70 L71 K72 P77 T78 R79 L82 N86 V87 I88 T98 Y99 Q100 D101 E104 H110 M114 H121 H128

L131 N133 H140 V141 H142 D145 I148 L149 S150 G151 R160 I161 H164 S165 F166 Y180 Y181 T182 S192 M193 R199 R200 R201 S204 S205 E206 A207 R212 R213 A214 Y215 R220 Q221 A236 Q237 Q238 R246 T253 T257 R258

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


Chain H: 

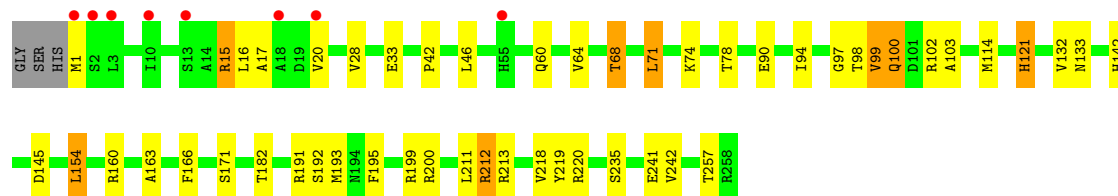
GLY SER HIS M1 S2 L3 I4 I9 R15 L16 D19 V20 Q21 V28 E33 I34 T38 I52 G53 N56 Y59 T68 P69 D70 L71 K72 Y73 T78 R79 L80 R89 E90 G91 T93 R96 G97 T98 Q100 D101 R102 A103 E104 I107 G108

D109 H110 A115 Y116 H121 I125 H128 V132 N133 M134 L137 V141 H142 L149 R160 I161 H164 S165 F166 M169 G170 S171 T182 V183 A188 M193 N194 G197 M198 R201 S205 R212 R220 Q221 G222 H223 E227 S235


Q238 T253 R258

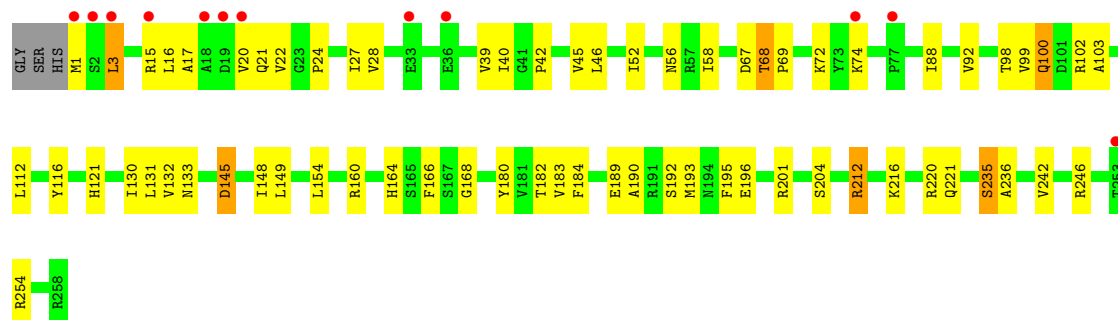
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain I: 




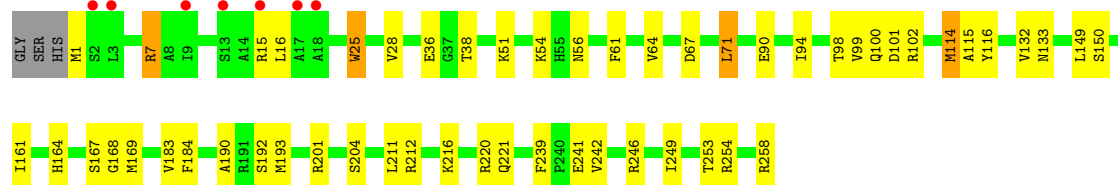
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain J: 




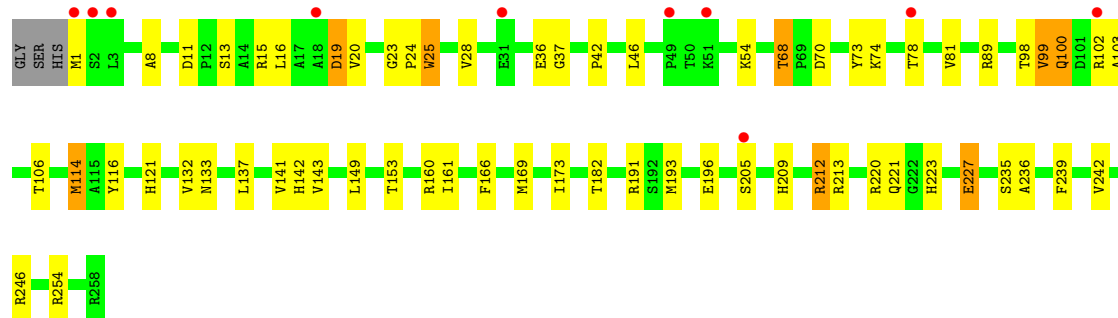
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain K: 

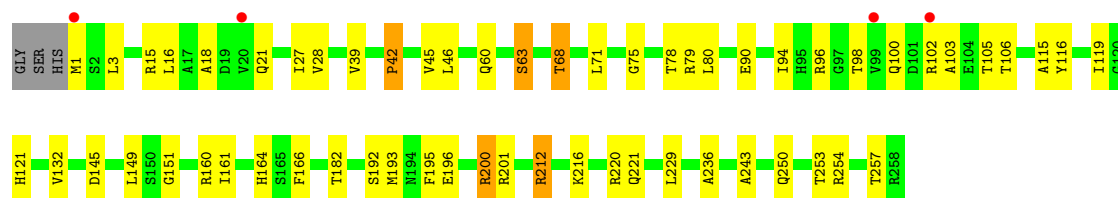
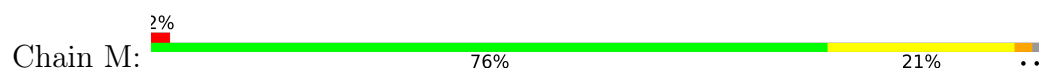


• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

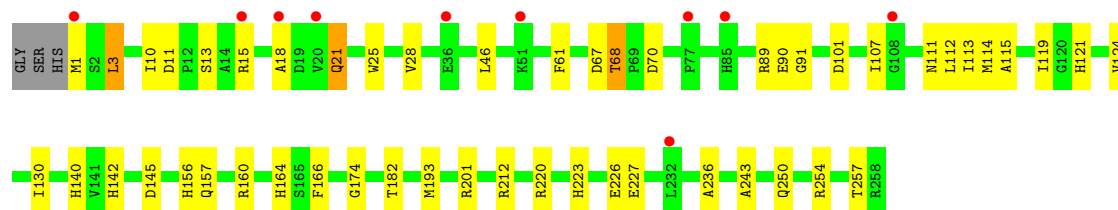
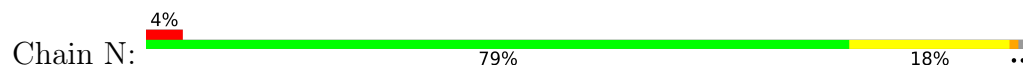
Chain L: 



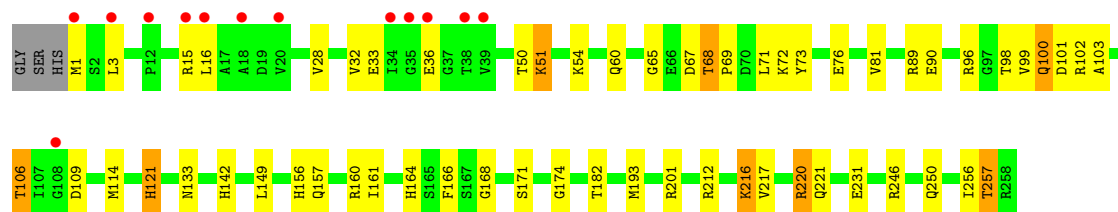
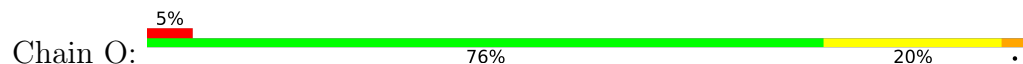
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



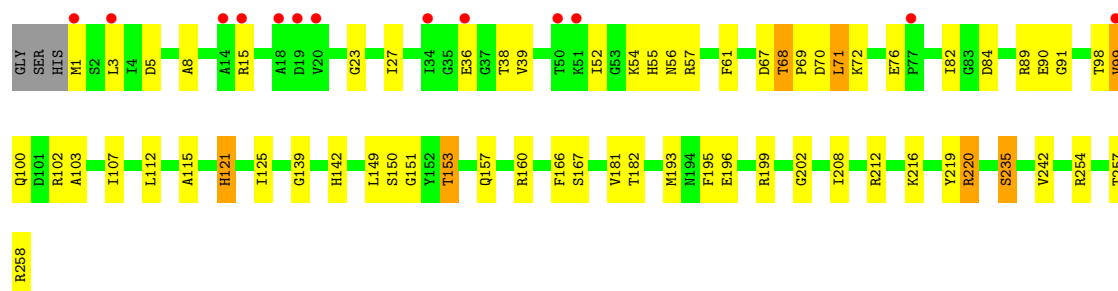
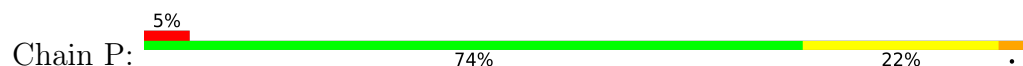
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



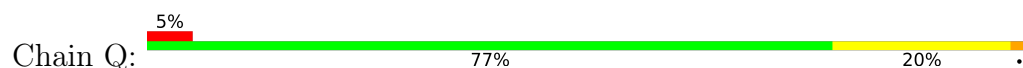
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

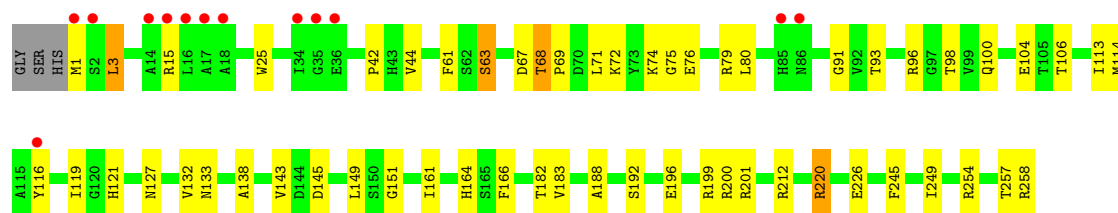


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

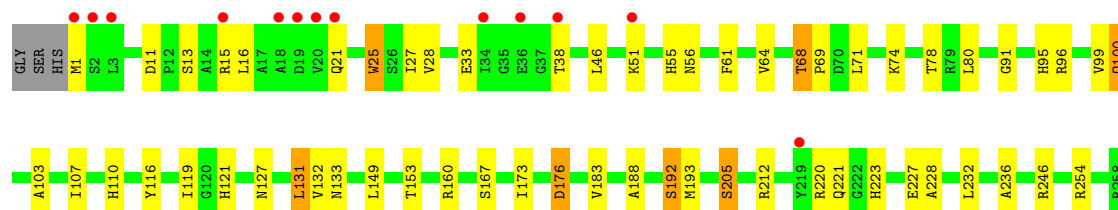
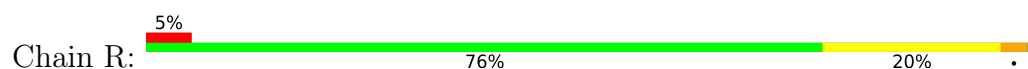


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

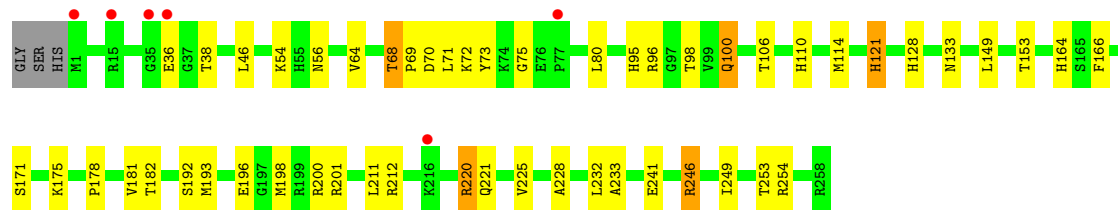
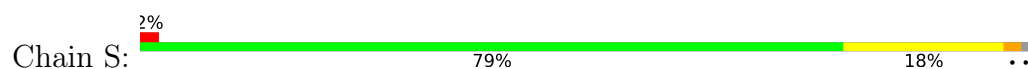




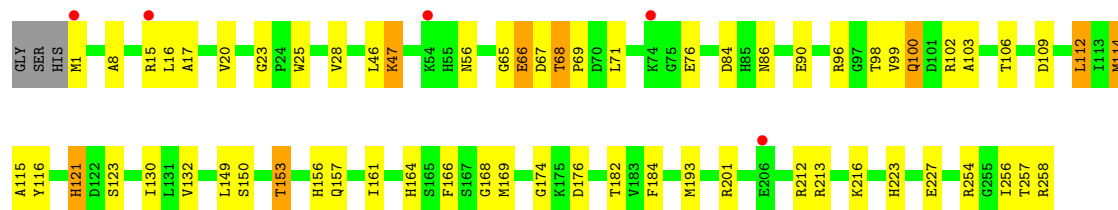
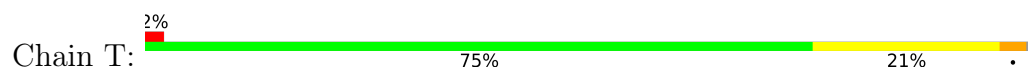
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



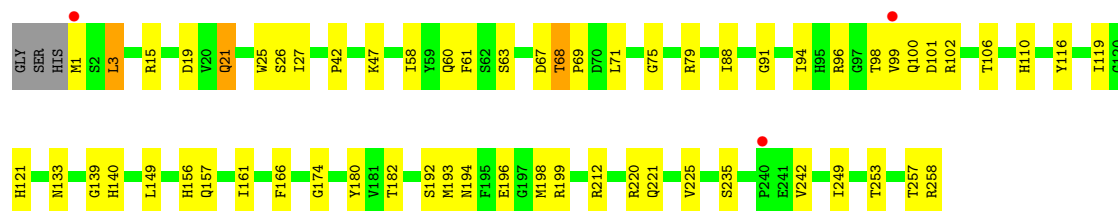
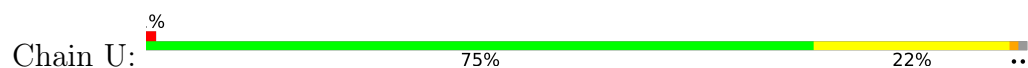
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase




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

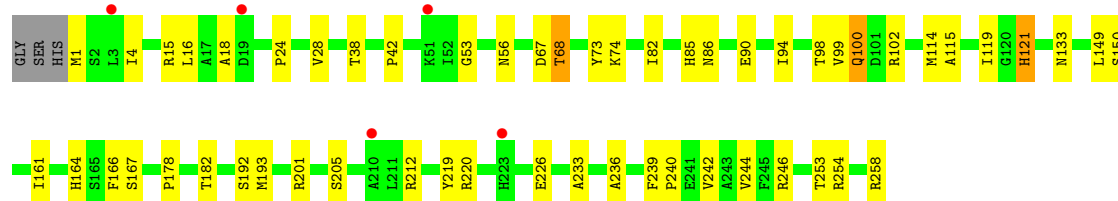


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase




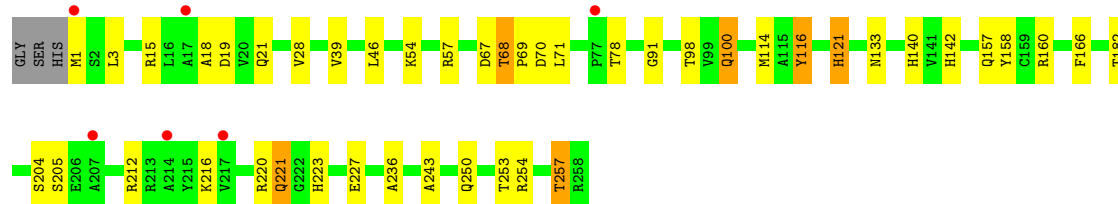
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain V:  2% 78% 20% ..




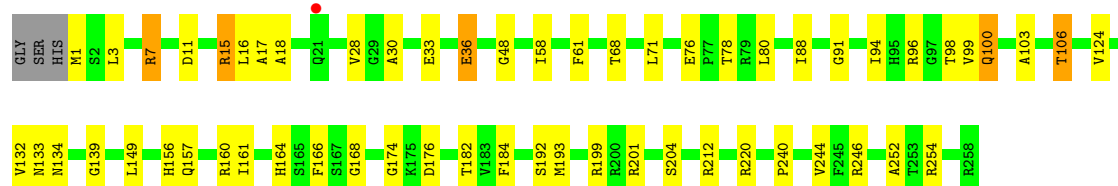
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain W:  2% 82% 15% ..




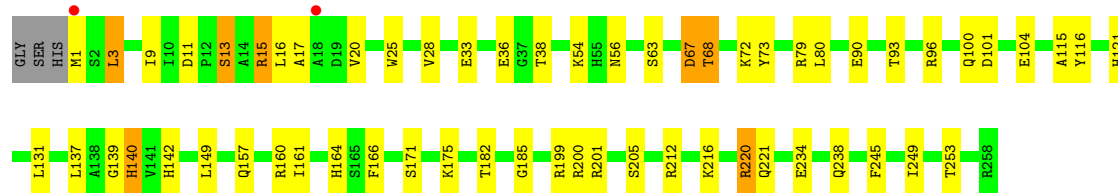
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain X:  77% 20% ..




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

Chain Y:  76% 20% ..



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

Chain Z:  76% 20% ..



V143	D144	D145	W146	T153	R160	H164	S165	F166	S167	G168	T182	V183	F184	S192	M193	R199	R200	R201	S205	R212	Q221	G222	H223	E234	P240	V244	D247	S248	I249	Q250	T253	R254	R258
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	247.29Å 367.65Å 372.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.45 – 2.89 49.45 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.45-2.89) 99.8 (49.45-2.89)	Depositor EDS
R_{merge}	0.59	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.192 , 0.231 0.225 , 0.263	Depositor DCC
R_{free} test set	18696 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	60216	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: VFN, SO4

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	1	0.53	0/2016	0.78	0/2734
1	2	0.53	0/2016	0.78	0/2734
1	3	0.52	0/2016	0.79	0/2734
1	4	0.53	0/2016	0.79	0/2734
1	A	0.52	0/2016	0.78	0/2734
1	B	0.51	0/2016	0.78	0/2734
1	C	0.51	0/2016	0.76	0/2734
1	D	0.55	0/2016	0.81	0/2734
1	E	0.54	0/2016	0.80	0/2734
1	F	0.51	0/2016	0.78	0/2734
1	G	0.52	0/2016	0.76	0/2734
1	H	0.49	0/2016	0.75	0/2734
1	I	0.51	0/2016	0.75	0/2734
1	J	0.52	0/2016	0.77	0/2734
1	K	0.50	0/2016	0.74	0/2734
1	L	0.48	0/2016	0.75	0/2734
1	M	0.52	0/2016	0.75	0/2734
1	N	0.50	0/2016	0.75	0/2734
1	O	0.51	0/2016	0.76	0/2734
1	P	0.50	0/2016	0.77	0/2734
1	Q	0.50	0/2016	0.77	0/2734
1	R	0.51	0/2016	0.78	0/2734
1	S	0.52	0/2016	0.78	0/2734
1	T	0.50	0/2016	0.77	0/2734
1	U	0.53	0/2016	0.80	0/2734
1	V	0.53	0/2016	0.80	0/2734
1	W	0.52	0/2016	0.78	0/2734
1	X	0.54	0/2016	0.81	0/2734
1	Y	0.52	0/2016	0.79	0/2734
1	Z	0.54	0/2016	0.79	0/2734
All	All	0.52	0/60480	0.78	0/82020

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1974	0	1947	23	0
1	2	1974	0	1947	20	0
1	3	1974	0	1947	35	0
1	4	1974	0	1947	20	0
1	A	1974	0	1947	22	0
1	B	1974	0	1947	32	0
1	C	1974	0	1947	19	0
1	D	1974	0	1947	34	0
1	E	1974	0	1947	20	0
1	F	1974	0	1947	34	0
1	G	1974	0	1947	33	0
1	H	1974	0	1947	29	0
1	I	1974	0	1947	23	0
1	J	1974	0	1947	36	0
1	K	1974	0	1947	23	0
1	L	1974	0	1947	33	0
1	M	1974	0	1947	28	0
1	N	1974	0	1947	18	0
1	O	1974	0	1947	29	0
1	P	1974	0	1947	34	0
1	Q	1974	0	1947	25	0
1	R	1974	0	1947	30	0
1	S	1974	0	1947	27	0
1	T	1974	0	1947	32	0
1	U	1974	0	1947	21	0
1	V	1974	0	1947	23	0
1	W	1974	0	1947	20	0
1	X	1974	0	1947	26	0
1	Y	1974	0	1947	28	0
1	Z	1974	0	1947	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1	56	0	0	0	0
2	2	28	0	0	1	0
2	3	56	0	0	3	0
2	A	56	0	0	0	0
2	B	28	0	0	0	0
2	D	56	0	0	0	0
2	F	28	0	0	0	0
2	G	28	0	0	1	0
2	H	56	0	0	3	0
2	J	28	0	0	0	0
2	K	28	0	0	1	0
2	L	28	0	0	0	0
2	N	28	0	0	1	0
2	O	56	0	0	0	0
2	P	56	0	0	3	0
2	R	28	0	0	1	0
2	S	56	0	0	0	0
2	T	28	0	0	0	0
2	V	28	0	0	0	0
2	W	56	0	0	1	0
2	Z	28	0	0	0	0
3	1	5	0	0	0	0
3	2	5	0	0	0	0
3	3	5	0	0	0	0
3	4	5	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
3	M	5	0	0	0	0
3	N	5	0	0	0	0
3	O	5	0	0	0	0
3	P	5	0	0	0	0
3	Q	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	5	0	0	0	0
3	S	5	0	0	0	0
3	T	5	0	0	0	0
3	U	5	0	0	0	0
3	V	5	0	0	0	0
3	W	5	0	0	0	0
3	X	5	0	0	0	0
3	Y	5	0	0	0	0
3	Z	5	0	0	0	0
4	B	1	0	0	0	0
All	All	60216	0	58410	757	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.

The worst 5 of 757 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:C:68:THR:HG21	1:C:121:HIS:HD2	1.36	0.89
1:H:164:HIS:CE1	1:H:201:ARG:HG3	2.09	0.88
1:3:98:THR:HB	1:3:100:GLN:HE21	1.38	0.88
1:1:249:ILE:O	1:1:253:THR:HG22	1.76	0.86
1:H:164:HIS:HE1	1:H:201:ARG:HG3	1.40	0.84

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	1	256/261 (98%)	225 (88%)	28 (11%)	3 (1%)	13	40
1	2	256/261 (98%)	224 (88%)	28 (11%)	4 (2%)	9	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	256/261 (98%)	220 (86%)	31 (12%)	5 (2%)	7	27
1	4	256/261 (98%)	218 (85%)	32 (12%)	6 (2%)	6	23
1	A	256/261 (98%)	229 (90%)	22 (9%)	5 (2%)	7	27
1	B	256/261 (98%)	222 (87%)	29 (11%)	5 (2%)	7	27
1	C	256/261 (98%)	224 (88%)	28 (11%)	4 (2%)	9	32
1	D	256/261 (98%)	221 (86%)	33 (13%)	2 (1%)	19	51
1	E	256/261 (98%)	223 (87%)	29 (11%)	4 (2%)	9	32
1	F	256/261 (98%)	230 (90%)	24 (9%)	2 (1%)	19	51
1	G	256/261 (98%)	225 (88%)	27 (10%)	4 (2%)	9	32
1	H	256/261 (98%)	227 (89%)	22 (9%)	7 (3%)	5	19
1	I	256/261 (98%)	226 (88%)	25 (10%)	5 (2%)	7	27
1	J	256/261 (98%)	219 (86%)	35 (14%)	2 (1%)	19	51
1	K	256/261 (98%)	218 (85%)	34 (13%)	4 (2%)	9	32
1	L	256/261 (98%)	229 (90%)	26 (10%)	1 (0%)	34	66
1	M	256/261 (98%)	225 (88%)	26 (10%)	5 (2%)	7	27
1	N	256/261 (98%)	228 (89%)	26 (10%)	2 (1%)	19	51
1	O	256/261 (98%)	223 (87%)	30 (12%)	3 (1%)	13	40
1	P	256/261 (98%)	223 (87%)	26 (10%)	7 (3%)	5	19
1	Q	256/261 (98%)	218 (85%)	31 (12%)	7 (3%)	5	19
1	R	256/261 (98%)	223 (87%)	28 (11%)	5 (2%)	7	27
1	S	256/261 (98%)	231 (90%)	20 (8%)	5 (2%)	7	27
1	T	256/261 (98%)	223 (87%)	31 (12%)	2 (1%)	19	51
1	U	256/261 (98%)	219 (86%)	31 (12%)	6 (2%)	6	23
1	V	256/261 (98%)	225 (88%)	26 (10%)	5 (2%)	7	27
1	W	256/261 (98%)	224 (88%)	28 (11%)	4 (2%)	9	32
1	X	256/261 (98%)	226 (88%)	27 (10%)	3 (1%)	13	40
1	Y	256/261 (98%)	228 (89%)	26 (10%)	2 (1%)	19	51
1	Z	256/261 (98%)	223 (87%)	29 (11%)	4 (2%)	9	32
All	All	7680/7830 (98%)	6719 (88%)	838 (11%)	123 (2%)	9	32

5 of 123 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	18	ALA
1	3	18	ALA
1	3	220	ARG
1	C	220	ARG
1	D	18	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1	206/208 (99%)	190 (92%)	16 (8%)	12	34
1	2	206/208 (99%)	192 (93%)	14 (7%)	16	42
1	3	206/208 (99%)	194 (94%)	12 (6%)	20	50
1	4	206/208 (99%)	193 (94%)	13 (6%)	18	46
1	A	206/208 (99%)	191 (93%)	15 (7%)	14	38
1	B	206/208 (99%)	189 (92%)	17 (8%)	11	32
1	C	206/208 (99%)	191 (93%)	15 (7%)	14	38
1	D	206/208 (99%)	187 (91%)	19 (9%)	9	27
1	E	206/208 (99%)	193 (94%)	13 (6%)	18	46
1	F	206/208 (99%)	192 (93%)	14 (7%)	16	42
1	G	206/208 (99%)	184 (89%)	22 (11%)	6	20
1	H	206/208 (99%)	188 (91%)	18 (9%)	10	30
1	I	206/208 (99%)	187 (91%)	19 (9%)	9	27
1	J	206/208 (99%)	186 (90%)	20 (10%)	8	25
1	K	206/208 (99%)	189 (92%)	17 (8%)	11	32
1	L	206/208 (99%)	183 (89%)	23 (11%)	6	18
1	M	206/208 (99%)	189 (92%)	17 (8%)	11	32
1	N	206/208 (99%)	187 (91%)	19 (9%)	9	27
1	O	206/208 (99%)	184 (89%)	22 (11%)	6	20
1	P	206/208 (99%)	188 (91%)	18 (9%)	10	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	206/208 (99%)	189 (92%)	17 (8%)	11	32
1	R	206/208 (99%)	188 (91%)	18 (9%)	10	30
1	S	206/208 (99%)	193 (94%)	13 (6%)	18	46
1	T	206/208 (99%)	181 (88%)	25 (12%)	5	15
1	U	206/208 (99%)	182 (88%)	24 (12%)	5	16
1	V	206/208 (99%)	187 (91%)	19 (9%)	9	27
1	W	206/208 (99%)	185 (90%)	21 (10%)	7	22
1	X	206/208 (99%)	185 (90%)	21 (10%)	7	22
1	Y	206/208 (99%)	191 (93%)	15 (7%)	14	38
1	Z	206/208 (99%)	187 (91%)	19 (9%)	9	27
All	All	6180/6240 (99%)	5645 (91%)	535 (9%)	10	30

5 of 535 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	54	LYS
1	W	221	GLN
1	W	19	ASP
1	Z	74	LYS
1	I	99	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	164	HIS
1	S	164	HIS
1	P	100	GLN
1	Q	164	HIS
1	T	164	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

61 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	VFN	3	302	-	26,30,30	0.99	2 (7%)	28,40,40	0.59	0
2	VFN	A	301	-	26,30,30	0.92	2 (7%)	28,40,40	0.90	1 (3%)
3	SO4	4	301	-	4,4,4	0.07	0	6,6,6	0.22	0
2	VFN	Z	301	-	26,30,30	0.96	1 (3%)	28,40,40	0.91	1 (3%)
3	SO4	C	302	-	4,4,4	0.22	0	6,6,6	0.18	0
3	SO4	U	301	-	4,4,4	0.12	0	6,6,6	0.29	0
3	SO4	M	301	-	4,4,4	0.14	0	6,6,6	0.15	0
2	VFN	N	301	-	26,30,30	0.85	1 (3%)	28,40,40	0.85	1 (3%)
2	VFN	D	302	-	26,30,30	0.81	1 (3%)	28,40,40	0.83	0
2	VFN	B	301	-	26,30,30	0.89	0	28,40,40	0.83	0
2	VFN	P	302	-	26,30,30	0.87	1 (3%)	28,40,40	1.03	1 (3%)
3	SO4	H	303	-	4,4,4	0.18	0	6,6,6	0.18	0
3	SO4	Q	301	-	4,4,4	0.15	0	6,6,6	0.22	0
2	VFN	R	301	-	26,30,30	0.94	2 (7%)	28,40,40	1.07	2 (7%)
3	SO4	O	303	-	4,4,4	0.19	0	6,6,6	0.09	0
3	SO4	R	302	-	4,4,4	0.21	0	6,6,6	0.29	0
2	VFN	K	301	-	26,30,30	0.98	2 (7%)	28,40,40	0.95	1 (3%)
2	VFN	A	302	-	26,30,30	0.89	1 (3%)	28,40,40	0.86	1 (3%)
2	VFN	J	301	-	26,30,30	1.01	1 (3%)	28,40,40	0.90	0
3	SO4	V	302	-	4,4,4	0.11	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	VFN	W	301	-	26,30,30	1.00	1 (3%)	28,40,40	1.18	3 (10%)
2	VFN	F	301	-	26,30,30	0.96	2 (7%)	28,40,40	1.05	1 (3%)
2	VFN	H	302	-	26,30,30	0.97	2 (7%)	28,40,40	1.14	2 (7%)
2	VFN	O	302	-	26,30,30	0.92	1 (3%)	28,40,40	0.83	1 (3%)
2	VFN	D	301	-	26,30,30	0.96	2 (7%)	28,40,40	0.88	0
2	VFN	P	301	-	26,30,30	0.94	2 (7%)	28,40,40	0.86	0
3	SO4	C	301	-	4,4,4	0.10	0	6,6,6	0.21	0
3	SO4	L	302	-	4,4,4	0.09	0	6,6,6	0.19	0
2	VFN	3	301	-	26,30,30	0.88	1 (3%)	28,40,40	0.85	1 (3%)
2	VFN	1	302	-	26,30,30	1.07	2 (7%)	28,40,40	1.21	4 (14%)
2	VFN	G	301	-	26,30,30	0.98	0	28,40,40	0.82	0
3	SO4	Y	301	-	4,4,4	0.19	0	6,6,6	0.17	0
3	SO4	K	302	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	3	303	-	4,4,4	0.16	0	6,6,6	0.14	0
3	SO4	2	302	-	4,4,4	0.25	0	6,6,6	0.29	0
3	SO4	F	302	-	4,4,4	0.25	0	6,6,6	0.15	0
2	VFN	2	301	-	26,30,30	0.93	1 (3%)	28,40,40	0.86	1 (3%)
2	VFN	O	301	-	26,30,30	0.87	1 (3%)	28,40,40	0.94	1 (3%)
3	SO4	X	301	-	4,4,4	0.24	0	6,6,6	0.13	0
2	VFN	S	301	-	26,30,30	0.85	0	28,40,40	0.97	1 (3%)
2	VFN	H	301	-	26,30,30	1.00	2 (7%)	28,40,40	1.06	2 (7%)
3	SO4	S	303	-	4,4,4	0.20	0	6,6,6	0.22	0
3	SO4	G	302	-	4,4,4	0.22	0	6,6,6	0.17	0
3	SO4	T	302	-	4,4,4	0.15	0	6,6,6	0.24	0
3	SO4	W	303	-	4,4,4	0.23	0	6,6,6	0.13	0
2	VFN	T	301	-	26,30,30	0.96	1 (3%)	28,40,40	1.06	1 (3%)
2	VFN	W	302	-	26,30,30	0.88	1 (3%)	28,40,40	1.25	4 (14%)
2	VFN	L	301	-	26,30,30	0.90	2 (7%)	28,40,40	0.90	1 (3%)
2	VFN	V	301	-	26,30,30	0.98	1 (3%)	28,40,40	1.05	1 (3%)
3	SO4	E	301	-	4,4,4	0.18	0	6,6,6	0.16	0
3	SO4	1	303	-	4,4,4	0.16	0	6,6,6	0.13	0
3	SO4	J	302	-	4,4,4	0.28	0	6,6,6	0.24	0
3	SO4	B	302	-	4,4,4	0.23	0	6,6,6	0.22	0
2	VFN	S	302	-	26,30,30	1.00	2 (7%)	28,40,40	0.95	1 (3%)
3	SO4	N	302	-	4,4,4	0.20	0	6,6,6	0.24	0
2	VFN	1	301	-	26,30,30	0.91	1 (3%)	28,40,40	0.88	0
3	SO4	I	301	-	4,4,4	0.20	0	6,6,6	0.15	0
3	SO4	A	303	-	4,4,4	0.20	0	6,6,6	0.18	0
3	SO4	P	303	-	4,4,4	0.25	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	303	-	4,4,4	0.28	0	6,6,6	0.26	0
3	SO4	Z	302	-	4,4,4	0.15	0	6,6,6	0.19	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	VFN	3	302	-	-	0/18/19/19	0/3/3/3
2	VFN	A	301	-	-	1/18/19/19	0/3/3/3
2	VFN	Z	301	-	-	0/18/19/19	0/3/3/3
2	VFN	N	301	-	-	0/18/19/19	0/3/3/3
2	VFN	D	302	-	-	0/18/19/19	0/3/3/3
2	VFN	B	301	-	-	0/18/19/19	0/3/3/3
2	VFN	P	302	-	-	0/18/19/19	0/3/3/3
2	VFN	R	301	-	-	0/18/19/19	0/3/3/3
2	VFN	K	301	-	-	0/18/19/19	0/3/3/3
2	VFN	A	302	-	-	0/18/19/19	0/3/3/3
2	VFN	J	301	-	-	0/18/19/19	0/3/3/3
2	VFN	W	301	-	-	0/18/19/19	0/3/3/3
2	VFN	F	301	-	-	0/18/19/19	0/3/3/3
2	VFN	H	302	-	-	0/18/19/19	0/3/3/3
2	VFN	O	302	-	-	0/18/19/19	0/3/3/3
2	VFN	D	301	-	-	0/18/19/19	0/3/3/3
2	VFN	P	301	-	-	0/18/19/19	0/3/3/3
2	VFN	3	301	-	-	0/18/19/19	0/3/3/3
2	VFN	1	302	-	-	0/18/19/19	0/3/3/3
2	VFN	G	301	-	-	0/18/19/19	0/3/3/3
2	VFN	2	301	-	-	1/18/19/19	0/3/3/3
2	VFN	O	301	-	-	0/18/19/19	0/3/3/3
2	VFN	S	301	-	-	0/18/19/19	0/3/3/3
2	VFN	H	301	-	-	0/18/19/19	0/3/3/3
2	VFN	T	301	-	-	1/18/19/19	0/3/3/3
2	VFN	W	302	-	-	0/18/19/19	0/3/3/3
2	VFN	L	301	-	-	0/18/19/19	0/3/3/3
2	VFN	V	301	-	-	0/18/19/19	0/3/3/3
2	VFN	S	302	-	-	0/18/19/19	0/3/3/3
2	VFN	1	301	-	-	0/18/19/19	0/3/3/3

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	302	VFN	C6-C5	-3.01	1.47	1.51
2	H	302	VFN	C6-C5	-3.01	1.47	1.51
2	3	302	VFN	C6-C5	-2.90	1.47	1.51
2	J	301	VFN	C6-C5	-2.86	1.47	1.51
2	V	301	VFN	C6-C5	-2.77	1.48	1.51

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	VFN	C19-S20-C21	3.65	108.21	102.61
2	V	301	VFN	C5-C6-N7	-3.33	108.05	113.64
2	H	301	VFN	C5-C6-N7	-3.13	108.39	113.64
2	S	302	VFN	C5-C6-N7	-3.07	108.48	113.64
2	A	301	VFN	C9-C8-N7	-2.84	108.56	113.13

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	VFN	N4-C5-C6-N7
2	2	301	VFN	C11-C12-C15-N16
2	T	301	VFN	C11-C12-C15-N16

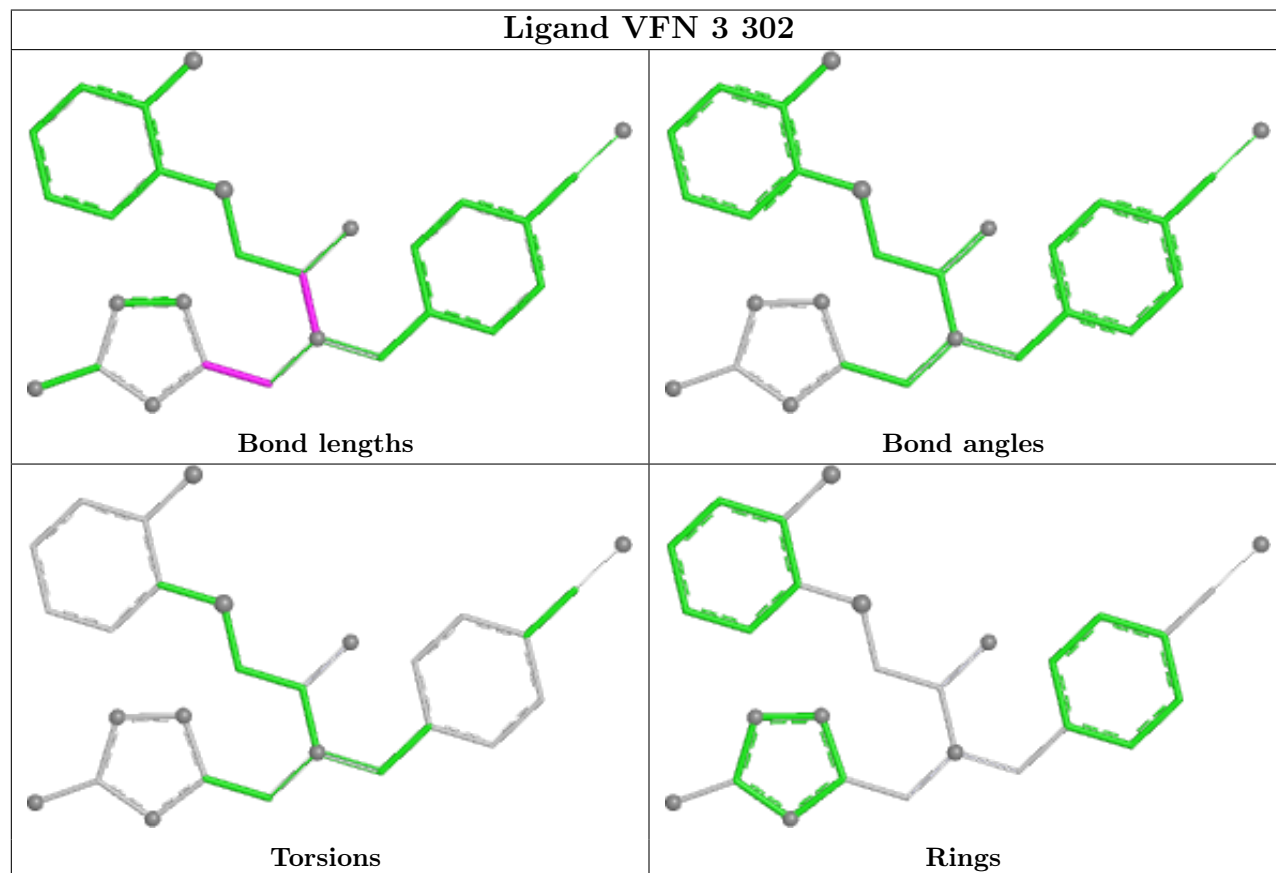
There are no ring outliers.

12 monomers are involved in 15 short contacts:

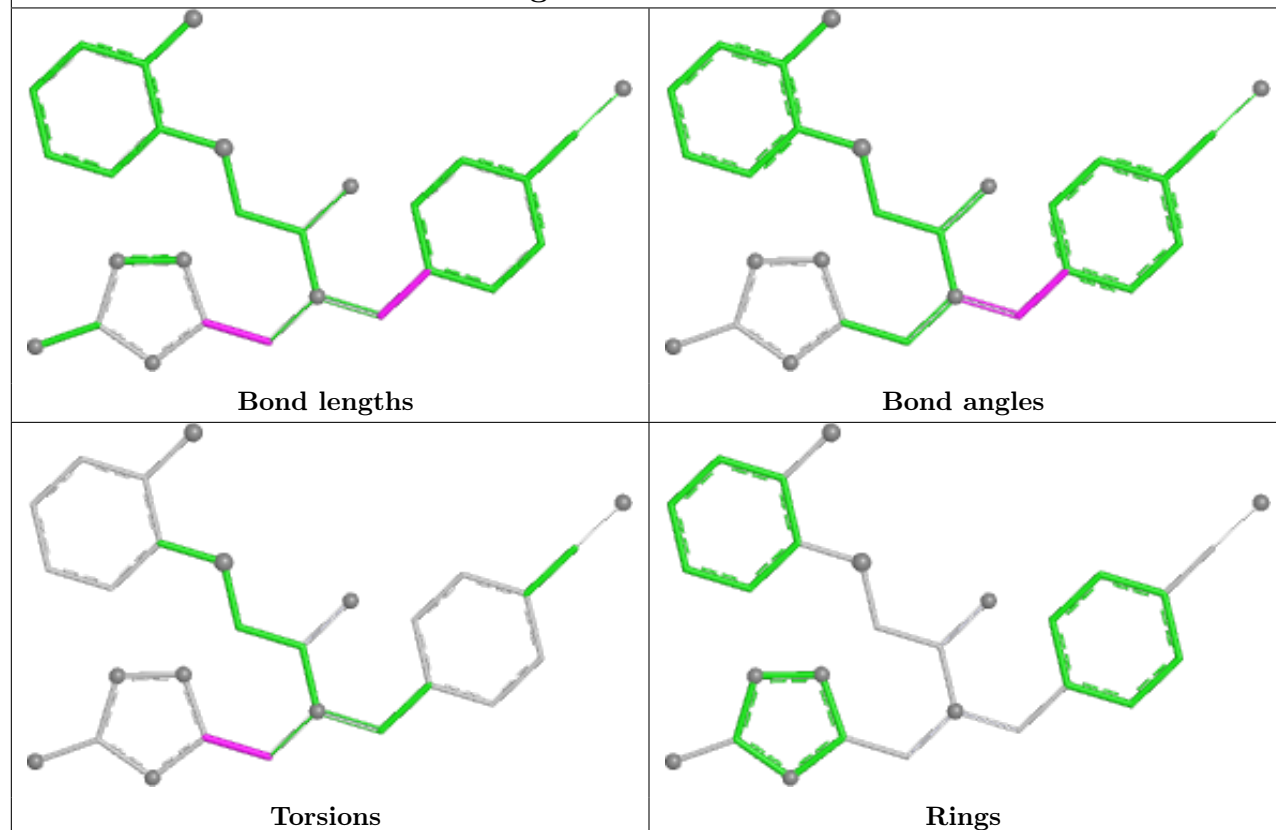
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	3	302	VFN	2	0
2	N	301	VFN	1	0
2	P	302	VFN	2	0
2	R	301	VFN	1	0
2	K	301	VFN	1	0
2	W	301	VFN	1	0
2	H	302	VFN	1	0
2	P	301	VFN	1	0
2	3	301	VFN	1	0
2	G	301	VFN	1	0
2	2	301	VFN	1	0
2	H	301	VFN	2	0

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

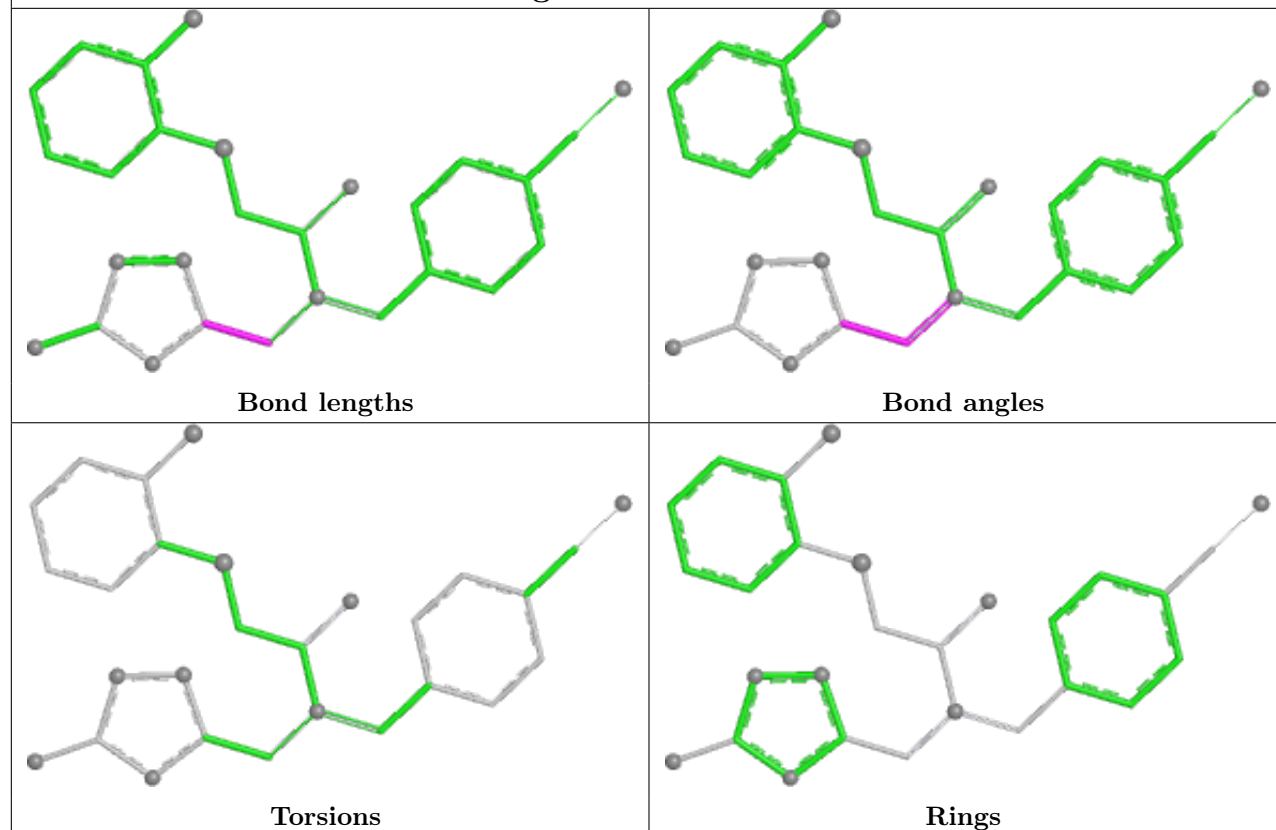
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

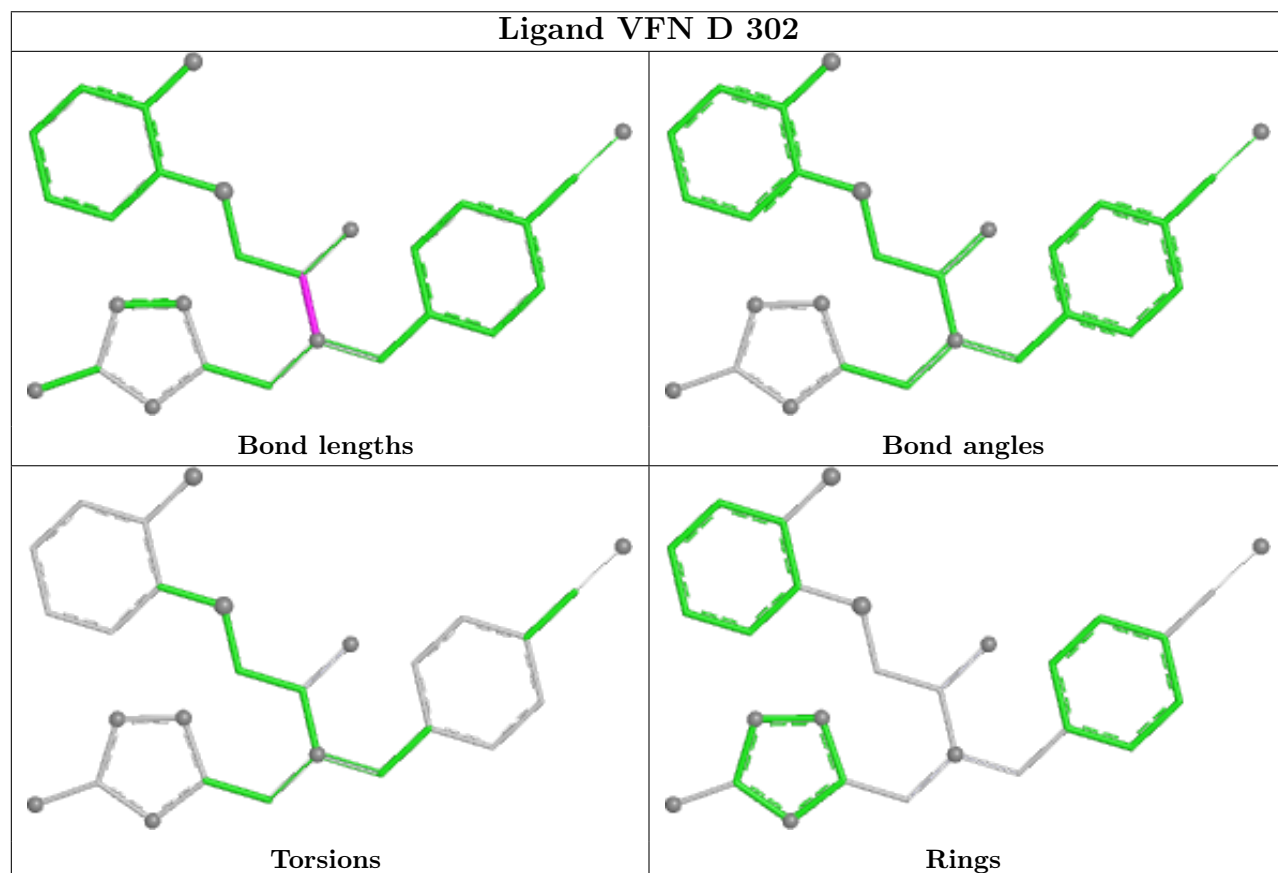
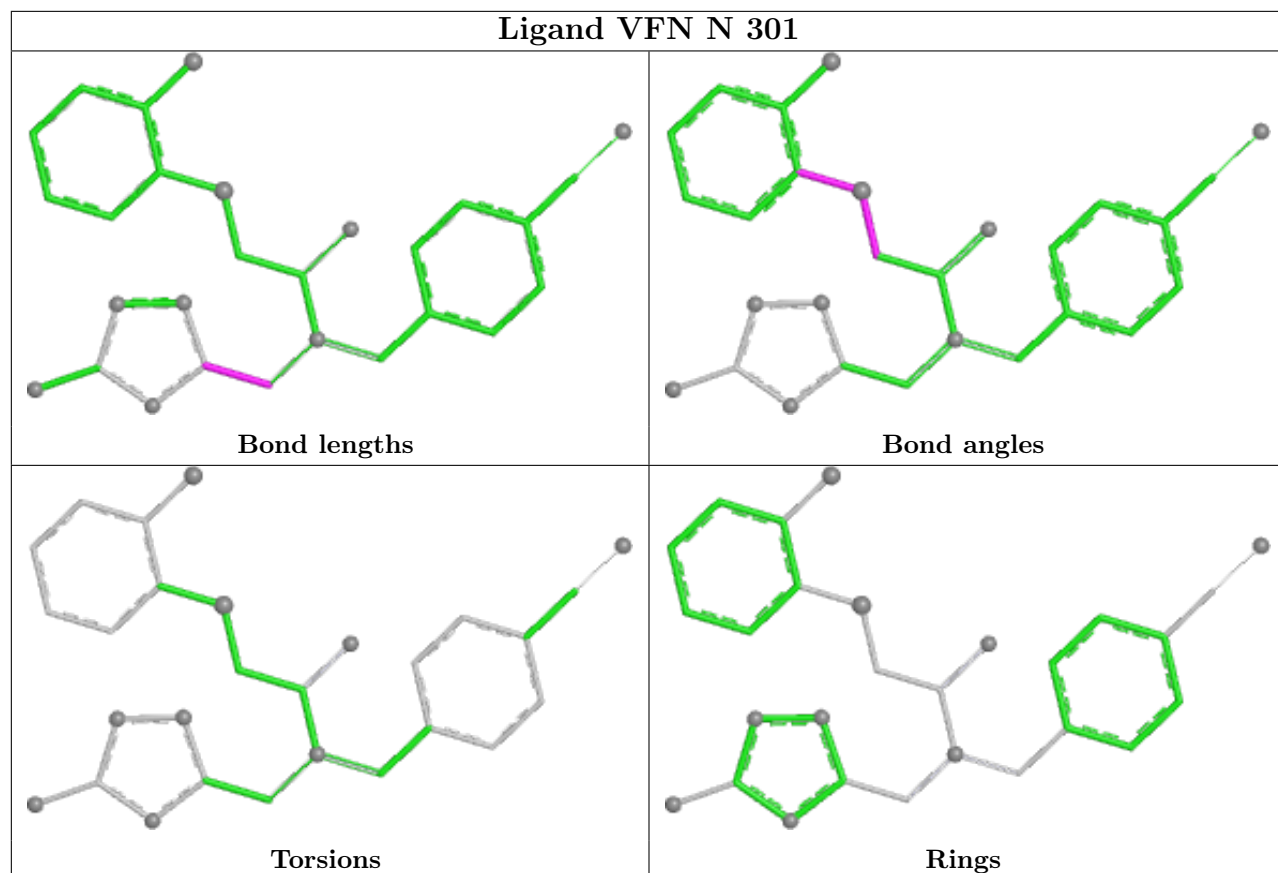


Ligand VFN A 301

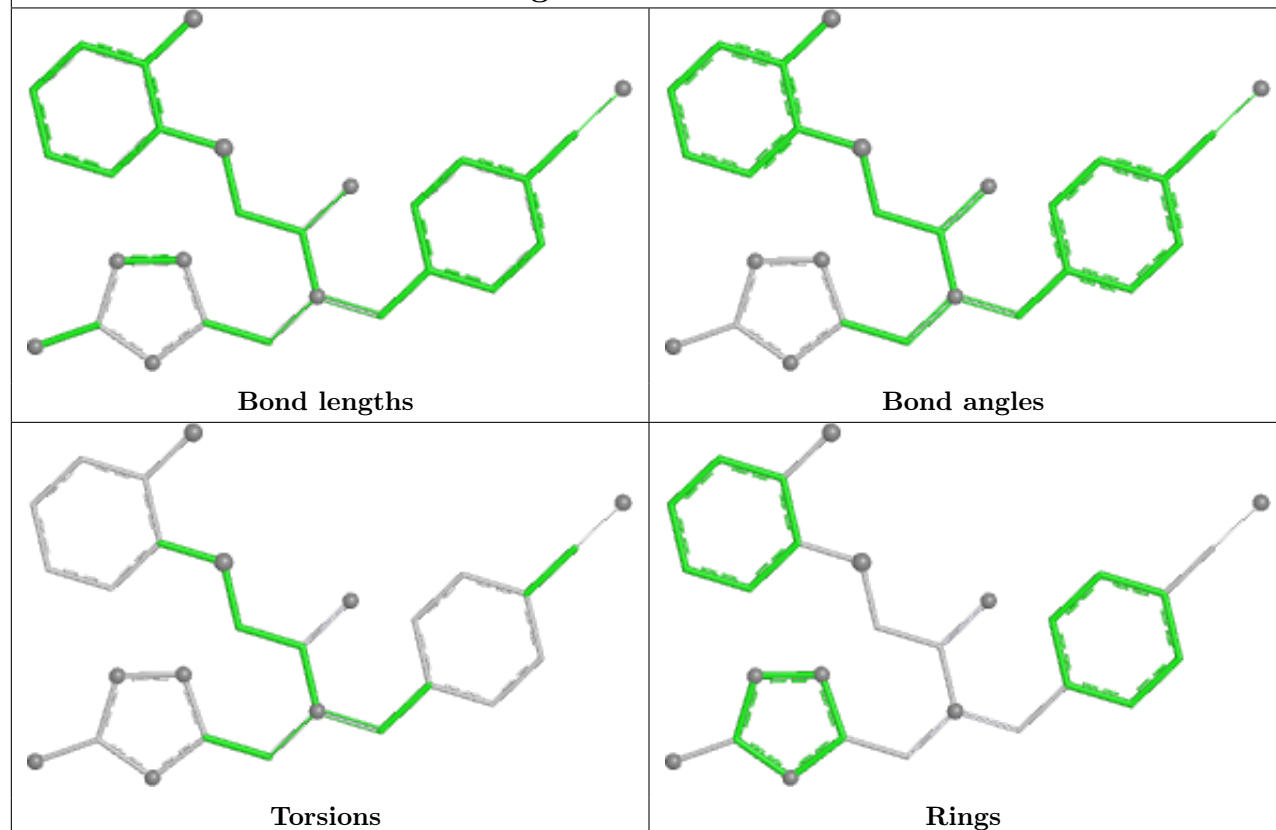


Ligand VFN Z 301

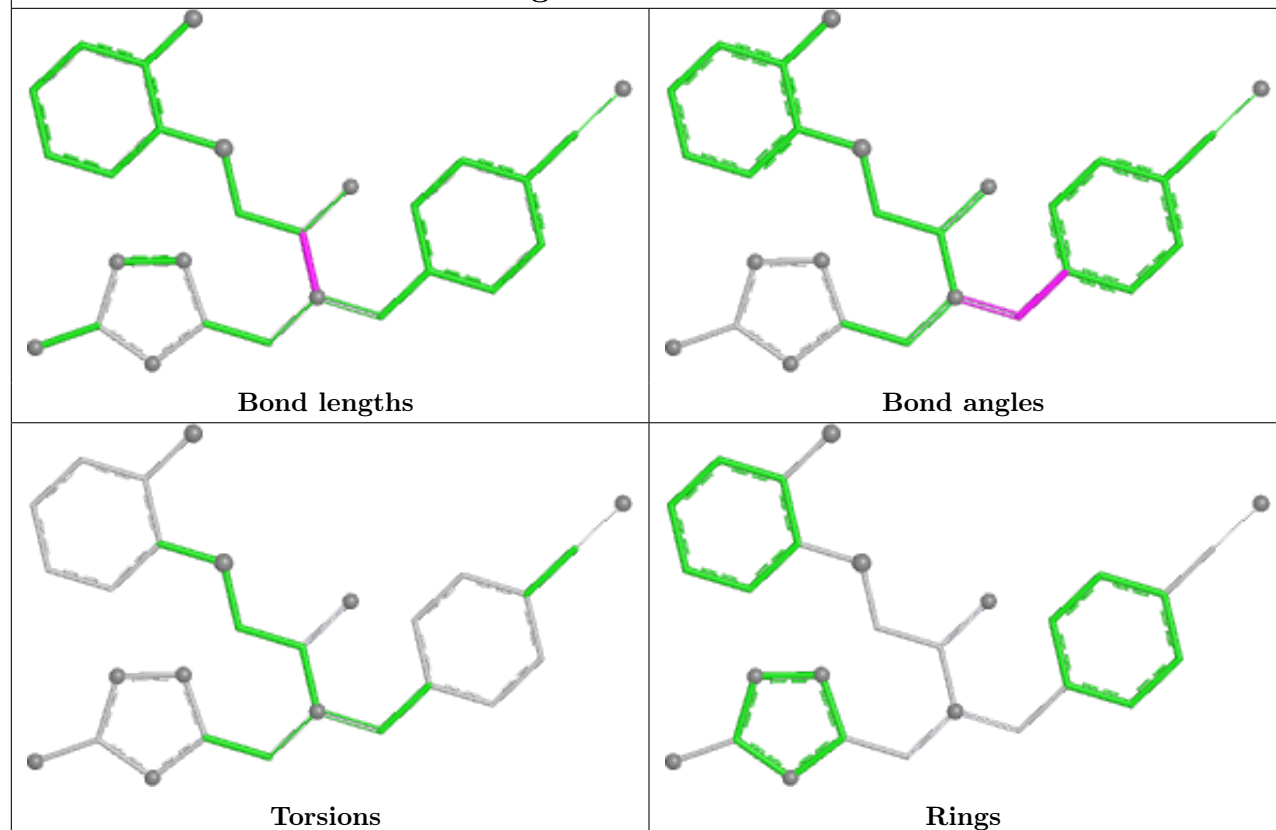




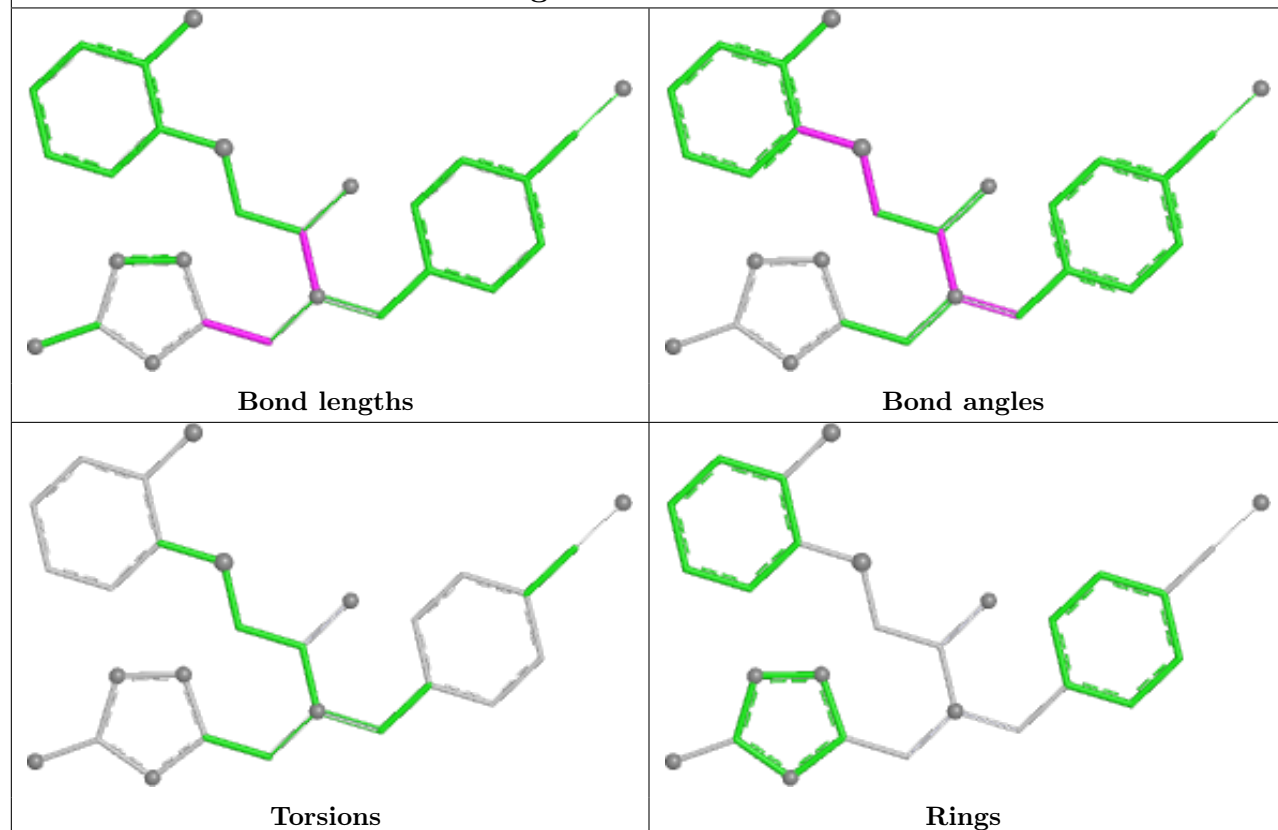
Ligand VFN B 301



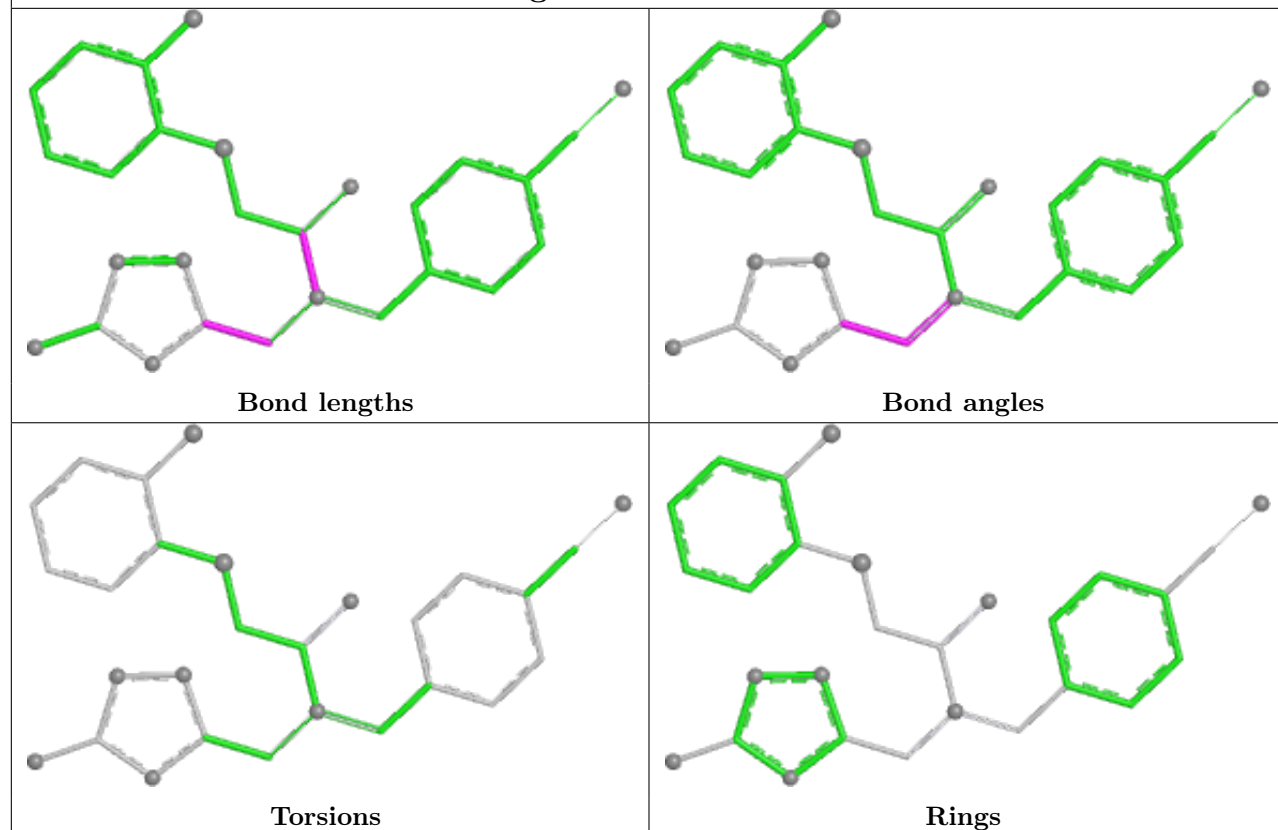
Ligand VFN P 302



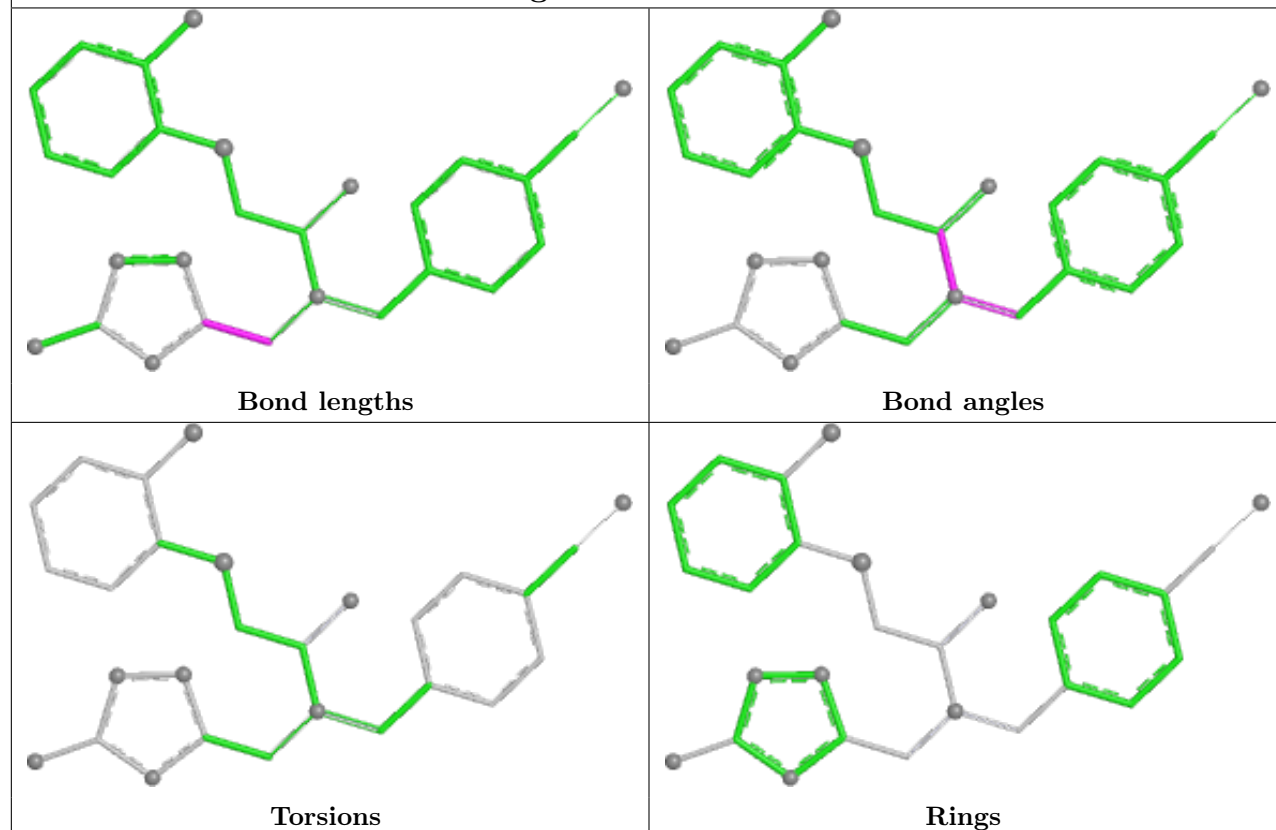
Ligand VFN R 301



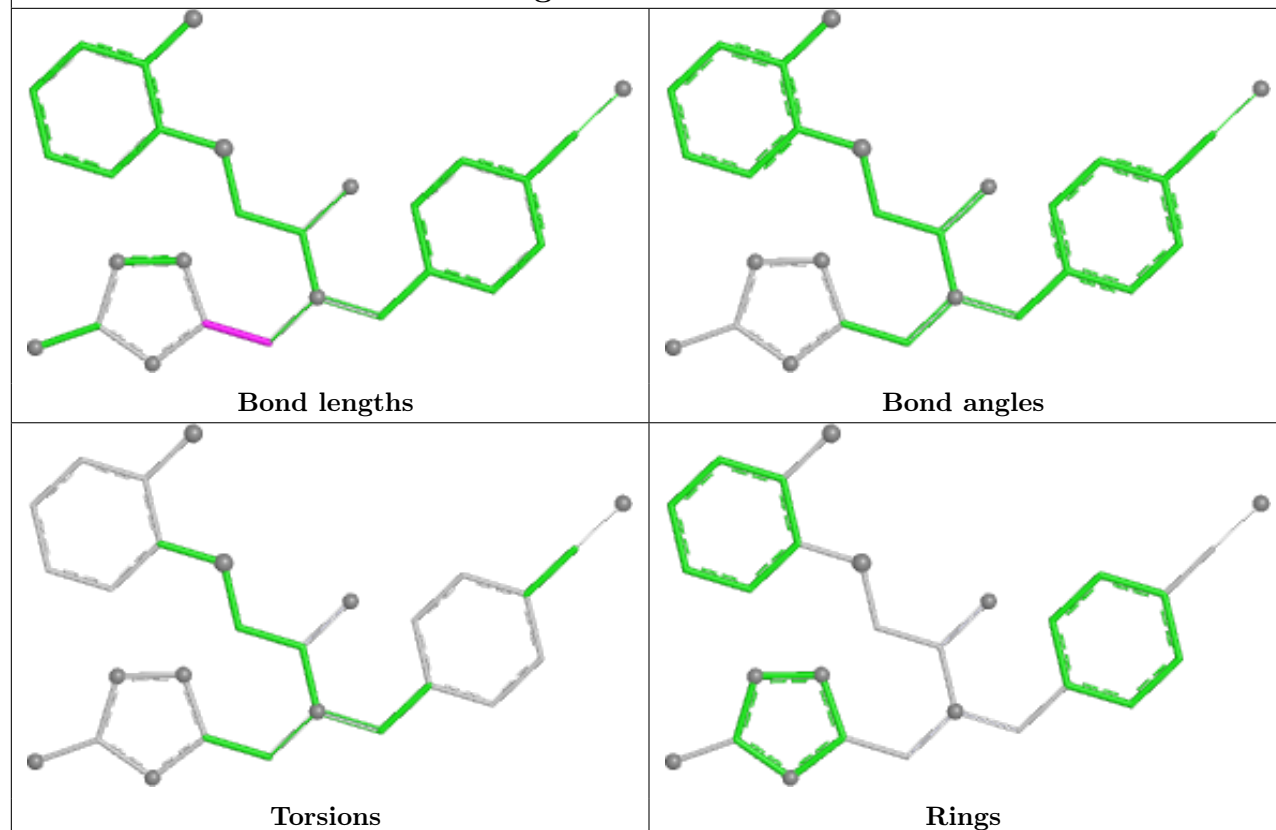
Ligand VFN K 301

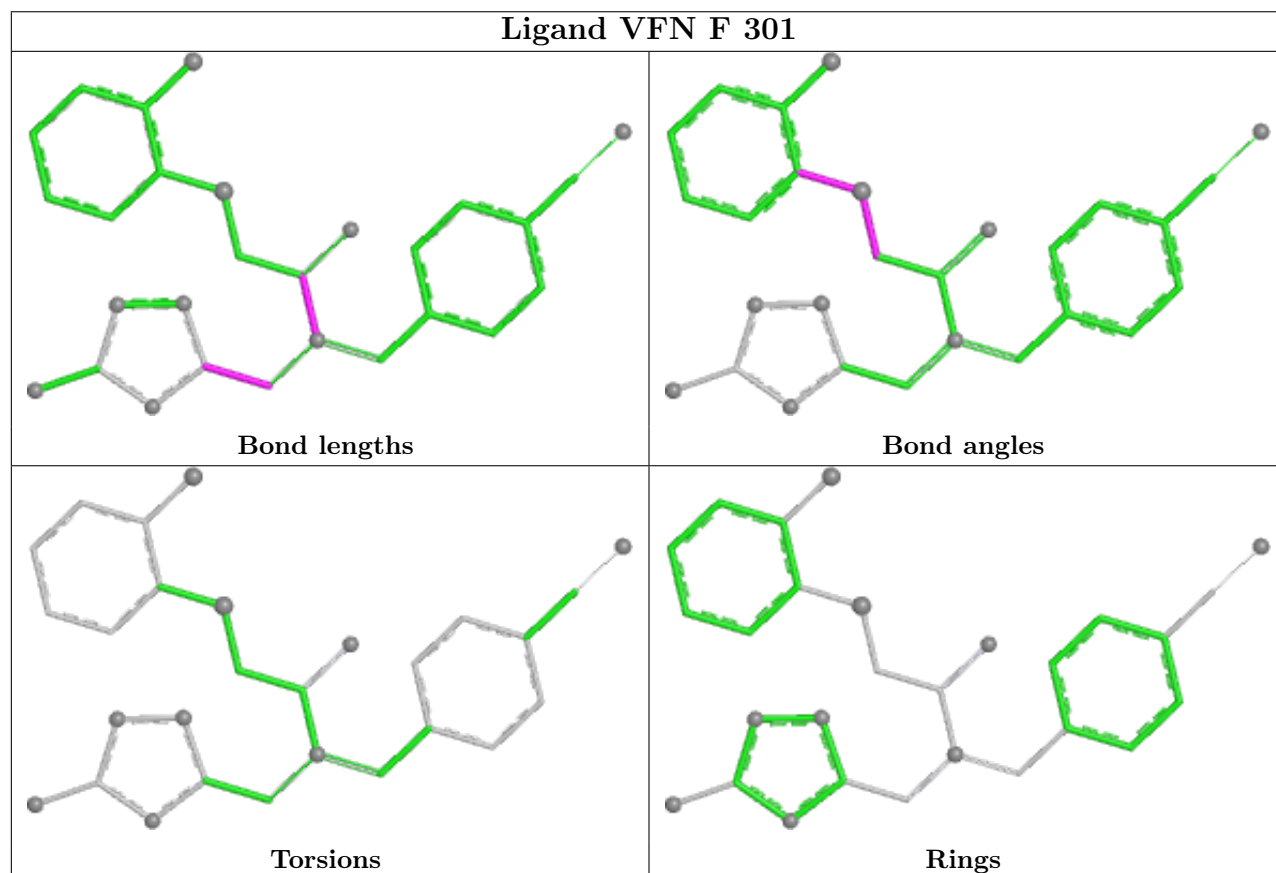
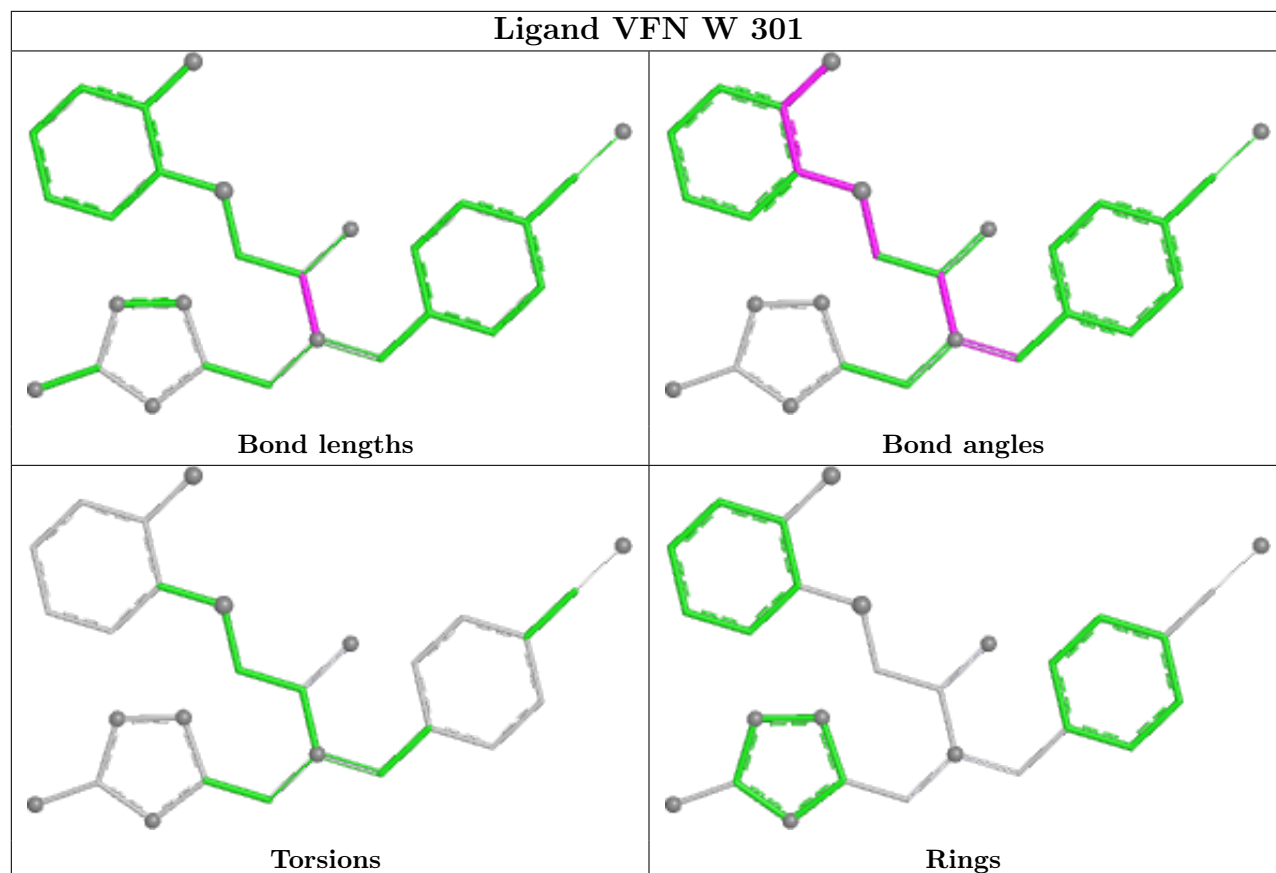


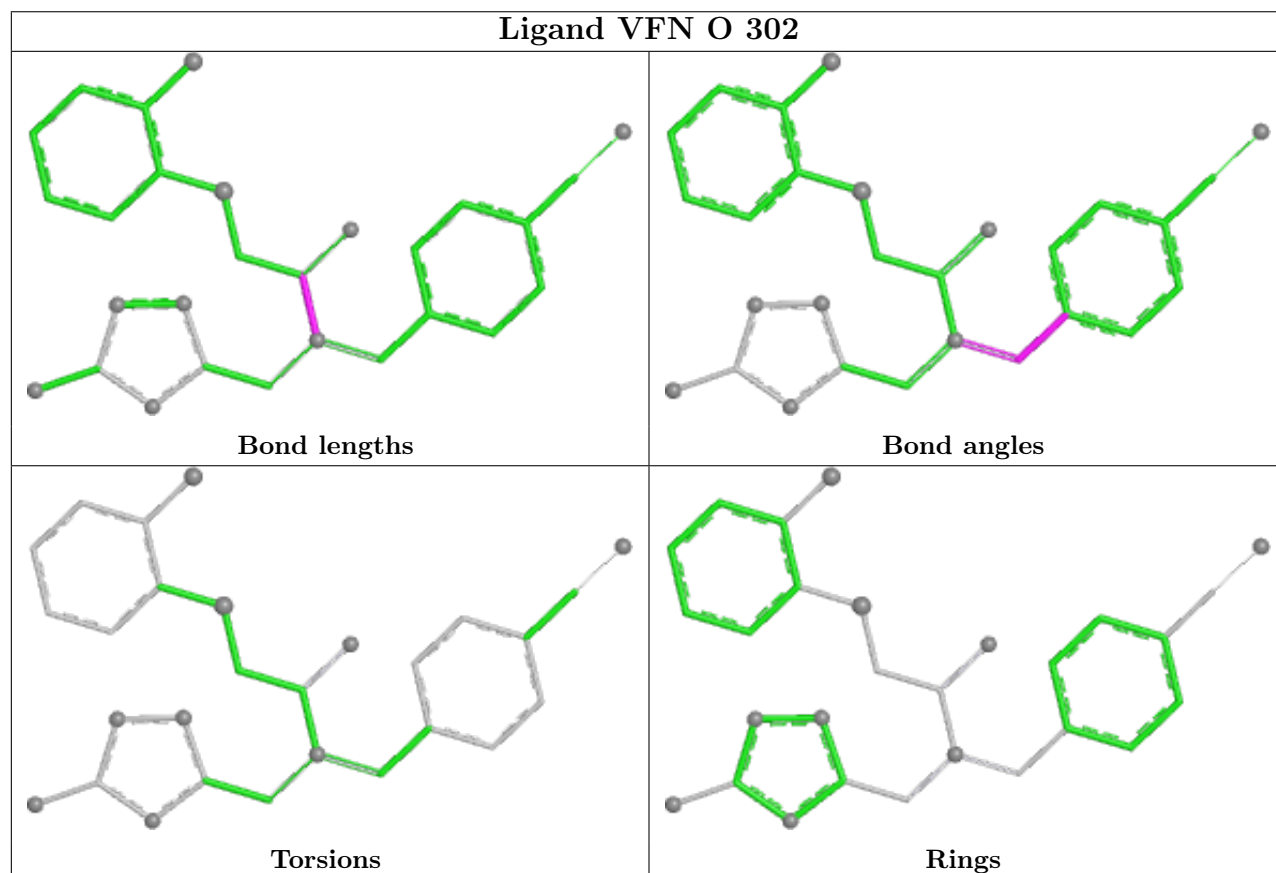
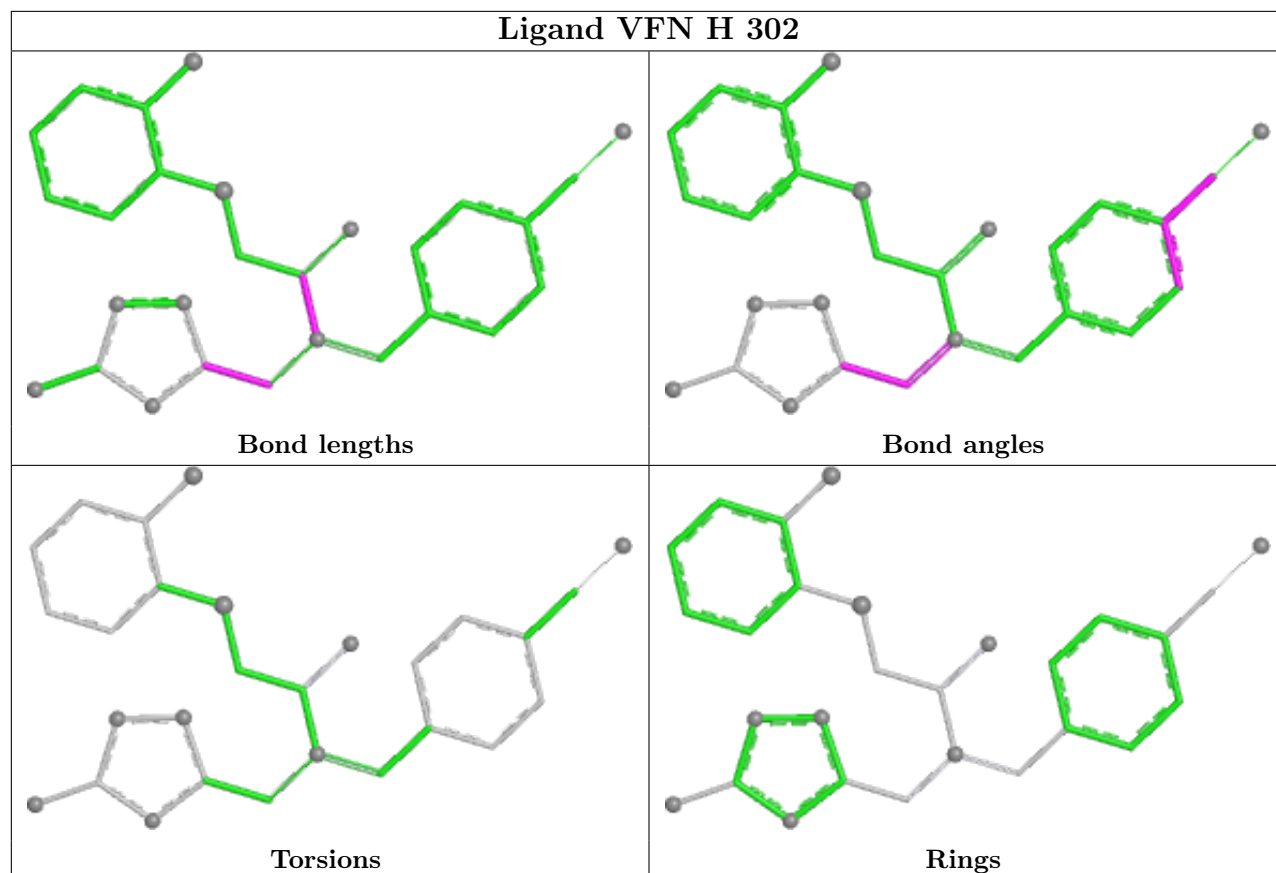
Ligand VFN A 302

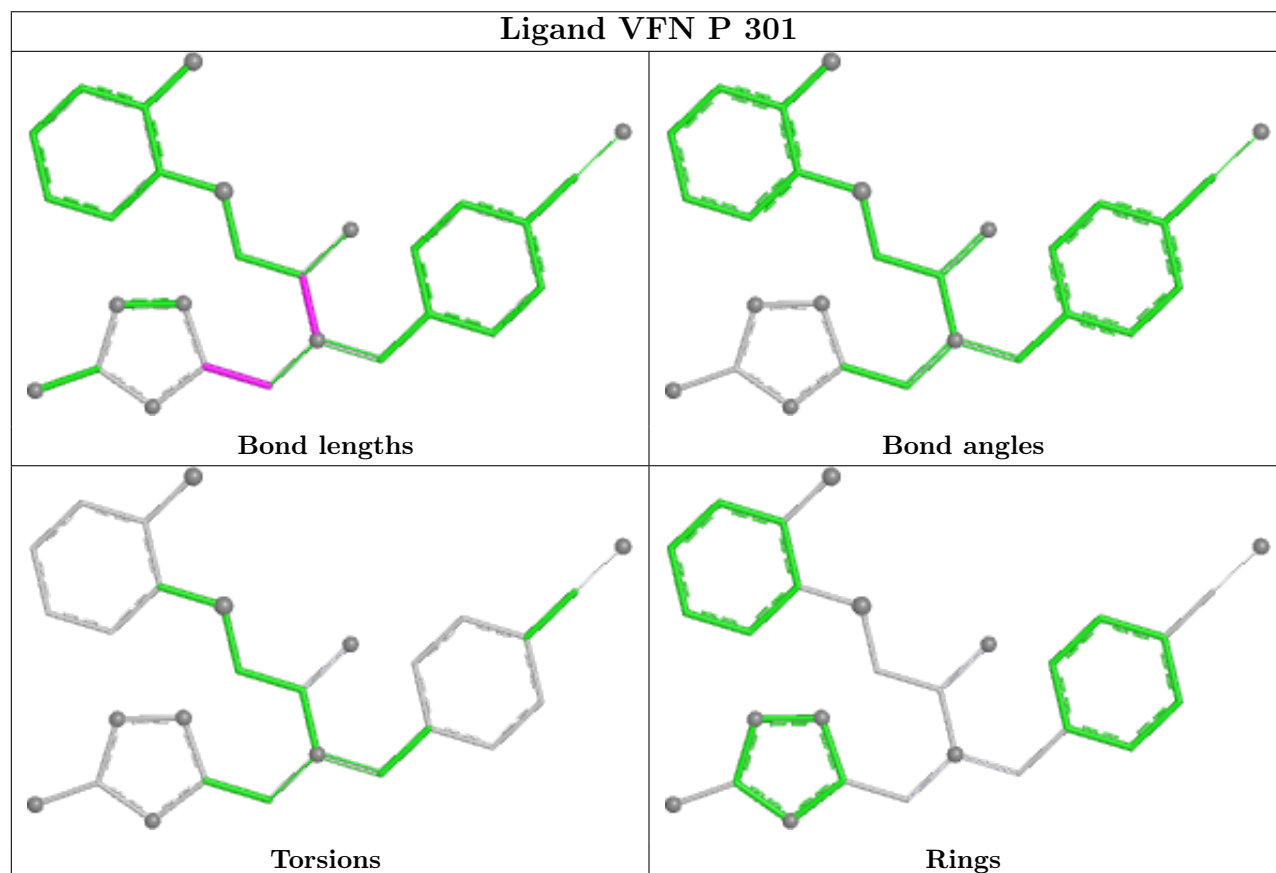
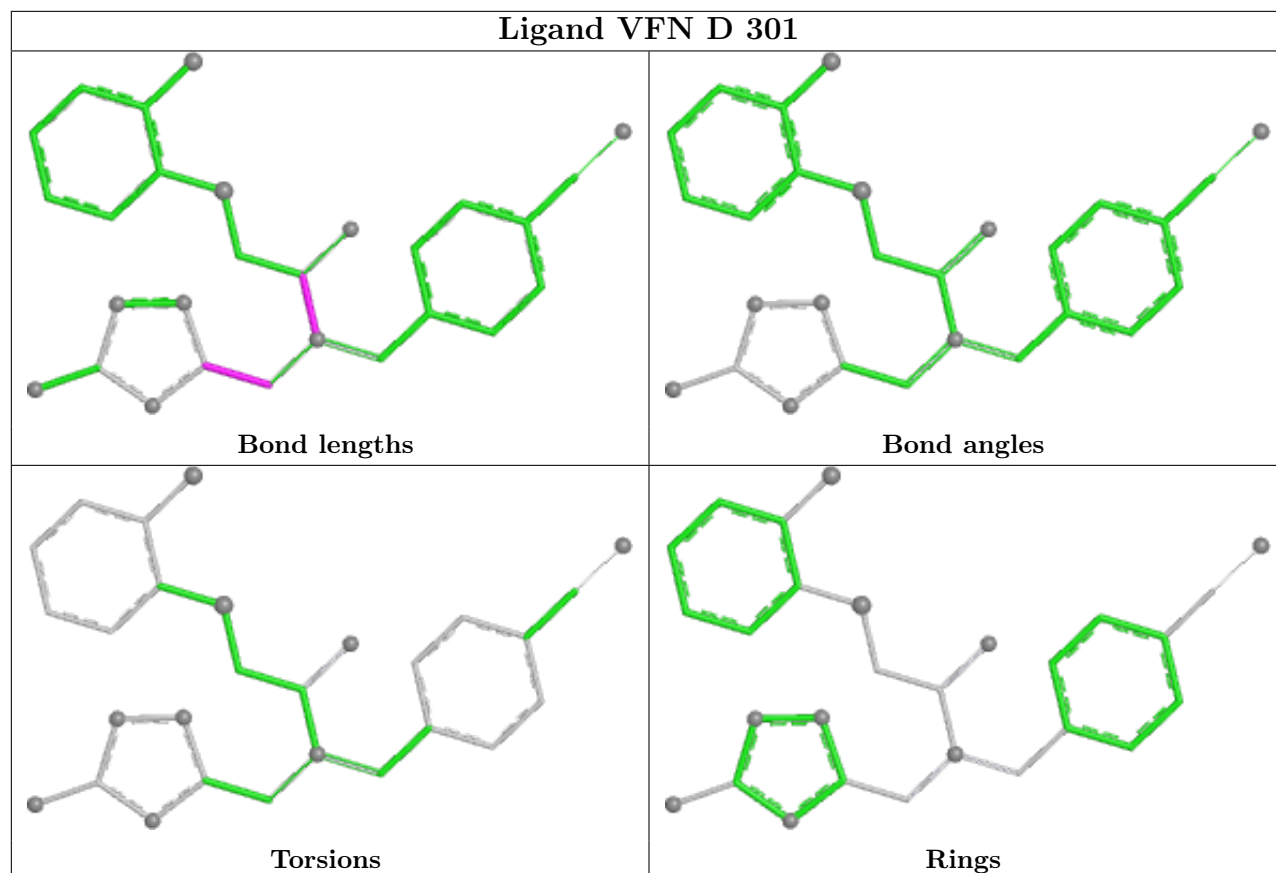


Ligand VFN J 301

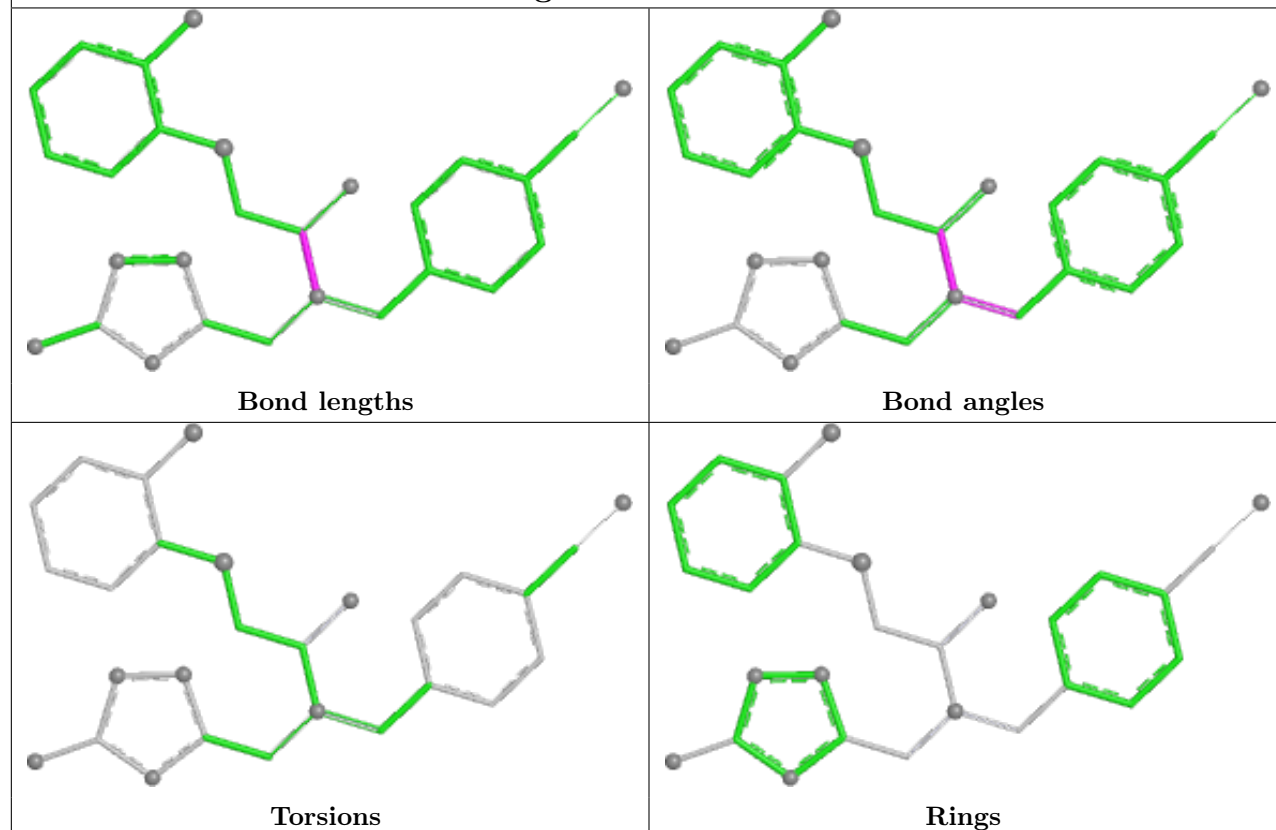




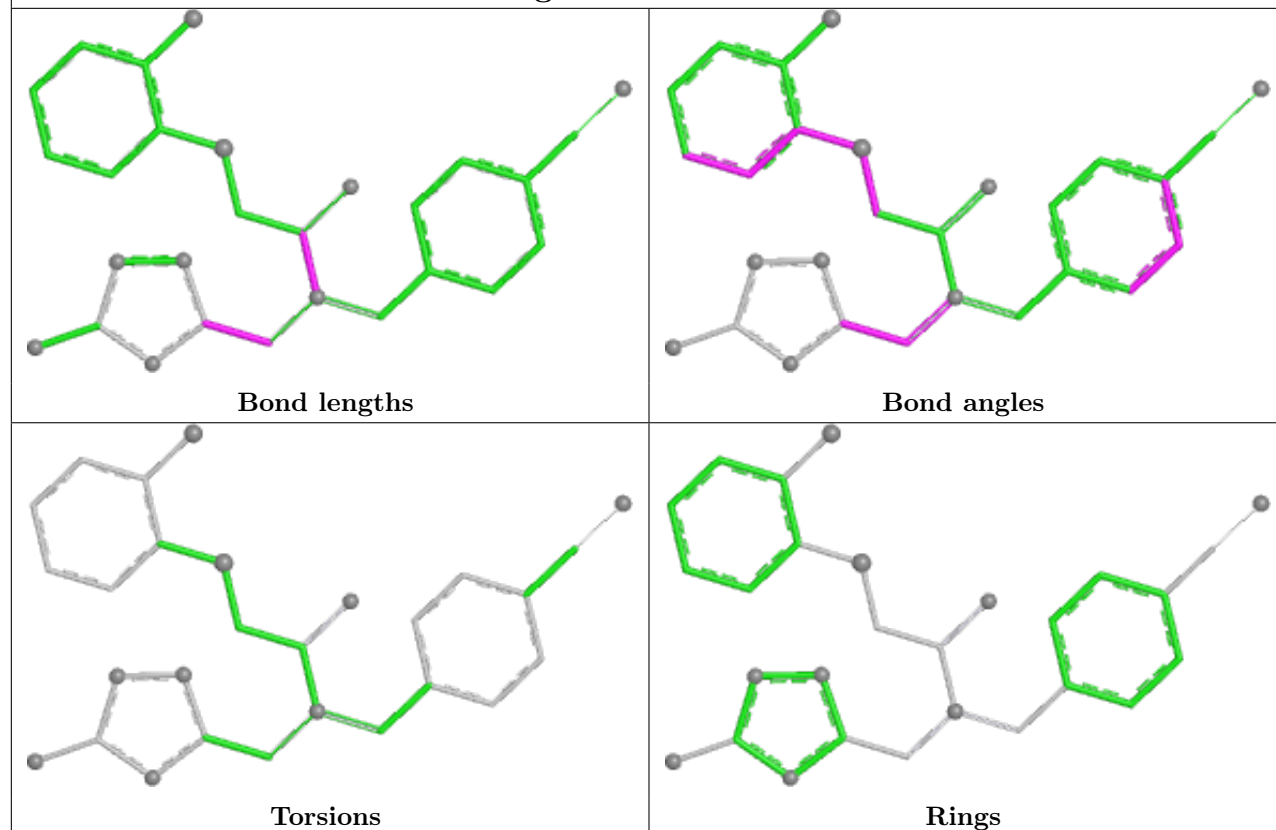


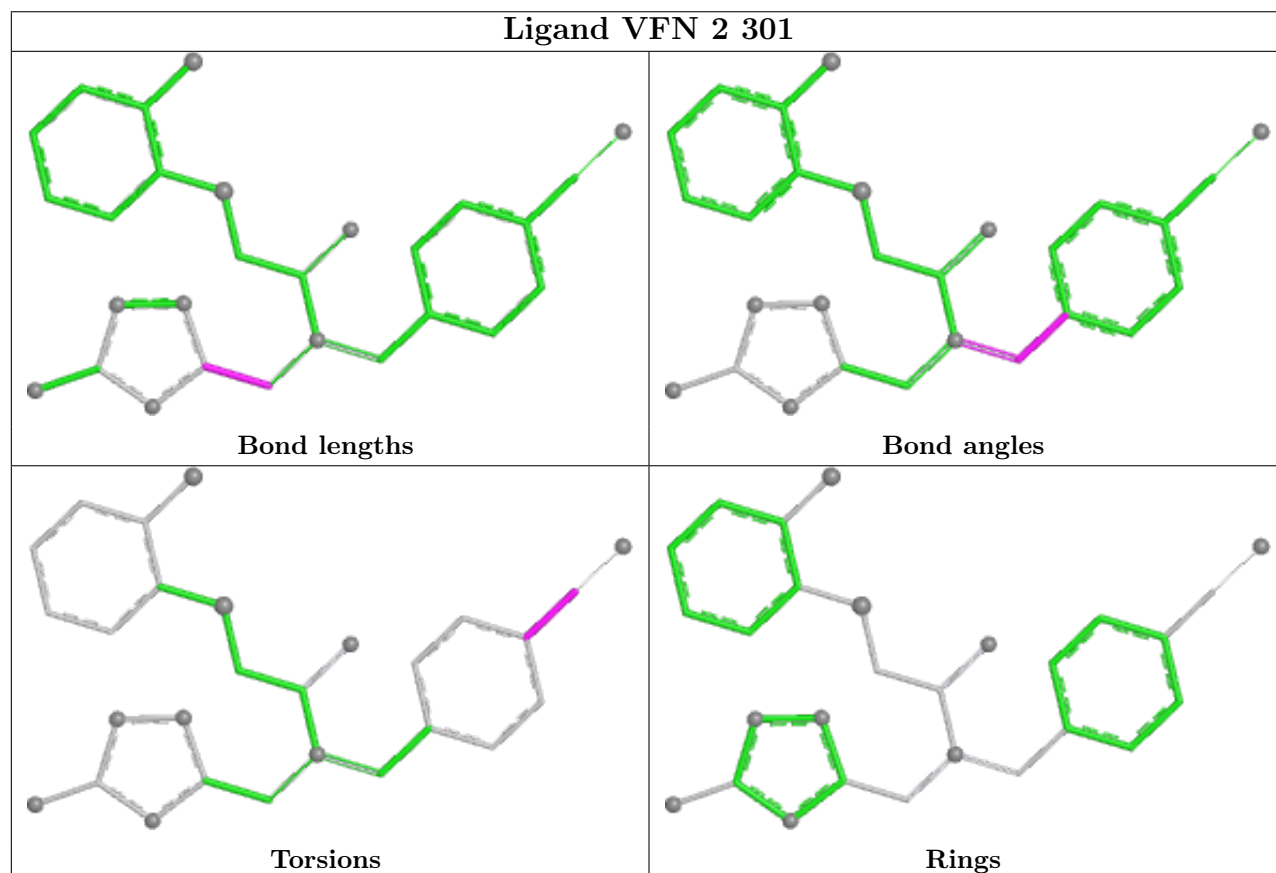
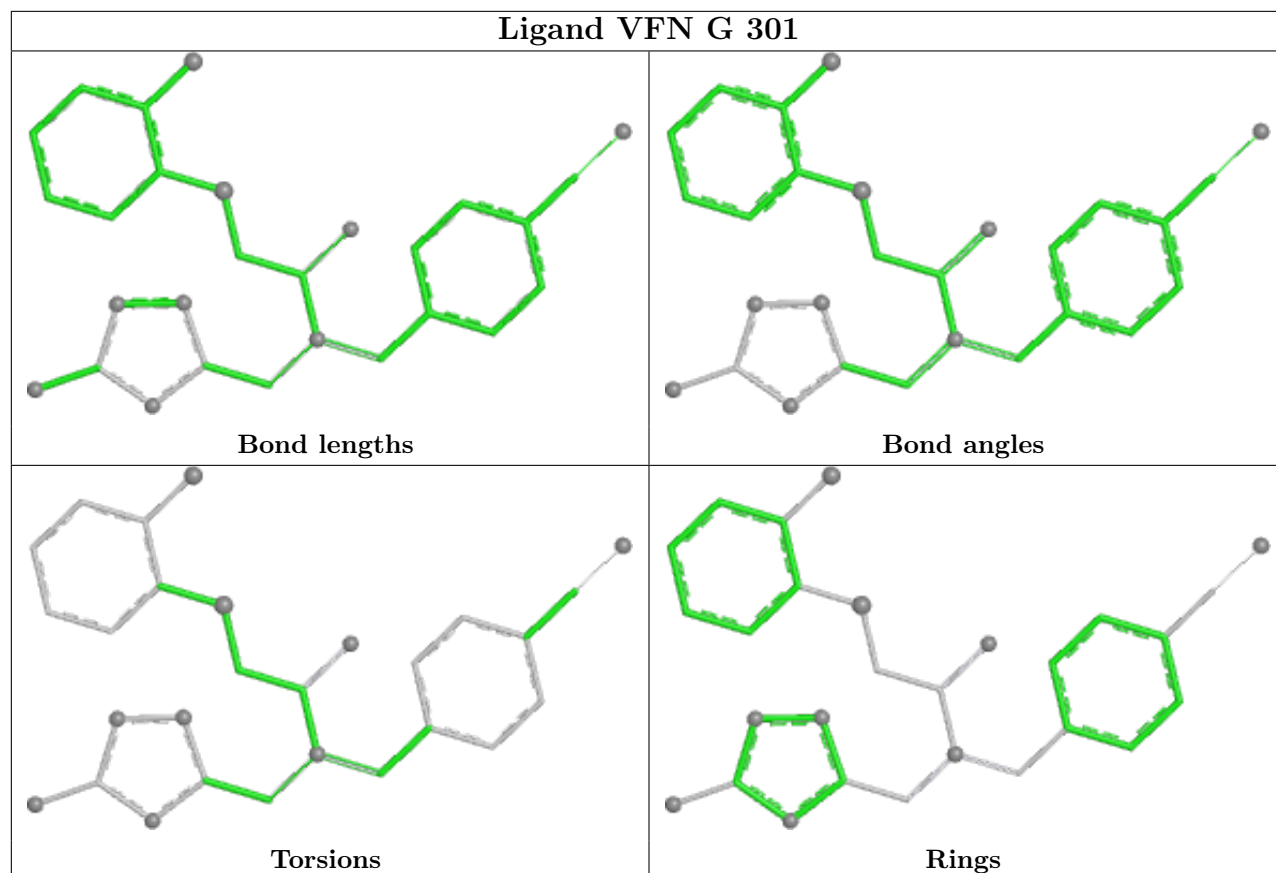


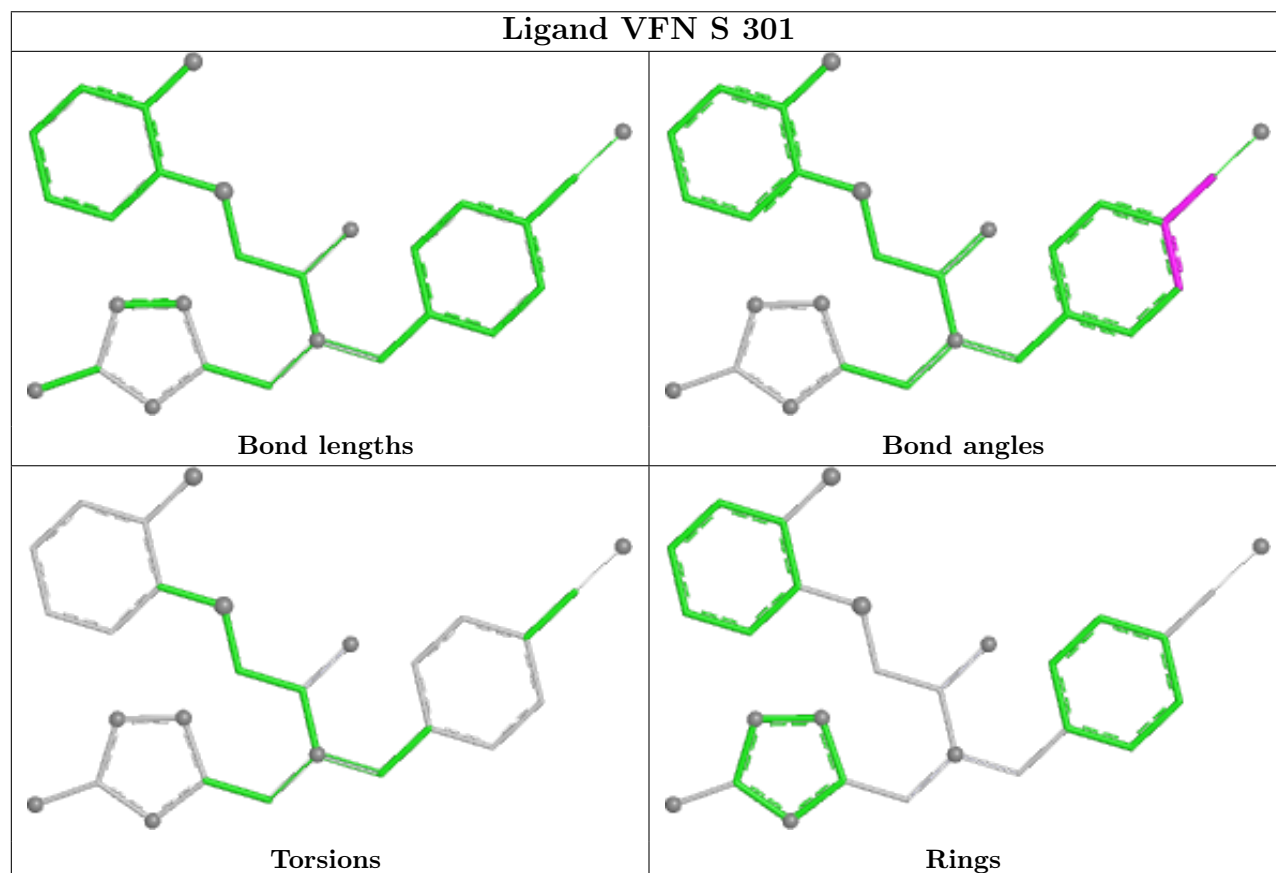
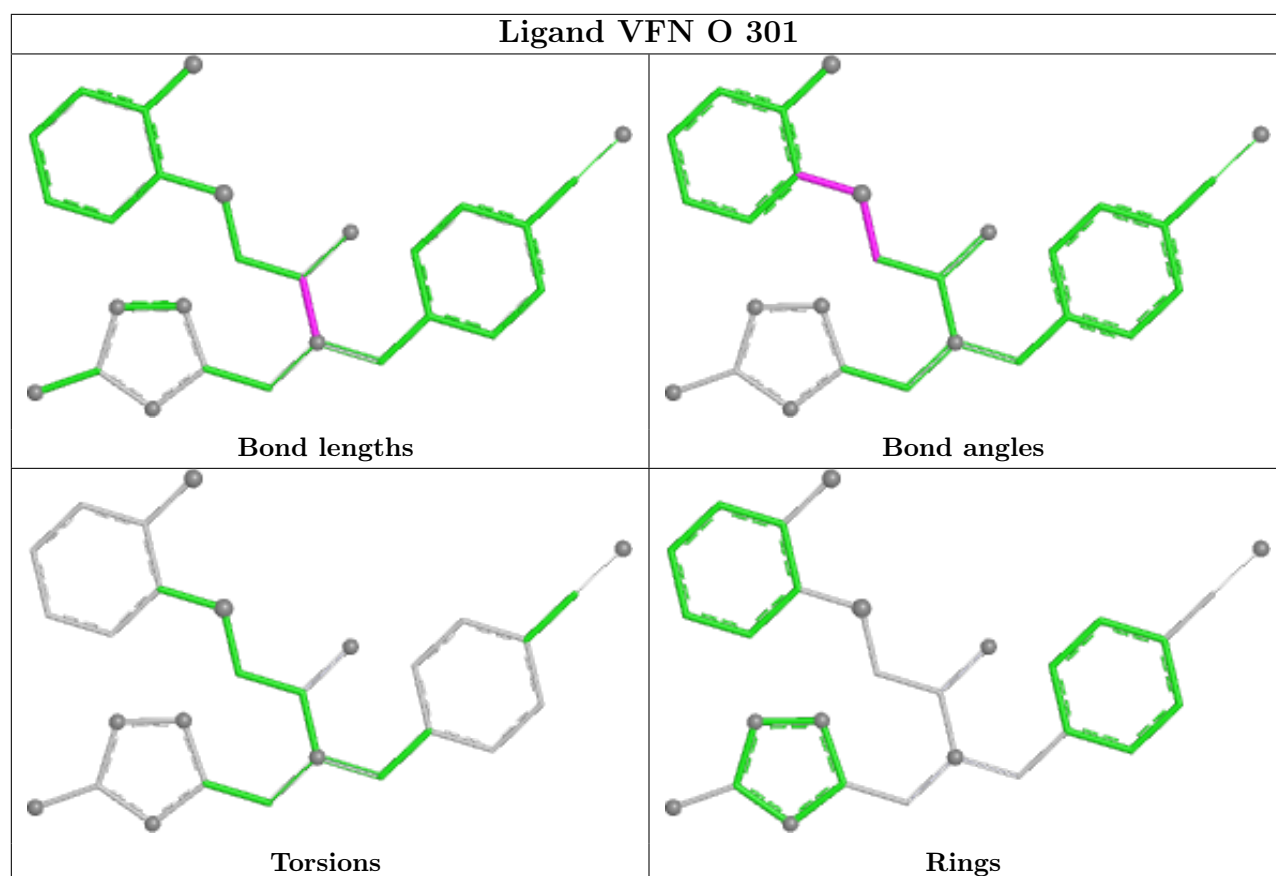
Ligand VFN 3 301

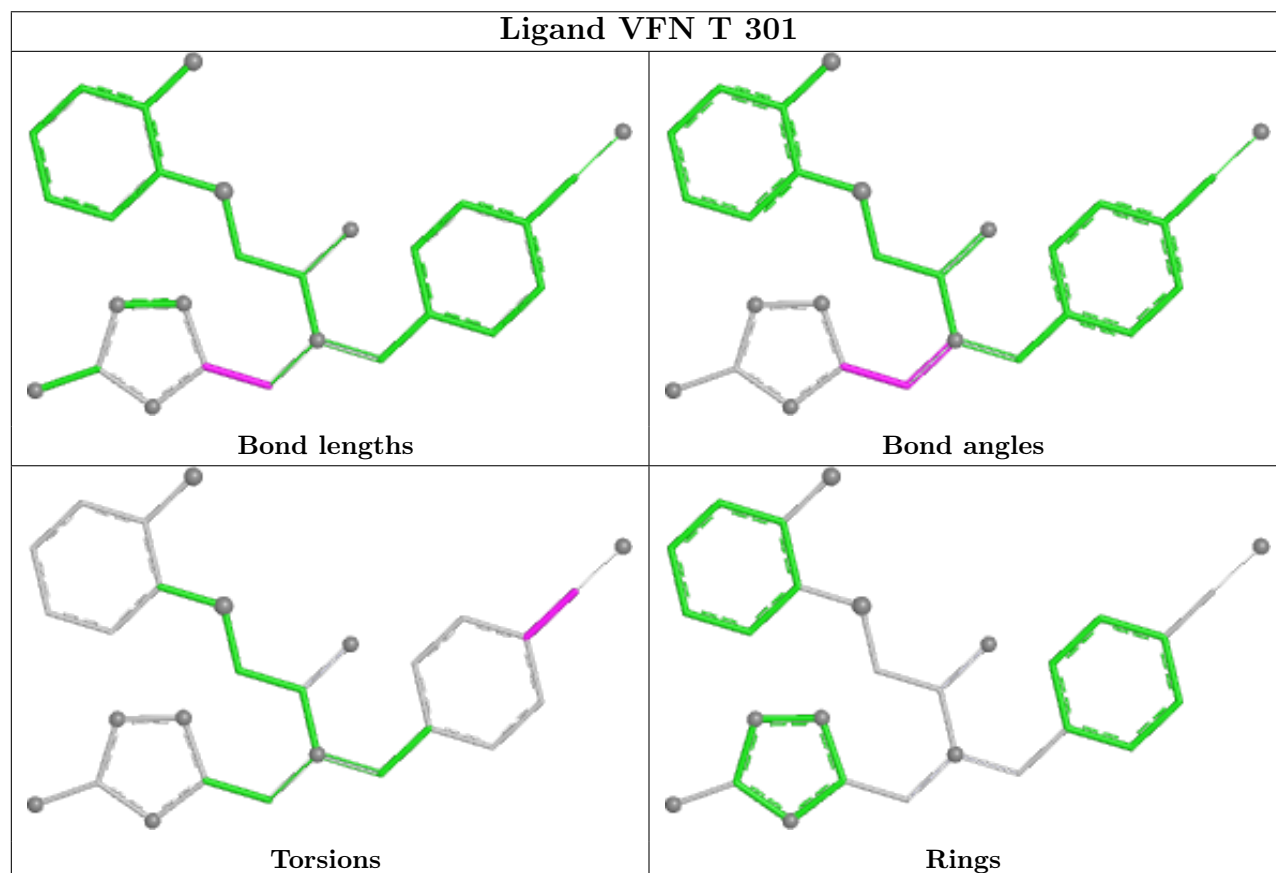
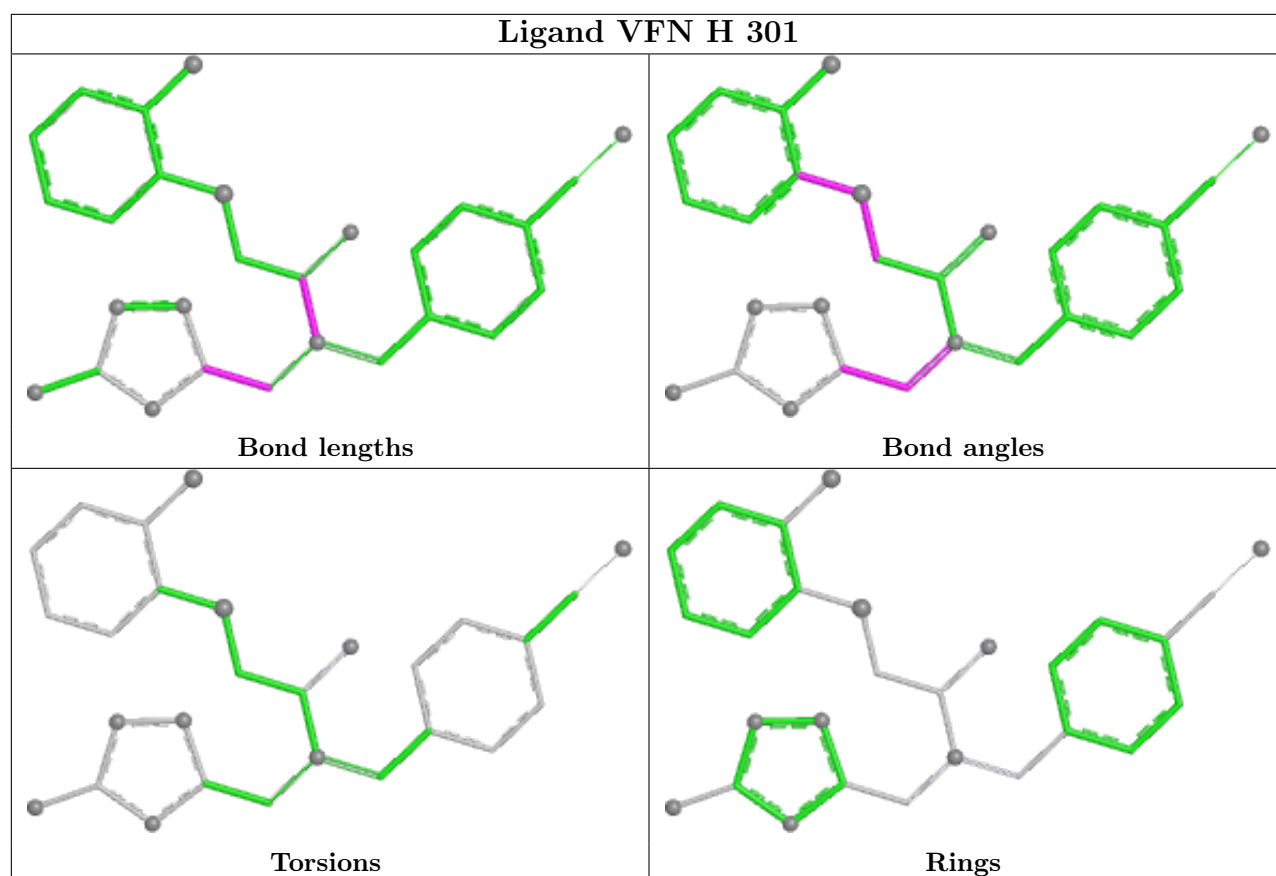


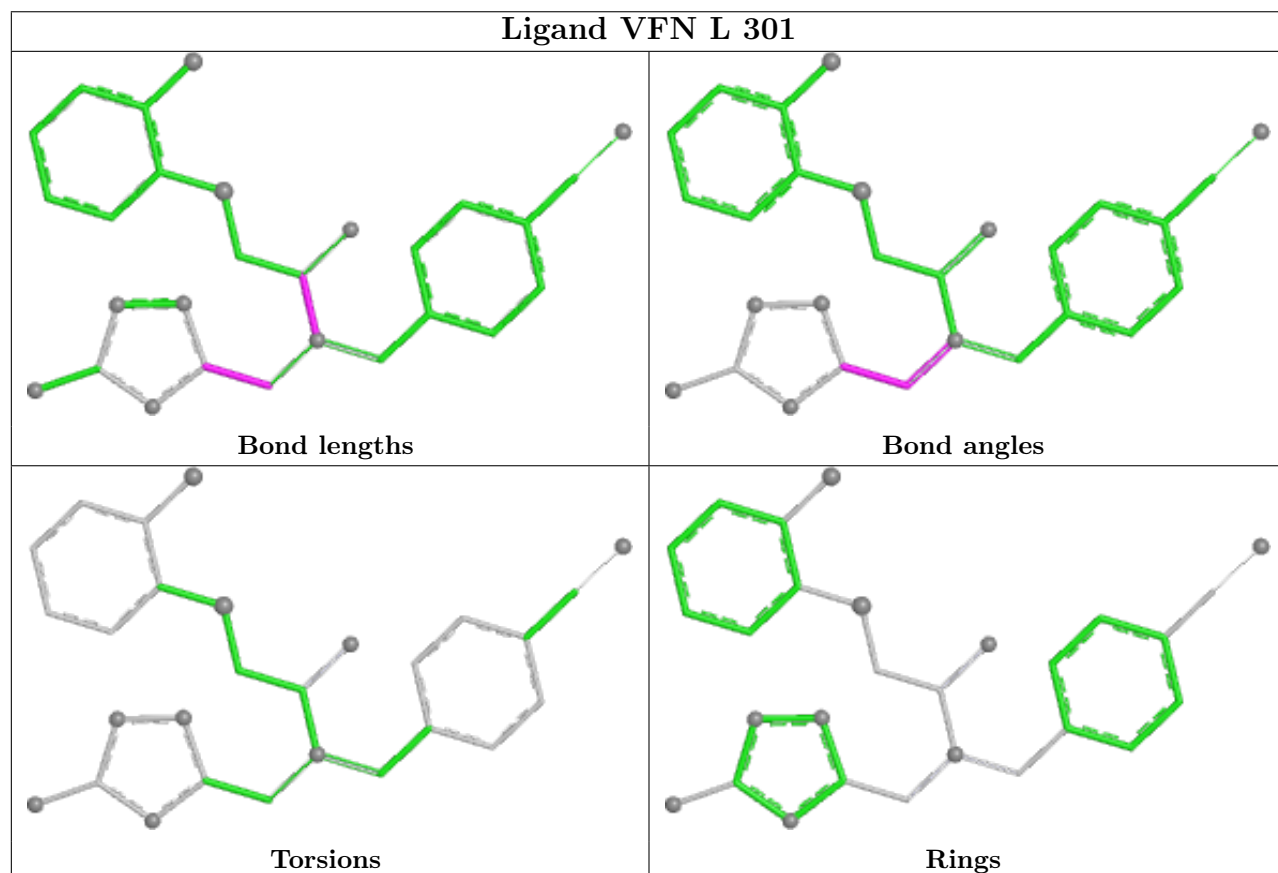
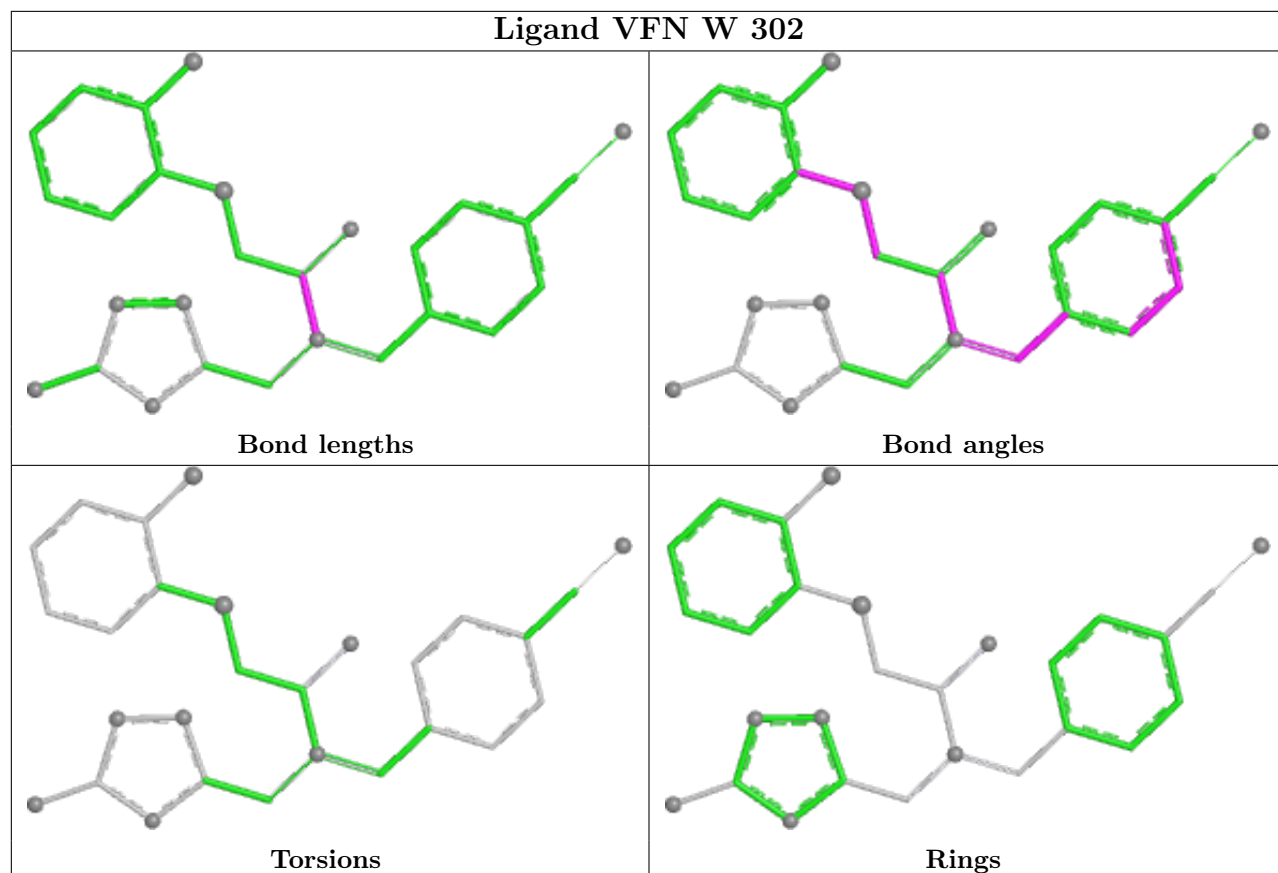
Ligand VFN 1 302



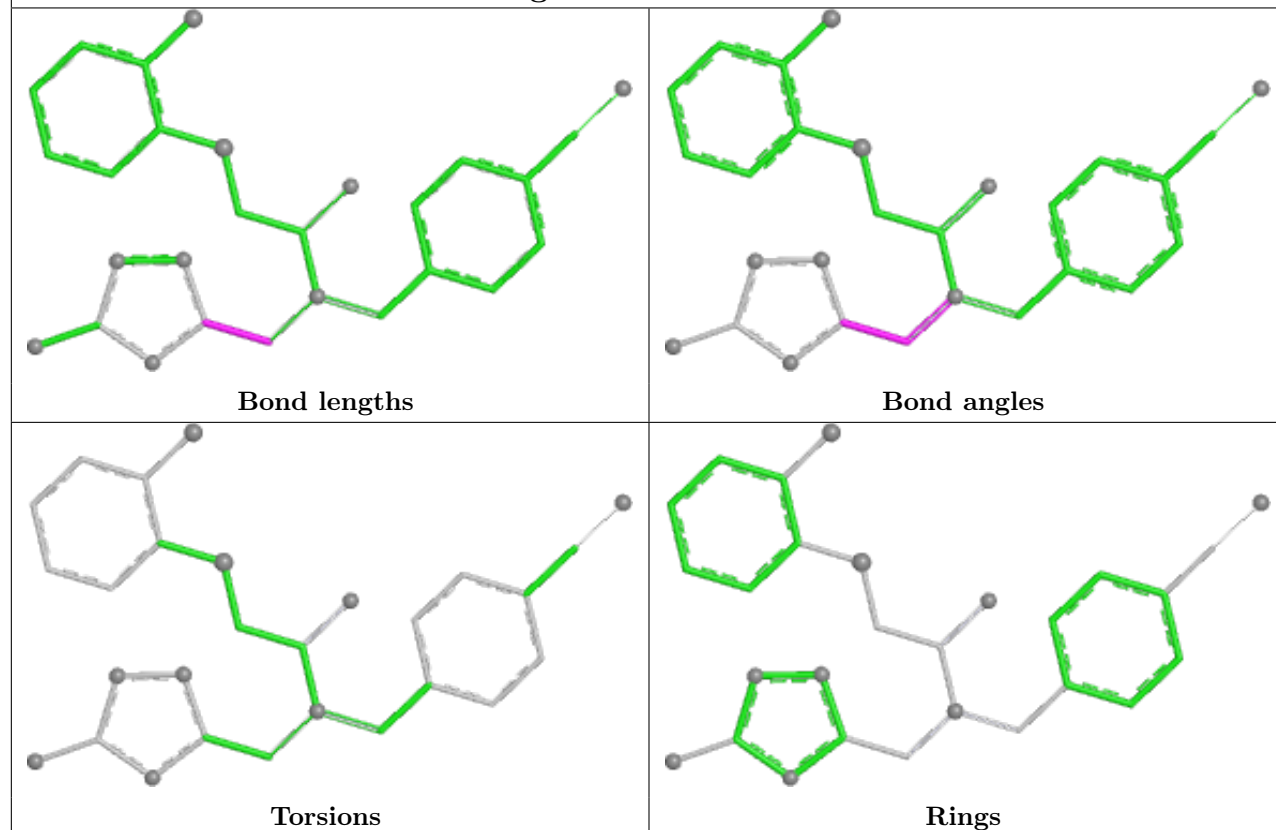




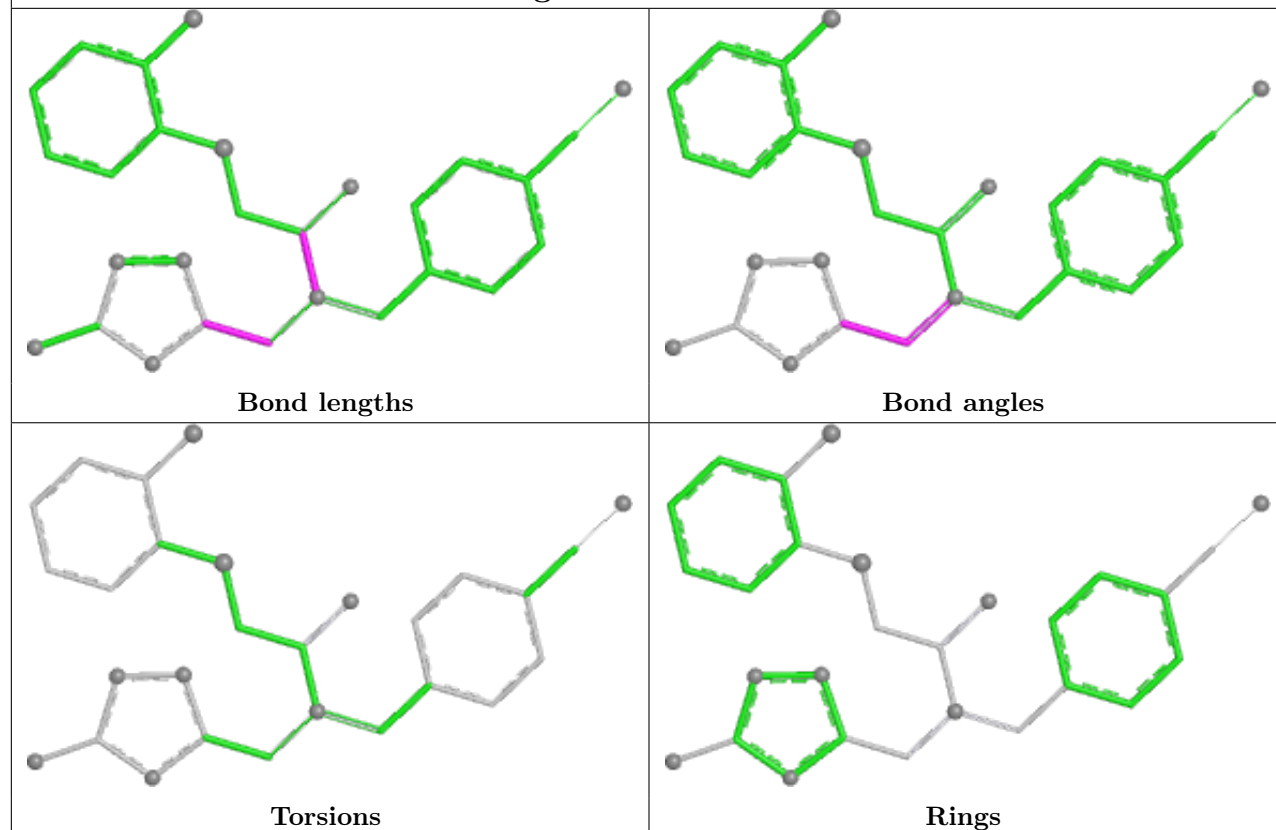


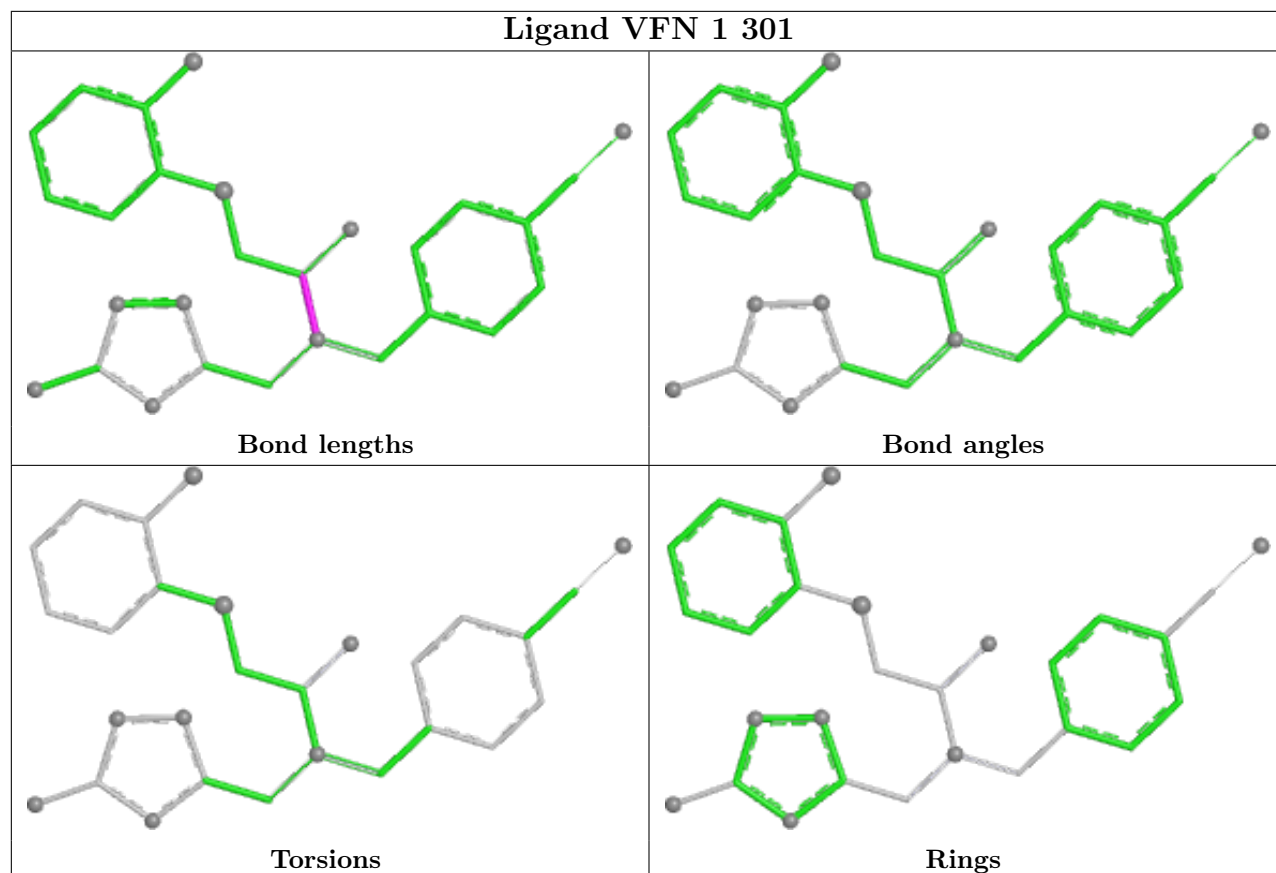


Ligand VFN V 301



Ligand VFN S 302





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	1	258/261 (98%)	0.45	4 (1%) 72 71	50, 66, 87, 119	0
1	2	258/261 (98%)	0.43	3 (1%) 79 79	50, 65, 86, 122	0
1	3	258/261 (98%)	0.42	8 (3%) 49 44	47, 65, 84, 111	0
1	4	258/261 (98%)	0.40	5 (1%) 66 65	46, 63, 82, 103	0
1	A	258/261 (98%)	0.32	0 100 100	51, 66, 87, 104	0
1	B	258/261 (98%)	0.36	4 (1%) 72 71	51, 65, 85, 105	0
1	C	258/261 (98%)	0.27	4 (1%) 72 71	52, 64, 85, 105	0
1	D	258/261 (98%)	0.35	3 (1%) 79 79	47, 63, 85, 111	0
1	E	258/261 (98%)	0.37	5 (1%) 66 65	47, 65, 83, 109	0
1	F	258/261 (98%)	0.38	2 (0%) 86 86	51, 66, 87, 116	0
1	G	258/261 (98%)	0.50	8 (3%) 49 44	54, 73, 99, 123	0
1	H	258/261 (98%)	0.51	11 (4%) 35 31	58, 75, 102, 116	0
1	I	258/261 (98%)	0.49	8 (3%) 49 44	53, 73, 100, 124	0
1	J	258/261 (98%)	0.59	12 (4%) 31 28	51, 74, 106, 130	0
1	K	258/261 (98%)	0.47	7 (2%) 54 50	58, 76, 101, 121	0
1	L	258/261 (98%)	0.46	10 (3%) 39 35	56, 73, 100, 135	0
1	M	258/261 (98%)	0.41	4 (1%) 72 71	55, 72, 102, 125	0
1	N	258/261 (98%)	0.48	10 (3%) 39 35	55, 74, 100, 118	0
1	O	258/261 (98%)	0.44	13 (5%) 28 25	52, 72, 103, 121	0
1	P	258/261 (98%)	0.55	13 (5%) 28 25	57, 73, 100, 131	0
1	Q	258/261 (98%)	0.49	13 (5%) 28 25	58, 74, 102, 124	0
1	R	258/261 (98%)	0.56	13 (5%) 28 25	53, 71, 100, 136	0
1	S	258/261 (98%)	0.37	6 (2%) 60 58	50, 66, 87, 112	0
1	T	258/261 (98%)	0.32	5 (1%) 66 65	51, 66, 86, 118	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	U	258/261 (98%)	0.31	3 (1%) 79 79	49, 64, 84, 104	0
1	V	258/261 (98%)	0.39	5 (1%) 66 65	52, 66, 85, 109	0
1	W	258/261 (98%)	0.47	6 (2%) 60 58	45, 65, 87, 119	0
1	X	258/261 (98%)	0.30	1 (0%) 92 93	48, 63, 81, 105	0
1	Y	258/261 (98%)	0.42	2 (0%) 86 86	48, 66, 85, 116	0
1	Z	258/261 (98%)	0.36	3 (1%) 79 79	48, 66, 83, 108	0
All	All	7740/7830 (98%)	0.42	191 (2%) 57 55	45, 68, 95, 136	0

The worst 5 of 191 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1	MET	5.5
1	J	1	MET	5.5
1	W	1	MET	5.3
1	M	1	MET	5.2
1	H	1	MET	5.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	302	5/5	0.87	0.28	98,99,100,100	0
2	VFN	K	301	28/28	0.92	0.26	77,90,93,93	0
2	VFN	3	302	28/28	0.92	0.28	61,72,76,76	0
2	VFN	2	301	28/28	0.93	0.24	56,65,72,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	VFN	R	301	28/28	0.93	0.25	71,75,81,82	0
2	VFN	H	302	28/28	0.93	0.24	73,77,84,85	0
2	VFN	B	301	28/28	0.94	0.25	68,72,76,77	0
2	VFN	D	302	28/28	0.94	0.26	59,66,70,72	0
2	VFN	G	301	28/28	0.94	0.24	64,73,79,83	0
2	VFN	3	301	28/28	0.94	0.25	60,65,68,69	0
2	VFN	1	302	28/28	0.94	0.24	56,65,72,75	0
2	VFN	O	302	28/28	0.94	0.22	80,84,88,89	0
2	VFN	P	301	28/28	0.94	0.24	77,83,86,88	0
2	VFN	A	301	28/28	0.94	0.23	61,66,71,72	0
2	VFN	S	301	28/28	0.94	0.25	64,71,74,76	0
2	VFN	W	302	28/28	0.94	0.23	57,74,83,84	0
2	VFN	A	302	28/28	0.94	0.23	65,73,76,76	0
3	SO4	F	302	5/5	0.94	0.20	84,84,85,88	0
2	VFN	F	301	28/28	0.95	0.23	51,62,70,75	0
2	VFN	P	302	28/28	0.95	0.22	67,73,76,77	0
2	VFN	1	301	28/28	0.95	0.21	54,61,67,71	0
2	VFN	L	301	28/28	0.95	0.23	78,81,87,87	0
2	VFN	W	301	28/28	0.95	0.24	56,64,72,73	0
2	VFN	N	301	28/28	0.95	0.22	64,72,85,86	0
2	VFN	O	301	28/28	0.95	0.25	66,74,77,80	0
2	VFN	H	301	28/28	0.95	0.22	73,77,81,84	0
3	SO4	H	303	5/5	0.95	0.22	92,93,93,96	0
3	SO4	O	303	5/5	0.95	0.20	85,87,87,87	0
3	SO4	Q	301	5/5	0.95	0.17	85,85,85,87	0
3	SO4	U	301	5/5	0.95	0.22	80,82,83,85	0
3	SO4	V	302	5/5	0.95	0.21	88,90,91,91	0
3	SO4	X	301	5/5	0.95	0.24	90,90,91,94	0
2	VFN	T	301	28/28	0.96	0.25	61,68,77,82	0
3	SO4	E	301	5/5	0.96	0.20	74,76,78,79	0
2	VFN	V	301	28/28	0.96	0.22	51,63,67,68	0
3	SO4	G	302	5/5	0.96	0.20	99,100,100,101	0
2	VFN	J	301	28/28	0.96	0.21	61,75,84,85	0
3	SO4	I	301	5/5	0.96	0.16	80,82,82,83	0
3	SO4	M	301	5/5	0.96	0.17	90,90,91,92	0
3	SO4	N	302	5/5	0.96	0.18	89,90,91,92	0
2	VFN	S	302	28/28	0.96	0.22	55,64,73,75	0
3	SO4	P	303	5/5	0.96	0.20	95,96,96,96	0
2	VFN	Z	301	28/28	0.96	0.21	60,67,78,79	0
3	SO4	1	303	5/5	0.96	0.15	91,92,92,93	0
3	SO4	3	303	5/5	0.96	0.23	92,92,94,94	0
3	SO4	W	303	5/5	0.96	0.17	91,93,93,94	0

Continued on next page...

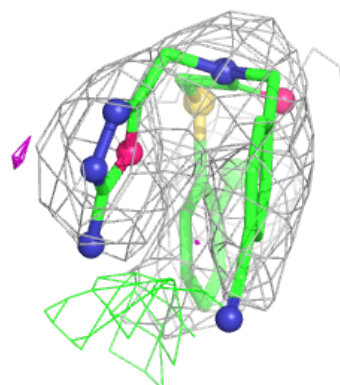
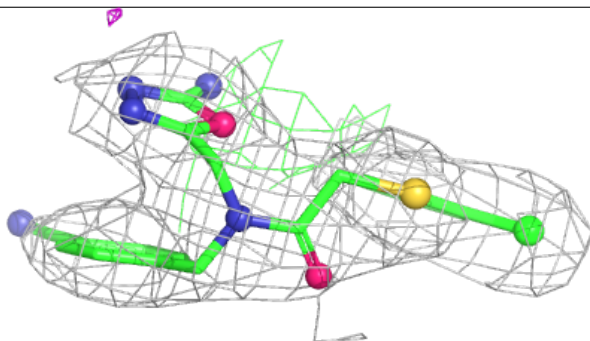
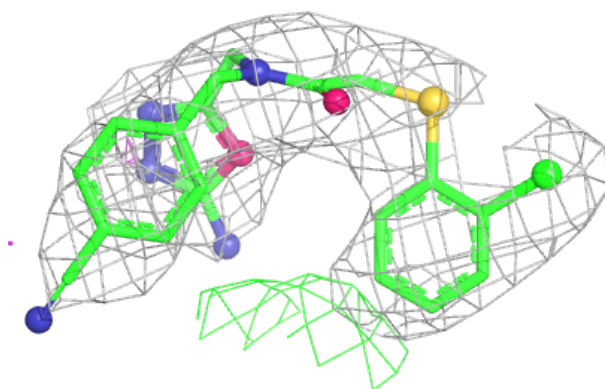
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	C	301	5/5	0.96	0.18	98,98,99,99	0
3	SO4	Y	301	5/5	0.96	0.20	91,91,93,94	0
2	VFN	D	301	28/28	0.97	0.23	57,65,73,74	0
3	SO4	D	303	5/5	0.97	0.18	81,83,84,84	0
3	SO4	S	303	5/5	0.97	0.22	76,76,78,79	0
3	SO4	T	302	5/5	0.97	0.17	78,78,80,82	0
3	SO4	J	302	5/5	0.97	0.17	83,86,87,89	0
3	SO4	L	302	5/5	0.97	0.18	93,93,95,95	0
3	SO4	4	301	5/5	0.97	0.17	85,86,87,89	0
3	SO4	A	303	5/5	0.97	0.19	88,88,89,89	0
3	SO4	2	302	5/5	0.97	0.17	94,96,98,98	0
3	SO4	Z	302	5/5	0.97	0.18	81,81,83,83	0
3	SO4	R	302	5/5	0.98	0.16	79,82,83,84	0
3	SO4	B	302	5/5	0.98	0.14	75,76,77,77	0
3	SO4	K	302	5/5	0.98	0.16	88,89,90,92	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.

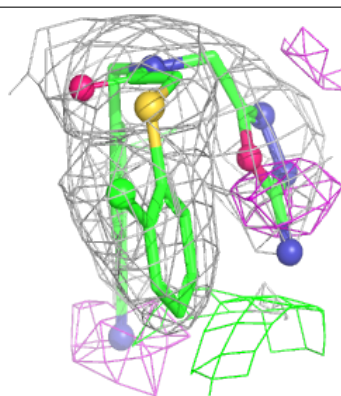
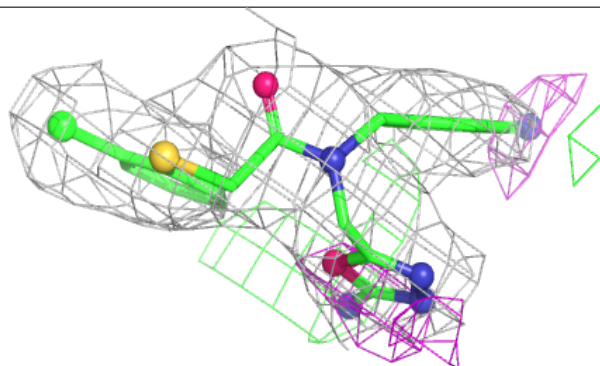
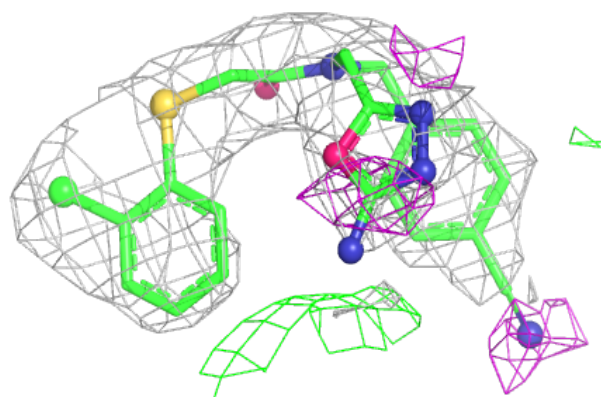
Electron density around VFN K 301:

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

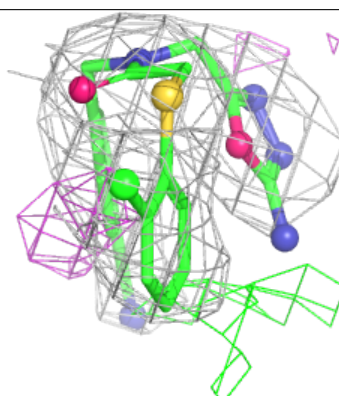
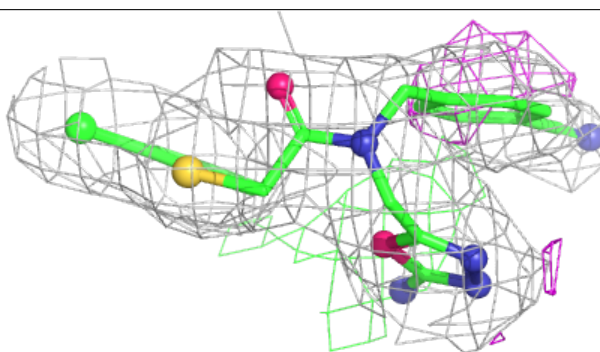
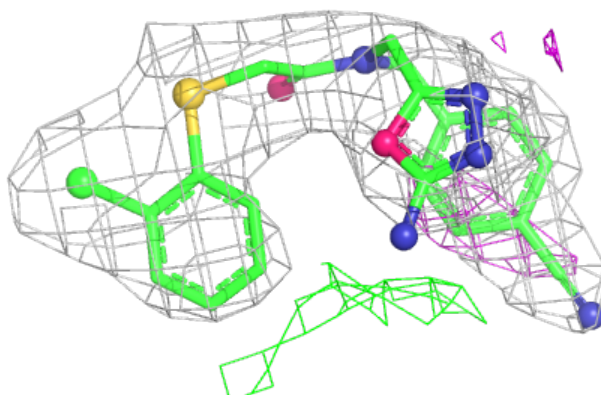


Electron density around VFN 3 302:

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

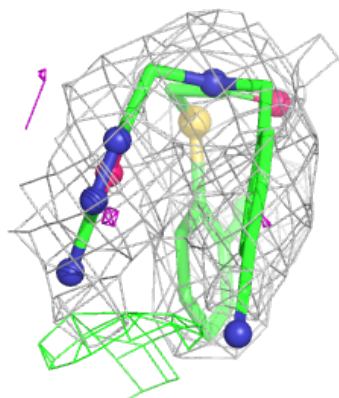
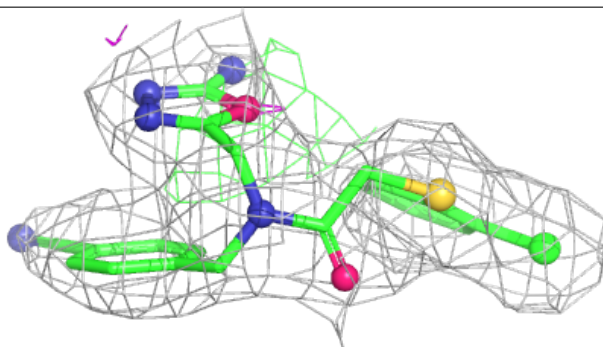
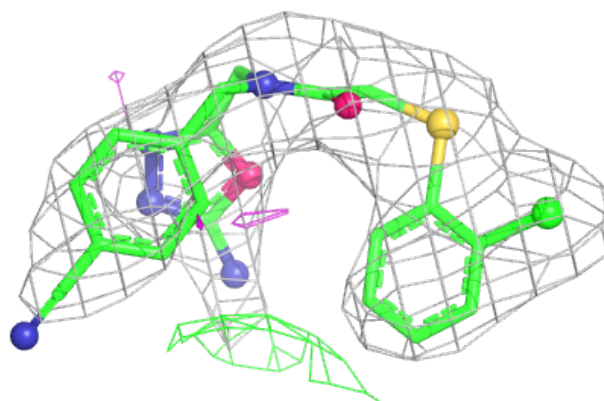
**Electron density around VFN 2 301:**

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

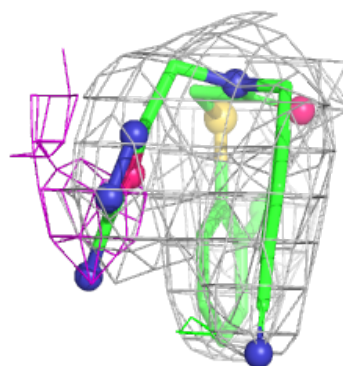
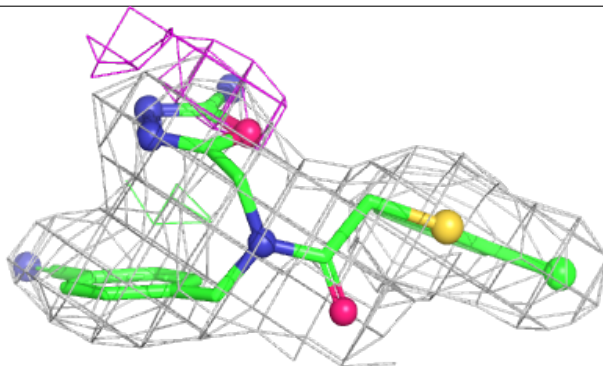
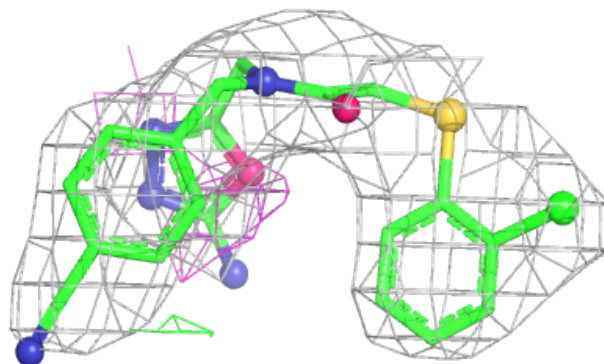


Electron density around VFN R 301:

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

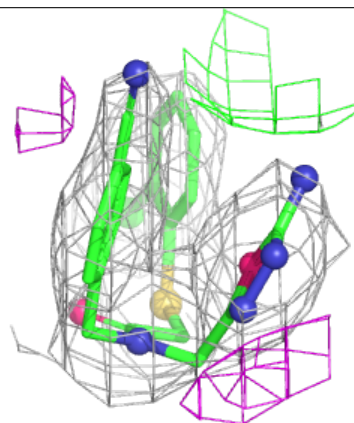
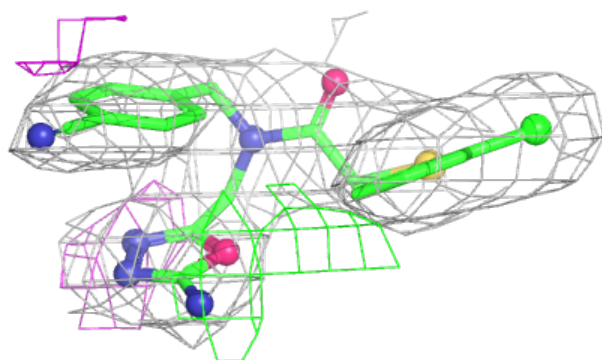
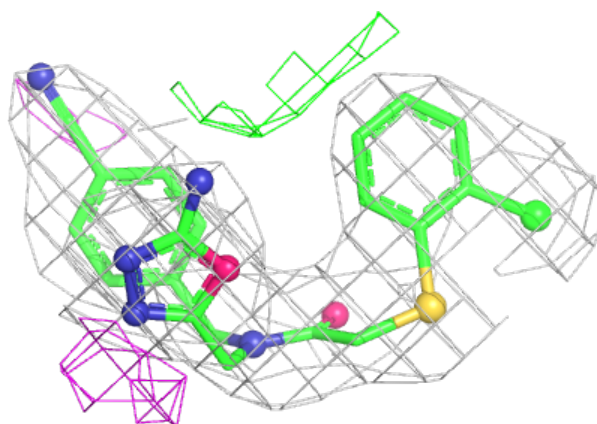
**Electron density around VFN H 302:**

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

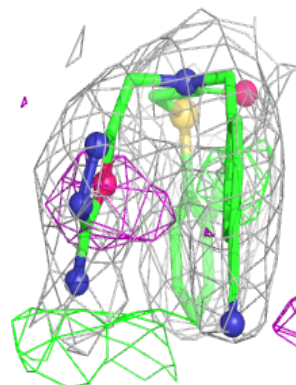
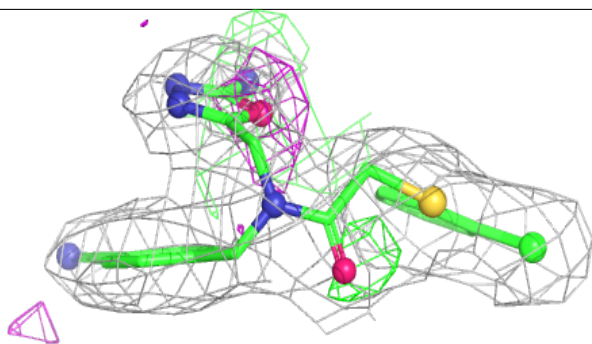
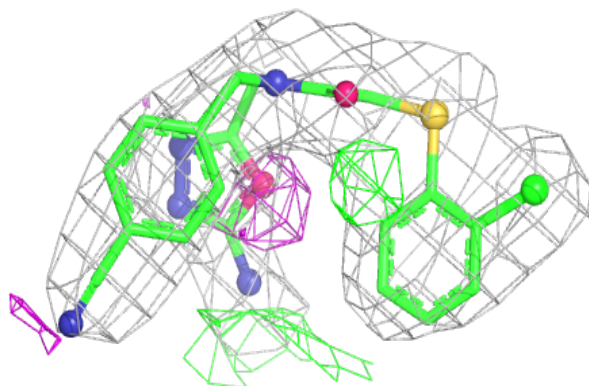


Electron density around VFN B 301:

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

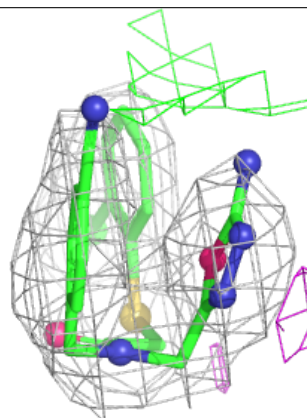
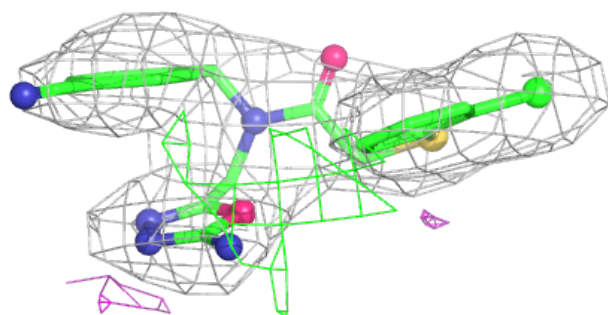
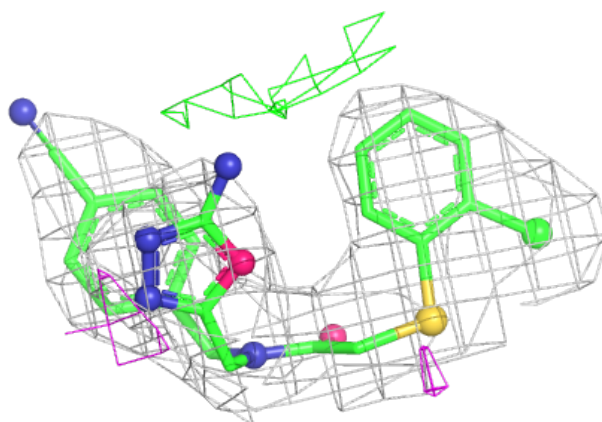
**Electron density around VFN D 302:**

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

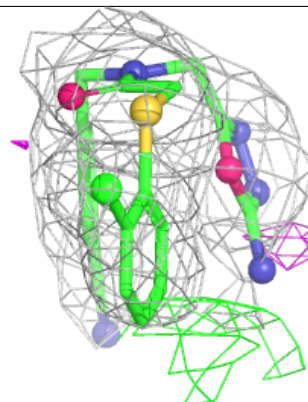
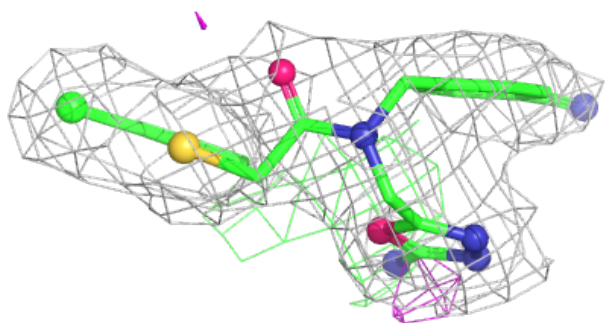
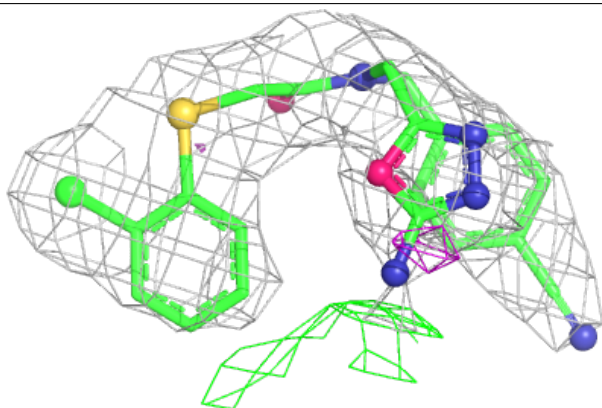


Electron density around VFN G 301:

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

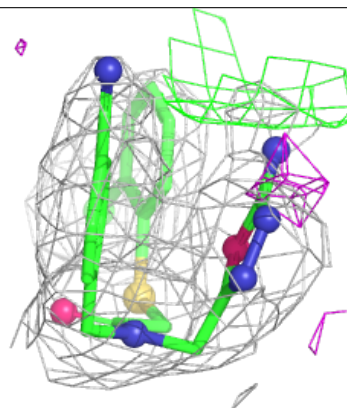
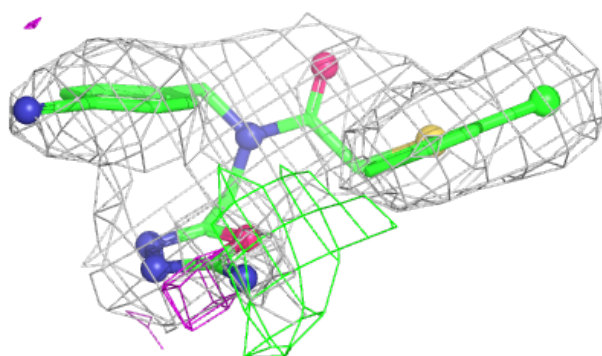
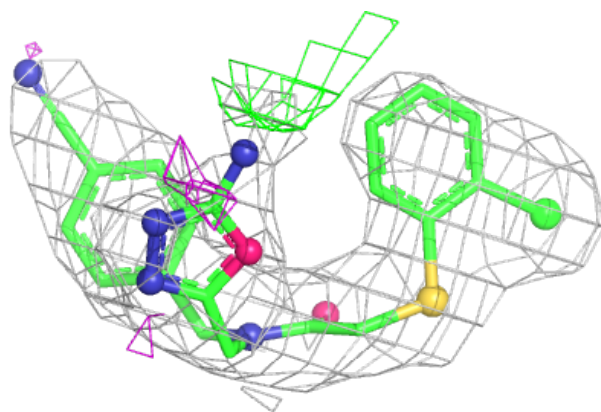
**Electron density around VFN 3 301:**

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

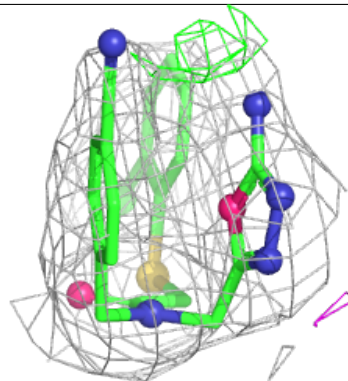
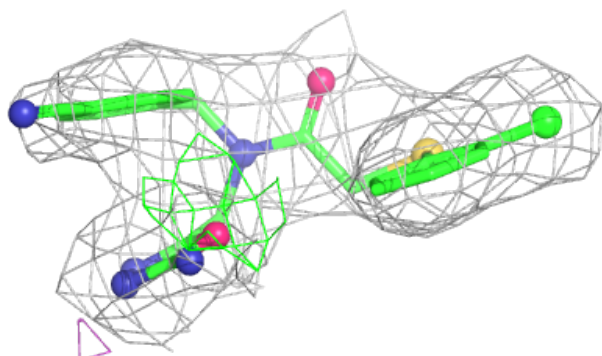
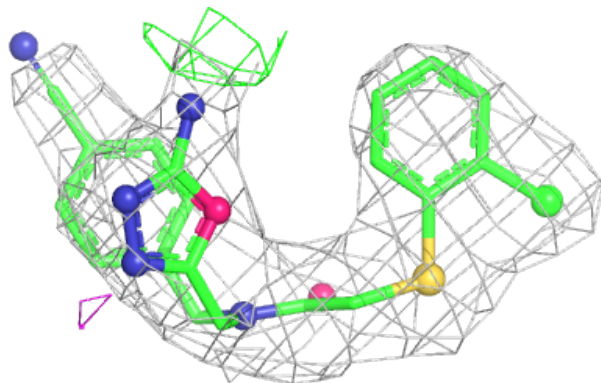


Electron density around VFN 1 302:

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

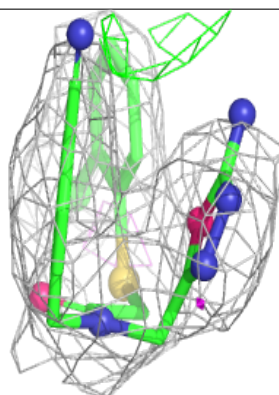
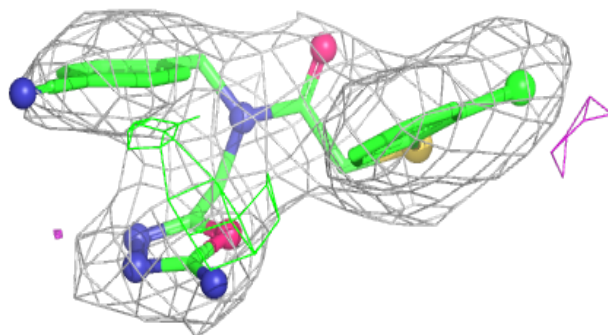
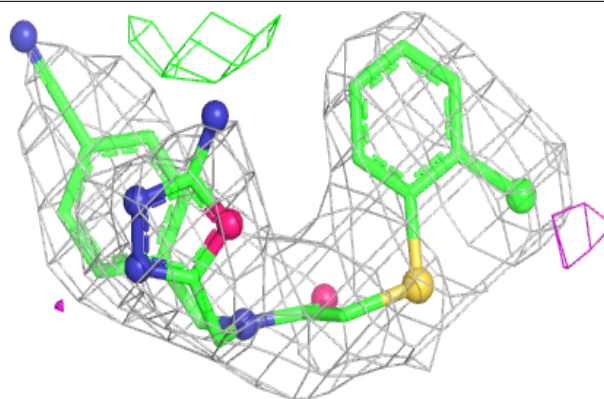
**Electron density around VFN O 302:**

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

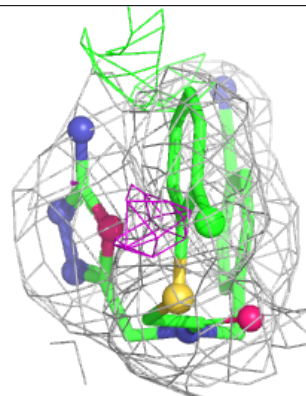
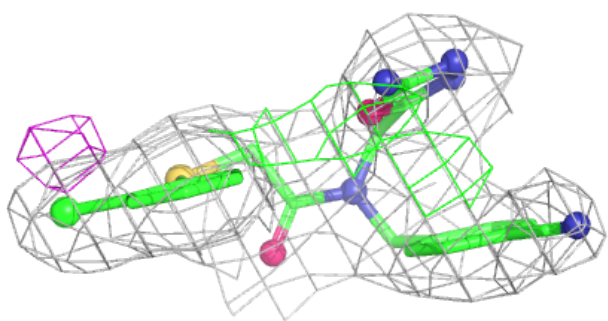
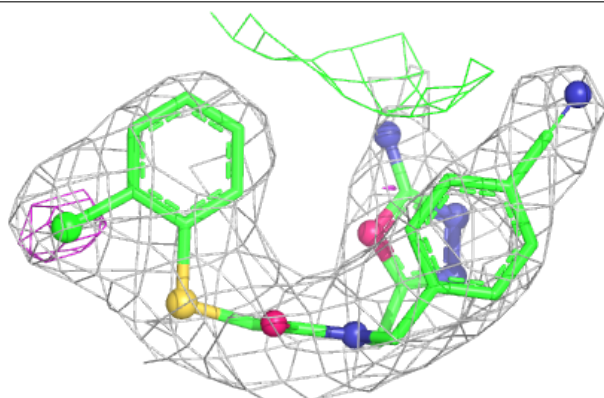


Electron density around VFN P 301:

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

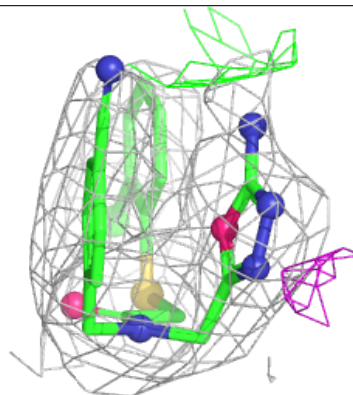
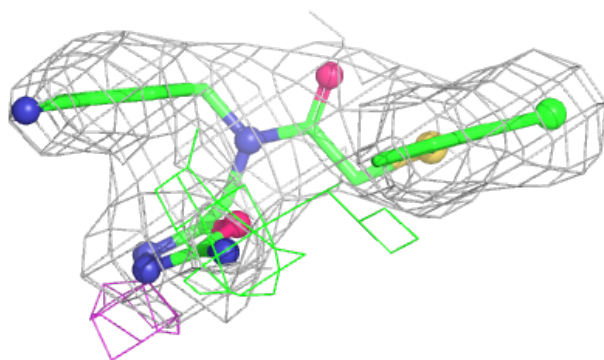
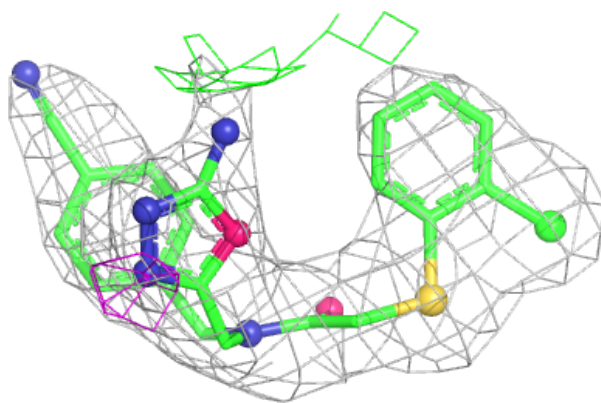
**Electron density around VFN A 301:**

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

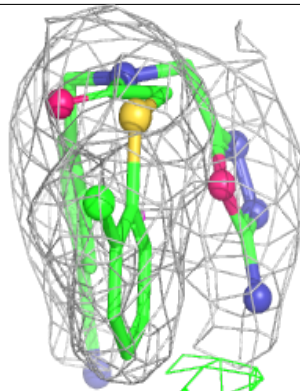
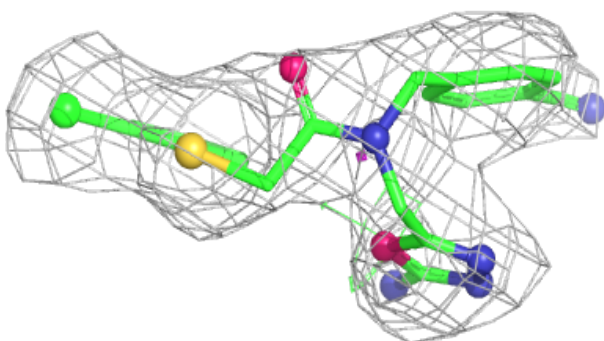
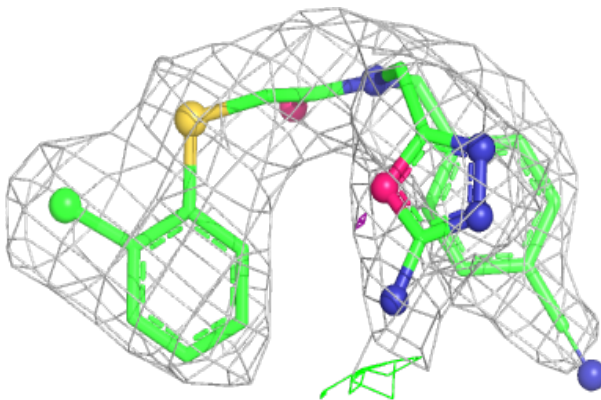


Electron density around VFN S 301:

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

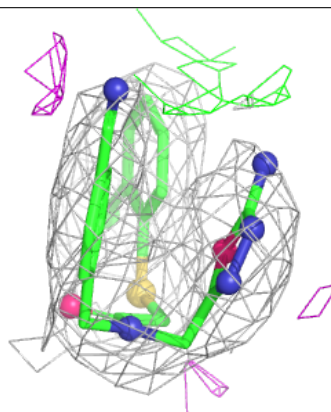
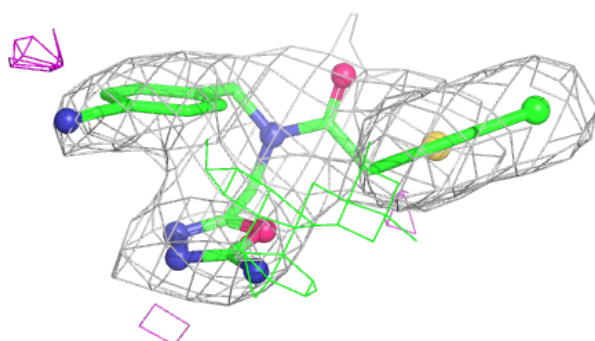
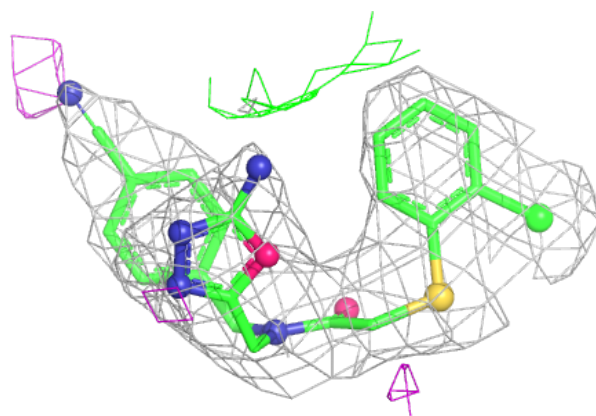
**Electron density around VFN W 302:**

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

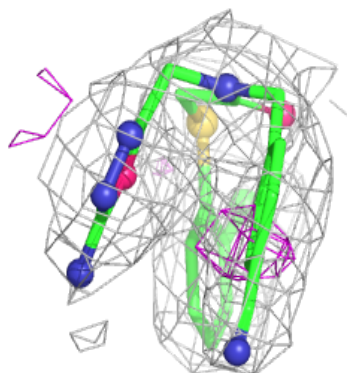
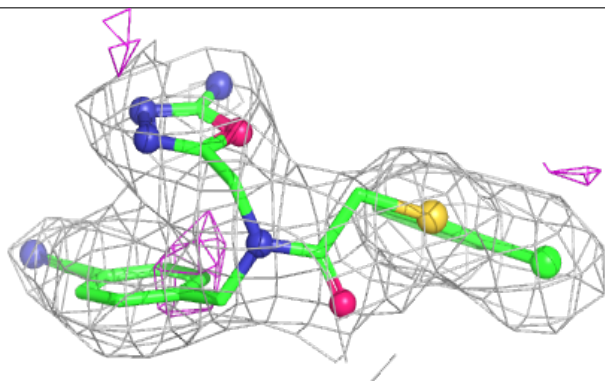
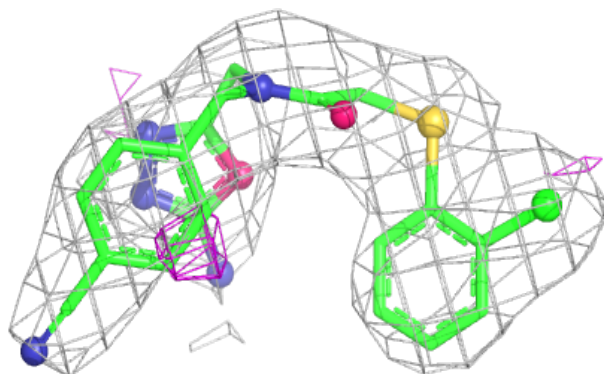


Electron density around VFN A 302:

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

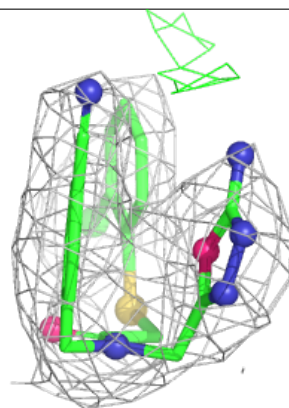
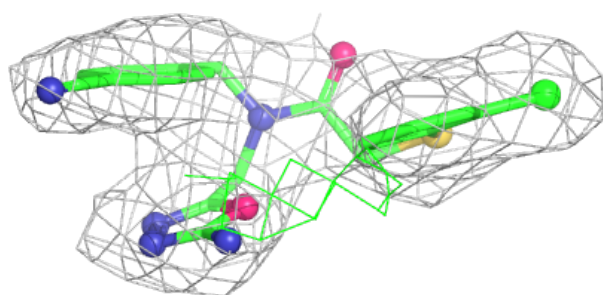
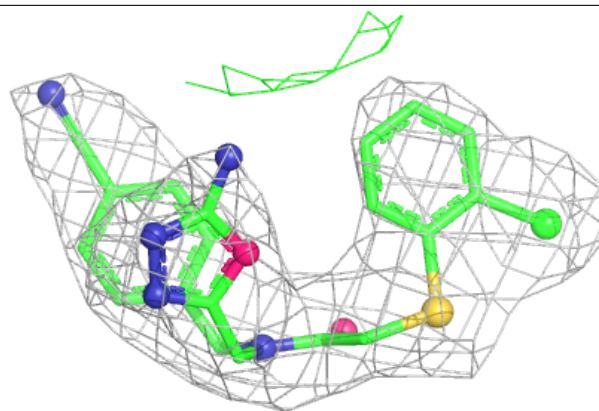
**Electron density around VFN F 301:**

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

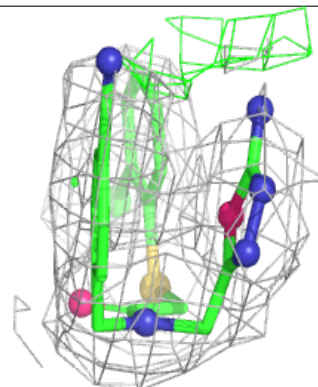
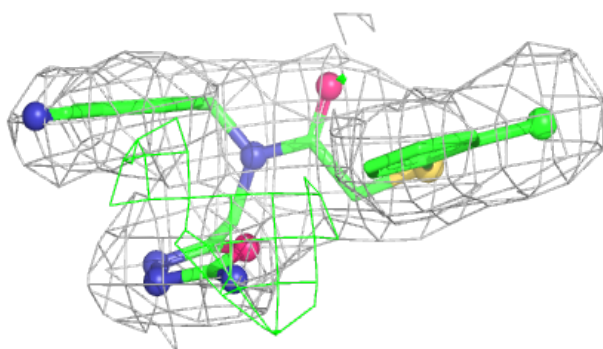
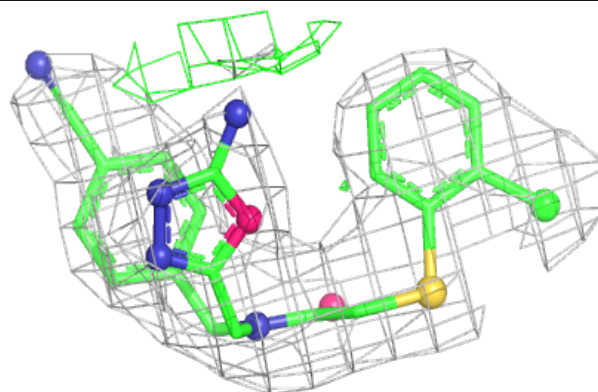


Electron density around VFN P 302:

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

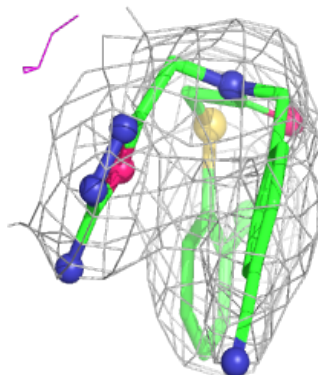
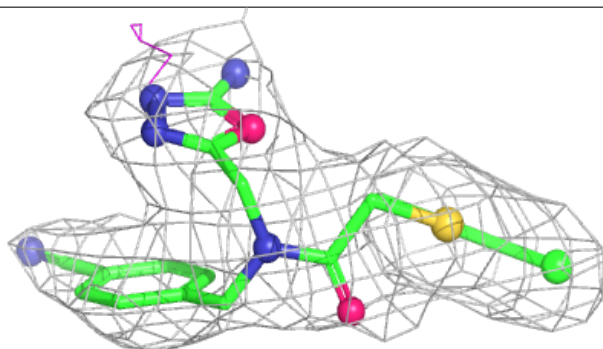
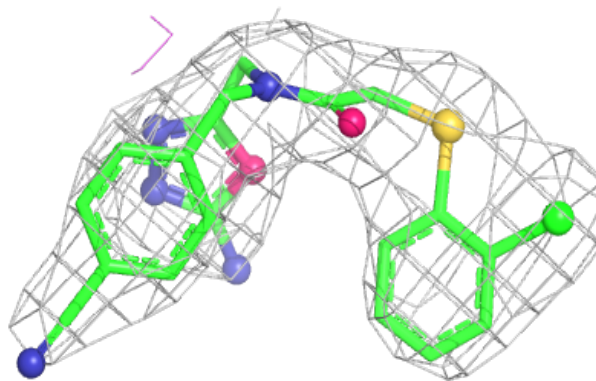
**Electron density around VFN 1 301:**

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

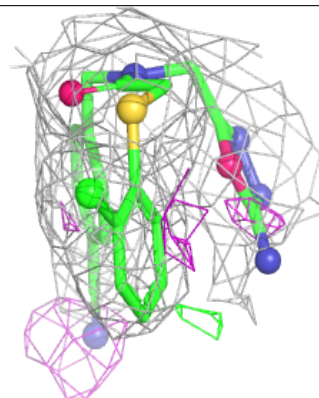
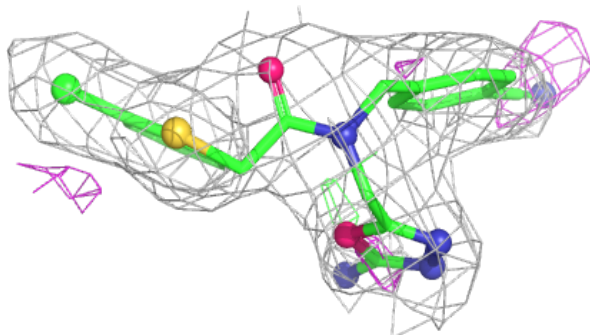
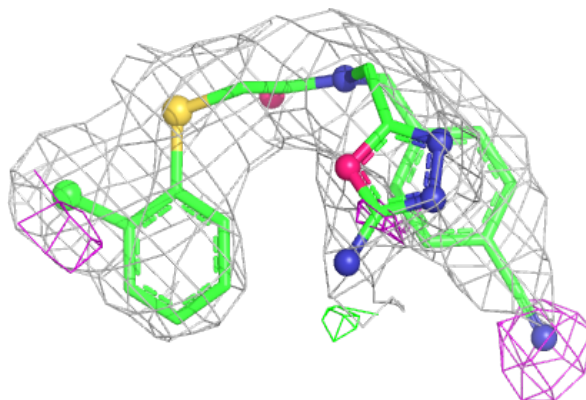


Electron density around VFN L 301:

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

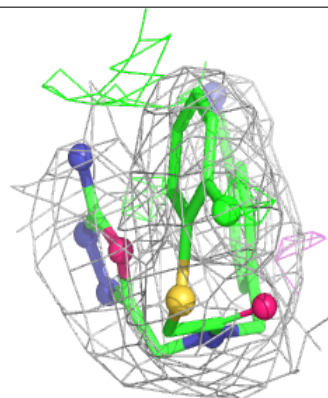
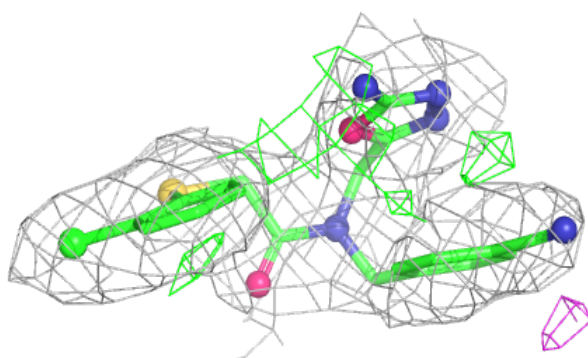
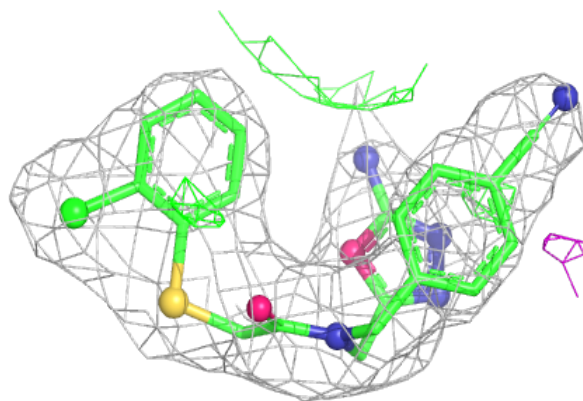
**Electron density around VFN W 301:**

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

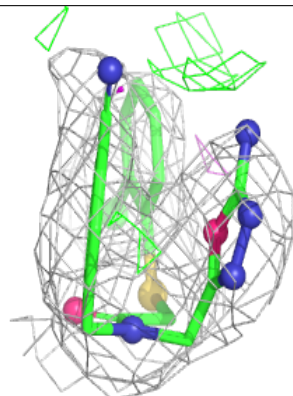
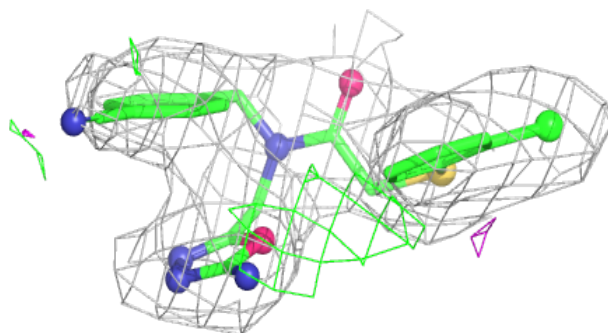
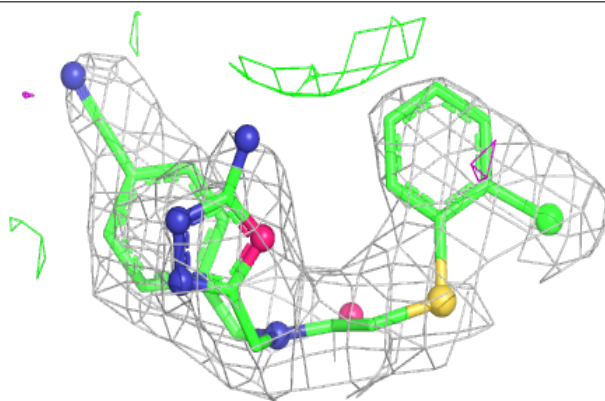


Electron density around VFN N 301:

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

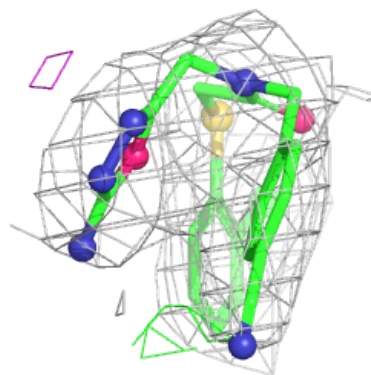
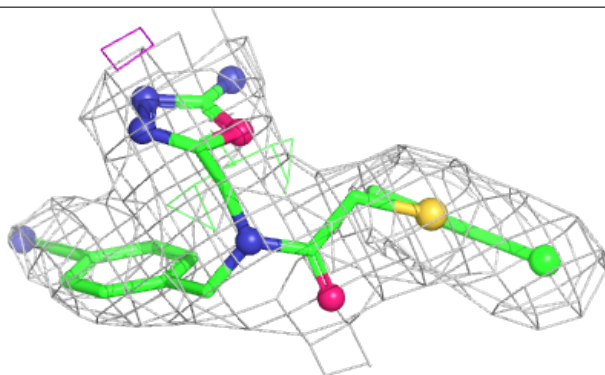
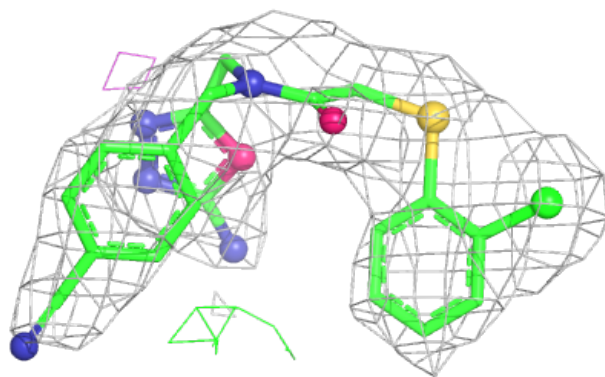
**Electron density around VFN O 301:**

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

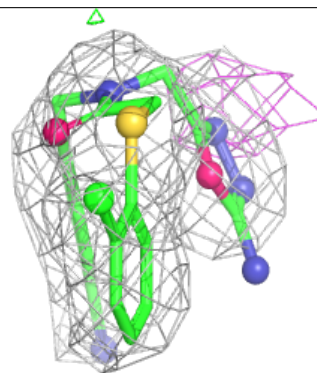
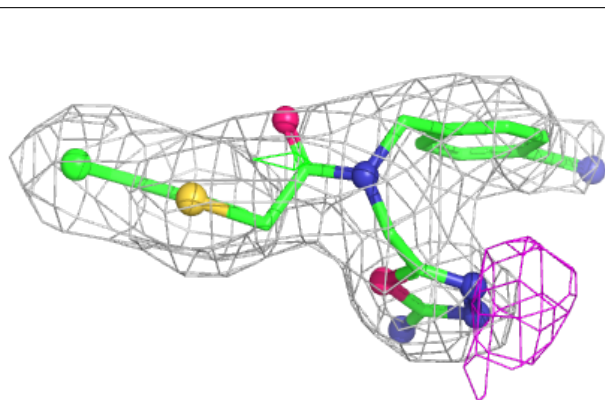
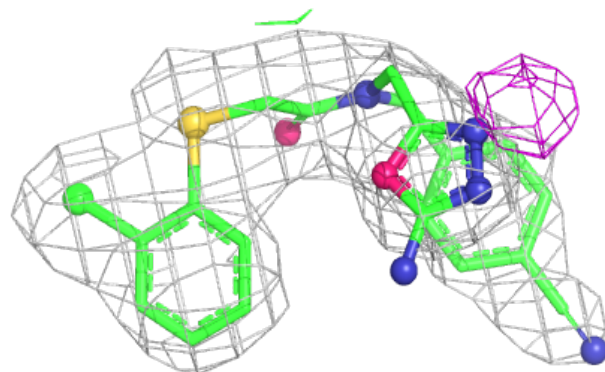


Electron density around VFN H 301:

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

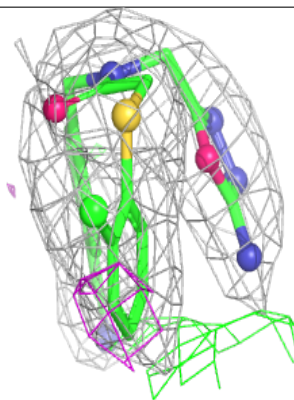
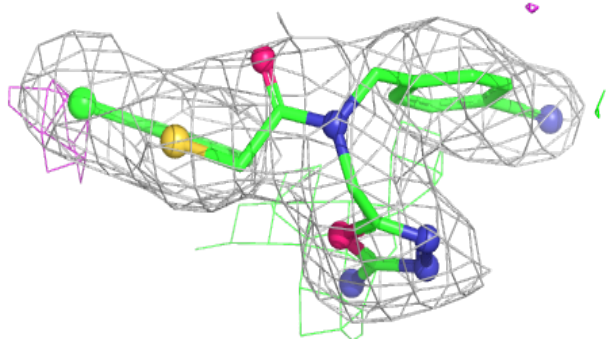
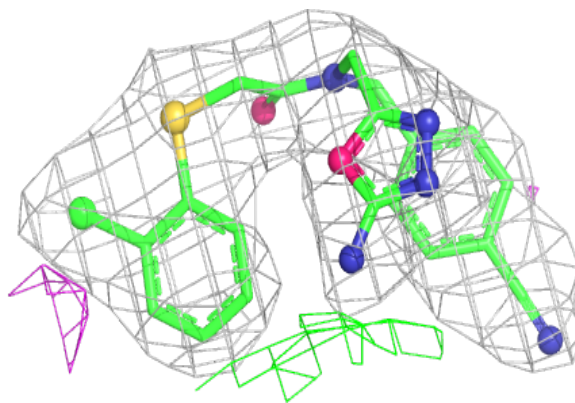
**Electron density around VFN T 301:**

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

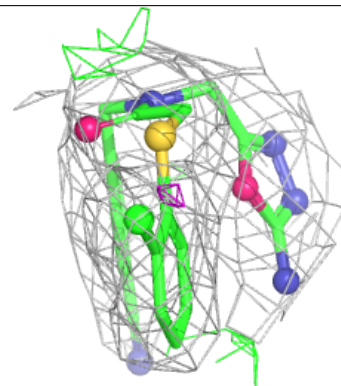
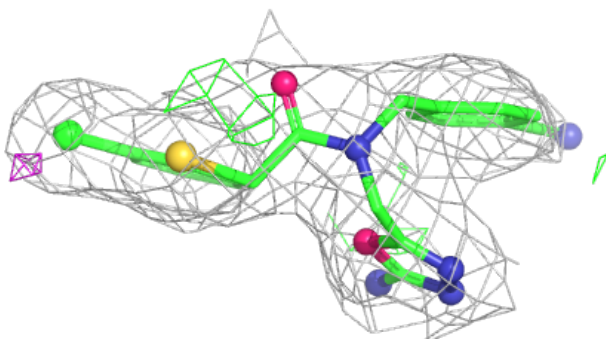
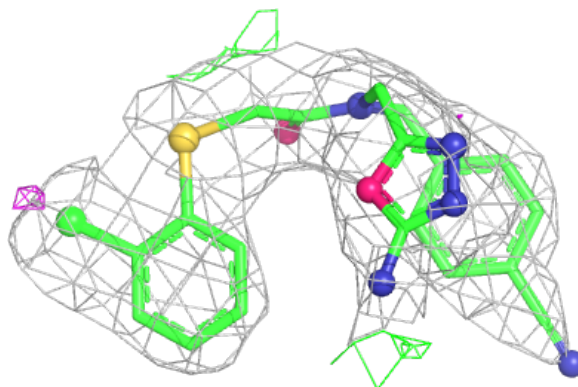


Electron density around VFN V 301:

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

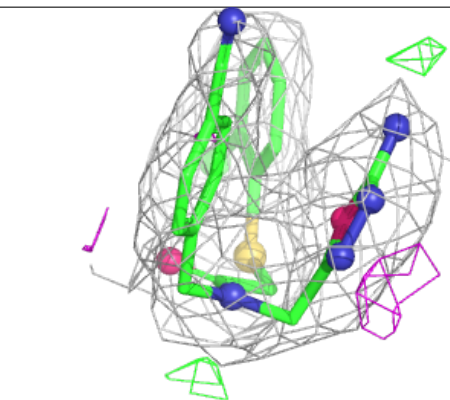
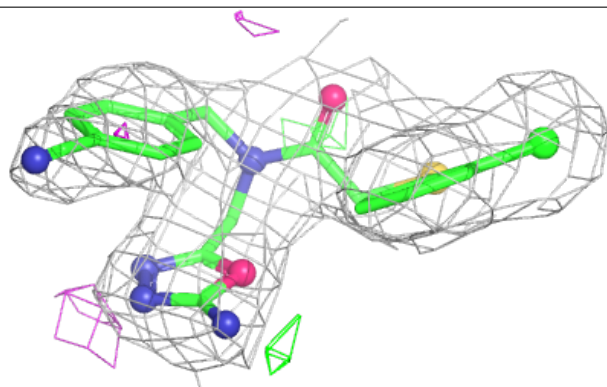
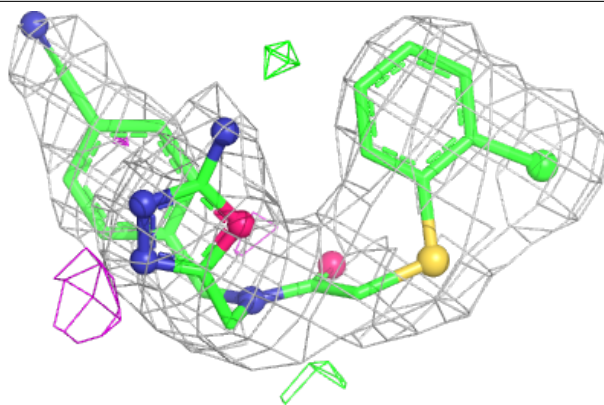
**Electron density around VFN J 301:**

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

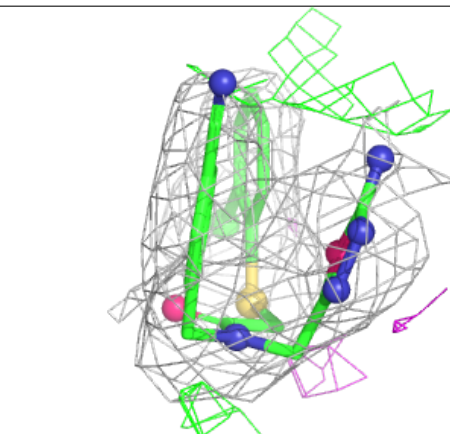
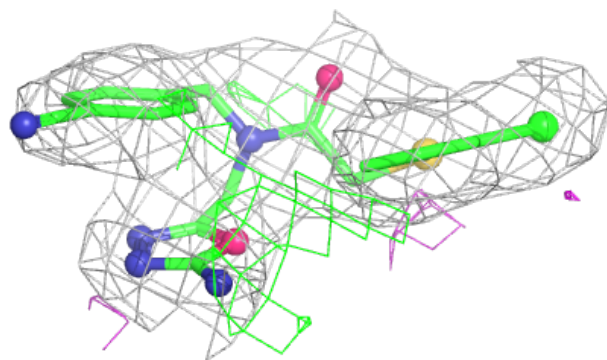
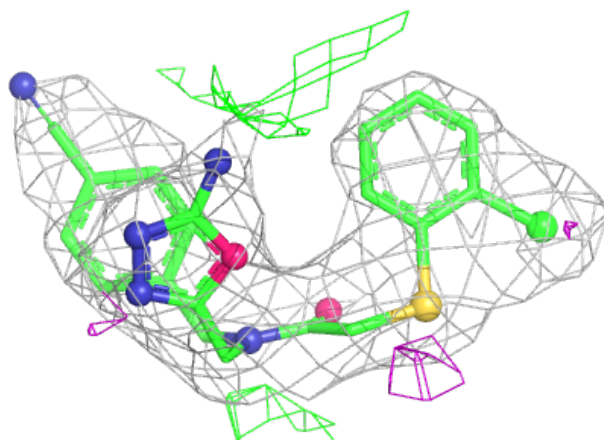


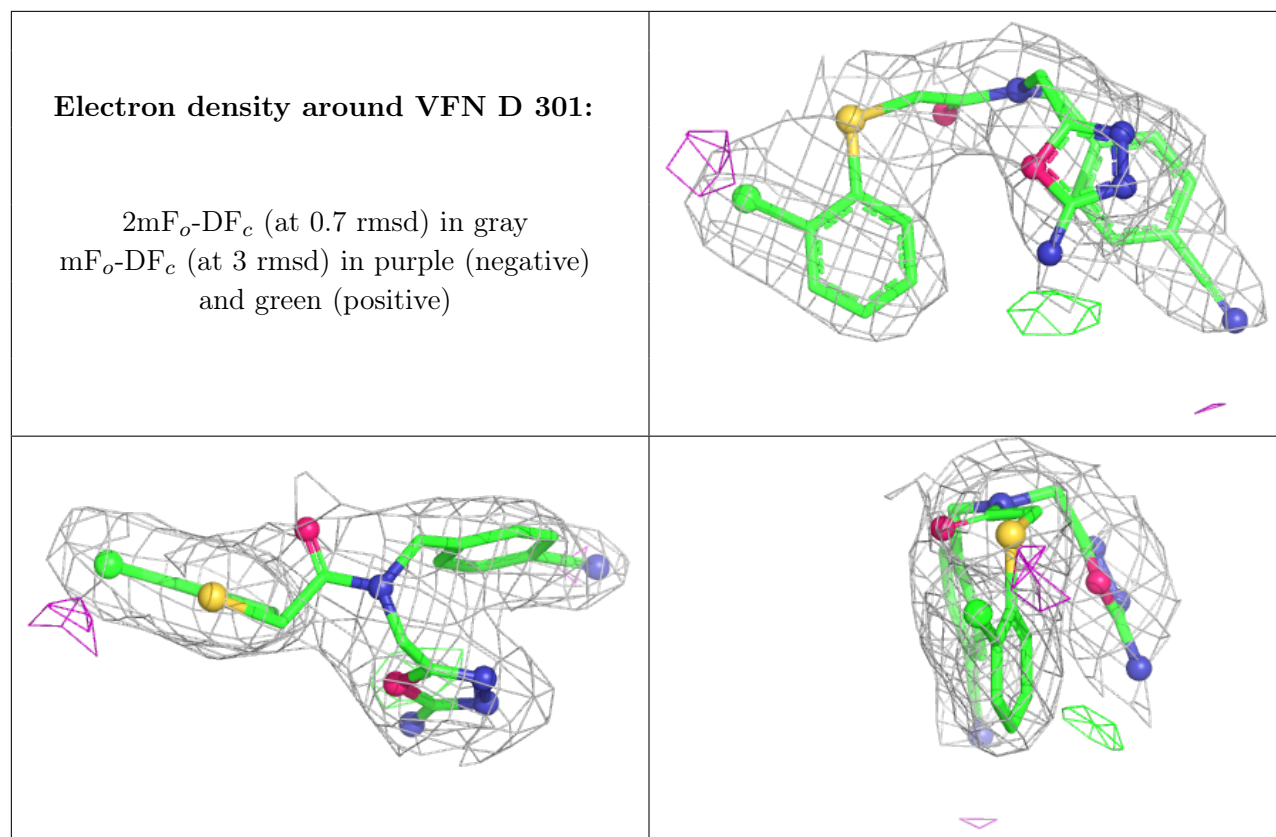
Electron density around VFN S 302:

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

**Electron density around VFN Z 301:**

$2mF_o-DF_c$ (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.