



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 6, 2023 – 05:36 PM EDT

PDB ID : 4FZB  
Title : Structure of thymidylate synthase ThyX complexed to a new inhibitor  
Authors : Basta, T.; Boum, Y.; Briffotiaux, J.; Becker, H.F.; Lamarre-Jouenne, I.; Lambry, J.C.; Skouloubris, S.; Liebl, U.; van Tilbeurgh, H.; Graille, M.; Myllykallio, H.  
Deposited on : 2012-07-06  
Resolution : 2.59 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.

The types of validation reports are described at

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

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

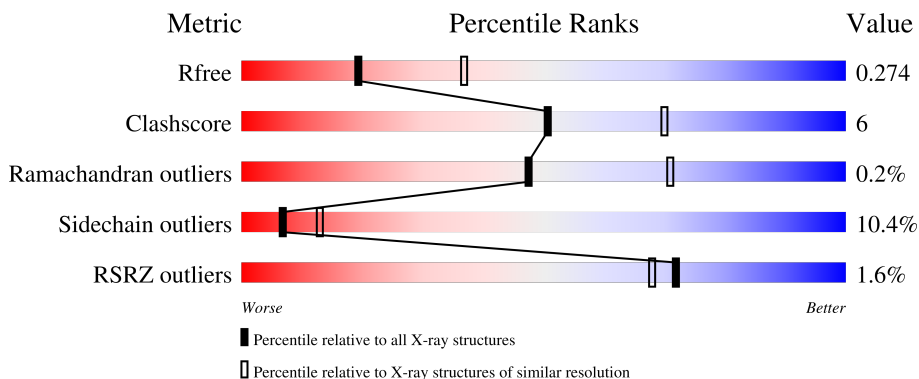
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	227	70% 12% • 16%
1	B	227	62% 19% • 17%
1	C	227	76% 13% • 9%
1	D	227	68% 21% • 11%

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Mol	Chain	Length	Quality of chain		
1	E	227		73%	15% 9%
1	F	227		70%	19% 9%
1	G	227		67%	14% 17%
1	H	227		65%	13% 21%
1	I	227		64%	20% 15%
1	J	227		64%	13% 21%
1	K	227		73%	15% 11%
1	L	227		67%	20% 11%
1	M	227		61%	23% 13%
1	N	227		59%	19% 22%
1	O	227		64%	22% 12%
1	P	227		69%	16% 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	0VJ	B	303	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 26503 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 Probable thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	191	Total 1544	C 984	N 267	O 287	S 6	0	0	0
1	B	188	Total 1519	C 971	N 264	O 278	S 6	0	0	0
1	C	207	Total 1667	C 1060	N 291	O 308	S 8	0	0	0
1	D	203	Total 1642	C 1047	N 285	O 303	S 7	0	0	0
1	E	206	Total 1668	C 1060	N 293	O 307	S 8	0	1	0
1	F	206	Total 1666	C 1062	N 289	O 307	S 8	0	0	0
1	G	188	Total 1519	C 971	N 264	O 278	S 6	0	0	0
1	H	179	Total 1446	C 928	N 250	O 262	S 6	0	0	0
1	I	193	Total 1558	C 995	N 270	O 286	S 7	0	0	0
1	J	179	Total 1449	C 931	N 251	O 261	S 6	0	0	0
1	K	201	Total 1624	C 1034	N 283	O 300	S 7	0	0	0
1	L	201	Total 1624	C 1034	N 283	O 300	S 7	0	0	0
1	M	197	Total 1592	C 1019	N 275	O 291	S 7	0	0	0
1	N	177	Total 1432	C 921	N 247	O 258	S 6	0	0	0
1	O	200	Total 1617	C 1029	N 282	O 299	S 7	0	0	0
1	P	197	Total 1592	C 1015	N 276	O 294	S 7	0	0	0



There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	expression tag	UNP O41156
A	-3	ALA	-	expression tag	UNP O41156
A	-2	SER	-	expression tag	UNP O41156
A	-1	MET	-	expression tag	UNP O41156
A	0	THR	-	expression tag	UNP O41156
A	1	GLY	-	expression tag	UNP O41156
A	217	HIS	-	expression tag	UNP O41156
A	218	HIS	-	expression tag	UNP O41156
A	219	HIS	-	expression tag	UNP O41156
A	220	HIS	-	expression tag	UNP O41156
A	221	HIS	-	expression tag	UNP O41156
A	222	HIS	-	expression tag	UNP O41156
B	-4	MET	-	expression tag	UNP O41156
B	-3	ALA	-	expression tag	UNP O41156
B	-2	SER	-	expression tag	UNP O41156
B	-1	MET	-	expression tag	UNP O41156
B	0	THR	-	expression tag	UNP O41156
B	1	GLY	-	expression tag	UNP O41156
B	217	HIS	-	expression tag	UNP O41156
B	218	HIS	-	expression tag	UNP O41156
B	219	HIS	-	expression tag	UNP O41156
B	220	HIS	-	expression tag	UNP O41156
B	221	HIS	-	expression tag	UNP O41156
B	222	HIS	-	expression tag	UNP O41156
C	-4	MET	-	expression tag	UNP O41156
C	-3	ALA	-	expression tag	UNP O41156
C	-2	SER	-	expression tag	UNP O41156
C	-1	MET	-	expression tag	UNP O41156
C	0	THR	-	expression tag	UNP O41156
C	1	GLY	-	expression tag	UNP O41156
C	217	HIS	-	expression tag	UNP O41156
C	218	HIS	-	expression tag	UNP O41156
C	219	HIS	-	expression tag	UNP O41156
C	220	HIS	-	expression tag	UNP O41156
C	221	HIS	-	expression tag	UNP O41156
C	222	HIS	-	expression tag	UNP O41156
D	-4	MET	-	expression tag	UNP O41156
D	-3	ALA	-	expression tag	UNP O41156
D	-2	SER	-	expression tag	UNP O41156
D	-1	MET	-	expression tag	UNP O41156
D	0	THR	-	expression tag	UNP O41156
D	1	GLY	-	expression tag	UNP O41156

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Chain	Residue	Modelled	Actual	Comment	Reference
D	217	HIS	-	expression tag	UNP O41156
D	218	HIS	-	expression tag	UNP O41156
D	219	HIS	-	expression tag	UNP O41156
D	220	HIS	-	expression tag	UNP O41156
D	221	HIS	-	expression tag	UNP O41156
D	222	HIS	-	expression tag	UNP O41156
E	-4	MET	-	expression tag	UNP O41156
E	-3	ALA	-	expression tag	UNP O41156
E	-2	SER	-	expression tag	UNP O41156
E	-1	MET	-	expression tag	UNP O41156
E	0	THR	-	expression tag	UNP O41156
E	1	GLY	-	expression tag	UNP O41156
E	217	HIS	-	expression tag	UNP O41156
E	218	HIS	-	expression tag	UNP O41156
E	219	HIS	-	expression tag	UNP O41156
E	220	HIS	-	expression tag	UNP O41156
E	221	HIS	-	expression tag	UNP O41156
E	222	HIS	-	expression tag	UNP O41156
F	-4	MET	-	expression tag	UNP O41156
F	-3	ALA	-	expression tag	UNP O41156
F	-2	SER	-	expression tag	UNP O41156
F	-1	MET	-	expression tag	UNP O41156
F	0	THR	-	expression tag	UNP O41156
F	1	GLY	-	expression tag	UNP O41156
F	217	HIS	-	expression tag	UNP O41156
F	218	HIS	-	expression tag	UNP O41156
F	219	HIS	-	expression tag	UNP O41156
F	220	HIS	-	expression tag	UNP O41156
F	221	HIS	-	expression tag	UNP O41156
F	222	HIS	-	expression tag	UNP O41156
G	-4	MET	-	expression tag	UNP O41156
G	-3	ALA	-	expression tag	UNP O41156
G	-2	SER	-	expression tag	UNP O41156
G	-1	MET	-	expression tag	UNP O41156
G	0	THR	-	expression tag	UNP O41156
G	1	GLY	-	expression tag	UNP O41156
G	217	HIS	-	expression tag	UNP O41156
G	218	HIS	-	expression tag	UNP O41156
G	219	HIS	-	expression tag	UNP O41156
G	220	HIS	-	expression tag	UNP O41156
G	221	HIS	-	expression tag	UNP O41156
G	222	HIS	-	expression tag	UNP O41156

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-4	MET	-	expression tag	UNP O41156
H	-3	ALA	-	expression tag	UNP O41156
H	-2	SER	-	expression tag	UNP O41156
H	-1	MET	-	expression tag	UNP O41156
H	0	THR	-	expression tag	UNP O41156
H	1	GLY	-	expression tag	UNP O41156
H	217	HIS	-	expression tag	UNP O41156
H	218	HIS	-	expression tag	UNP O41156
H	219	HIS	-	expression tag	UNP O41156
H	220	HIS	-	expression tag	UNP O41156
H	221	HIS	-	expression tag	UNP O41156
H	222	HIS	-	expression tag	UNP O41156
I	-4	MET	-	expression tag	UNP O41156
I	-3	ALA	-	expression tag	UNP O41156
I	-2	SER	-	expression tag	UNP O41156
I	-1	MET	-	expression tag	UNP O41156
I	0	THR	-	expression tag	UNP O41156
I	1	GLY	-	expression tag	UNP O41156
I	217	HIS	-	expression tag	UNP O41156
I	218	HIS	-	expression tag	UNP O41156
I	219	HIS	-	expression tag	UNP O41156
I	220	HIS	-	expression tag	UNP O41156
I	221	HIS	-	expression tag	UNP O41156
I	222	HIS	-	expression tag	UNP O41156
J	-4	MET	-	expression tag	UNP O41156
J	-3	ALA	-	expression tag	UNP O41156
J	-2	SER	-	expression tag	UNP O41156
J	-1	MET	-	expression tag	UNP O41156
J	0	THR	-	expression tag	UNP O41156
J	1	GLY	-	expression tag	UNP O41156
J	217	HIS	-	expression tag	UNP O41156
J	218	HIS	-	expression tag	UNP O41156
J	219	HIS	-	expression tag	UNP O41156
J	220	HIS	-	expression tag	UNP O41156
J	221	HIS	-	expression tag	UNP O41156
J	222	HIS	-	expression tag	UNP O41156
K	-4	MET	-	expression tag	UNP O41156
K	-3	ALA	-	expression tag	UNP O41156
K	-2	SER	-	expression tag	UNP O41156
K	-1	MET	-	expression tag	UNP O41156
K	0	THR	-	expression tag	UNP O41156
K	1	GLY	-	expression tag	UNP O41156

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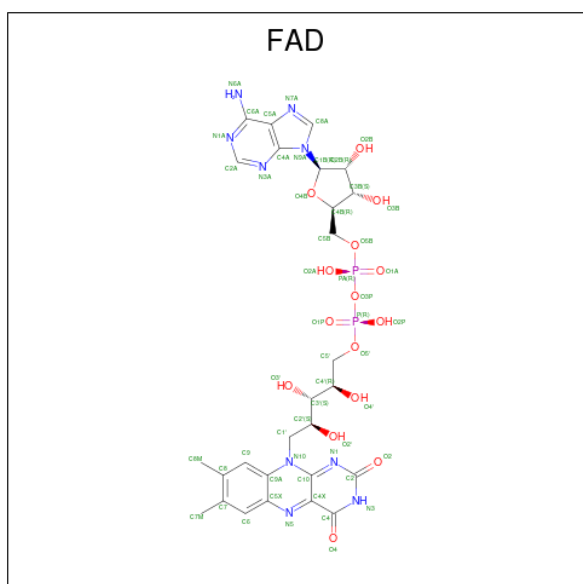
Chain	Residue	Modelled	Actual	Comment	Reference
K	217	HIS	-	expression tag	UNP O41156
K	218	HIS	-	expression tag	UNP O41156
K	219	HIS	-	expression tag	UNP O41156
K	220	HIS	-	expression tag	UNP O41156
K	221	HIS	-	expression tag	UNP O41156
K	222	HIS	-	expression tag	UNP O41156
L	-4	MET	-	expression tag	UNP O41156
L	-3	ALA	-	expression tag	UNP O41156
L	-2	SER	-	expression tag	UNP O41156
L	-1	MET	-	expression tag	UNP O41156
L	0	THR	-	expression tag	UNP O41156
L	1	GLY	-	expression tag	UNP O41156
L	217	HIS	-	expression tag	UNP O41156
L	218	HIS	-	expression tag	UNP O41156
L	219	HIS	-	expression tag	UNP O41156
L	220	HIS	-	expression tag	UNP O41156
L	221	HIS	-	expression tag	UNP O41156
L	222	HIS	-	expression tag	UNP O41156
M	-4	MET	-	expression tag	UNP O41156
M	-3	ALA	-	expression tag	UNP O41156
M	-2	SER	-	expression tag	UNP O41156
M	-1	MET	-	expression tag	UNP O41156
M	0	THR	-	expression tag	UNP O41156
M	1	GLY	-	expression tag	UNP O41156
M	217	HIS	-	expression tag	UNP O41156
M	218	HIS	-	expression tag	UNP O41156
M	219	HIS	-	expression tag	UNP O41156
M	220	HIS	-	expression tag	UNP O41156
M	221	HIS	-	expression tag	UNP O41156
M	222	HIS	-	expression tag	UNP O41156
N	-4	MET	-	expression tag	UNP O41156
N	-3	ALA	-	expression tag	UNP O41156
N	-2	SER	-	expression tag	UNP O41156
N	-1	MET	-	expression tag	UNP O41156
N	0	THR	-	expression tag	UNP O41156
N	1	GLY	-	expression tag	UNP O41156
N	217	HIS	-	expression tag	UNP O41156
N	218	HIS	-	expression tag	UNP O41156
N	219	HIS	-	expression tag	UNP O41156
N	220	HIS	-	expression tag	UNP O41156
N	221	HIS	-	expression tag	UNP O41156
N	222	HIS	-	expression tag	UNP O41156

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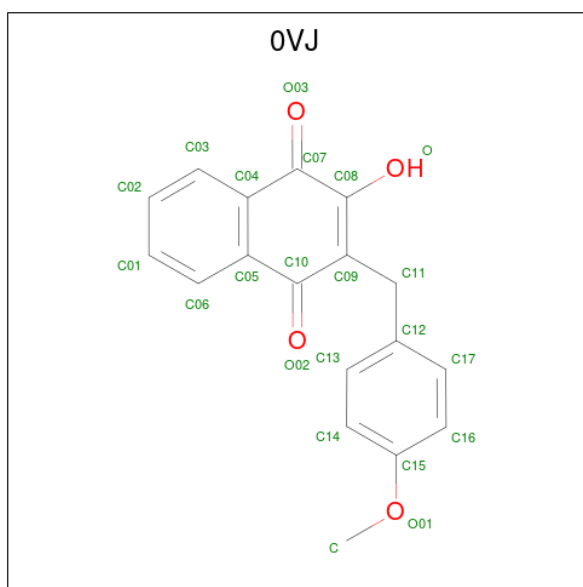
Chain	Residue	Modelled	Actual	Comment	Reference
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O	-3	ALA	-	expression tag	UNP O41156
O	-2	SER	-	expression tag	UNP O41156
O	-1	MET	-	expression tag	UNP O41156
O	0	THR	-	expression tag	UNP O41156
O	1	GLY	-	expression tag	UNP O41156
O	217	HIS	-	expression tag	UNP O41156
O	218	HIS	-	expression tag	UNP O41156
O	219	HIS	-	expression tag	UNP O41156
O	220	HIS	-	expression tag	UNP O41156
O	221	HIS	-	expression tag	UNP O41156
O	222	HIS	-	expression tag	UNP O41156
P	-4	MET	-	expression tag	UNP O41156
P	-3	ALA	-	expression tag	UNP O41156
P	-2	SER	-	expression tag	UNP O41156
P	-1	MET	-	expression tag	UNP O41156
P	0	THR	-	expression tag	UNP O41156
P	1	GLY	-	expression tag	UNP O41156
P	217	HIS	-	expression tag	UNP O41156
P	218	HIS	-	expression tag	UNP O41156
P	219	HIS	-	expression tag	UNP O41156
P	220	HIS	-	expression tag	UNP O41156
P	221	HIS	-	expression tag	UNP O41156
P	222	HIS	-	expression tag	UNP O41156

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0
2	A	1	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0
2	C	1	53	27	9	15	2	0	0
2	E	1	53	27	9	15	2	0	0
2	F	1	53	27	9	15	2	0	0
2	F	1	53	27	9	15	2	0	0
2	H	1	53	27	9	15	2	0	0
2	I	1	53	27	9	15	2	0	0
2	I	1	53	27	9	15	2	0	0
2	J	1	53	27	9	15	2	0	0
2	K	1	53	27	9	15	2	0	0
2	M	1	53	27	9	15	2	0	0
2	N	1	53	27	9	15	2	0	0
2	O	1	53	27	9	15	2	0	0
2	P	1	53	27	9	15	2	0	0

- Molecule 3 is 2-hydroxy-3-(4-methoxybenzyl)naphthalene-1,4-dione (three-letter code: 0VJ) (formula: C<sub>18</sub>H<sub>14</sub>O<sub>4</sub>).



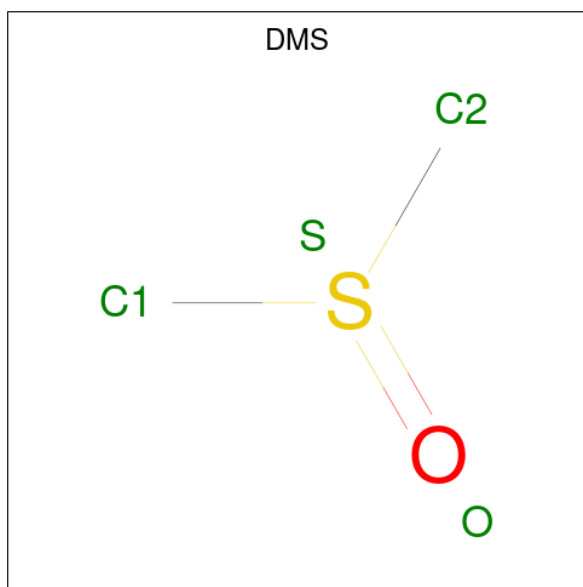
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	18	4		
3	A	1	Total	C	O	0	0
			22	18	4		
3	B	1	Total	C	O	0	0
			22	18	4		
3	D	1	Total	C	O	0	0
			22	18	4		
3	E	1	Total	C	O	0	0
			22	18	4		
3	F	1	Total	C	O	0	0
			22	18	4		
3	G	1	Total	C	O	0	0
			22	18	4		
3	H	1	Total	C	O	0	0
			22	18	4		
3	I	1	Total	C	O	0	0
			22	18	4		
3	J	1	Total	C	O	0	0
			22	18	4		
3	K	1	Total	C	O	0	0
			22	18	4		
3	L	1	Total	C	O	0	0
			22	18	4		
3	M	1	Total	C	O	0	0
			22	18	4		
3	N	1	Total	C	O	0	0
			22	18	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	C	O	0	0
			22	18	4		
3	P	1	Total	C	O	0	0
			22	18	4		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	K	1	Total	C	O	S	0	0
			4	2	1	1		
4	M	1	Total	C	O	S	0	0
			4	2	1	1		
4	O	1	Total	C	O	S	0	0
			4	2	1	1		
4	P	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	7	Total	O	0	0
			7	7		
5	C	2	Total	O	0	0
			2	2		
5	D	7	Total	O	0	0
			7	7		
5	E	8	Total	O	0	0
			8	8		
5	F	13	Total	O	0	0
			13	13		
5	G	13	Total	O	0	0
			13	13		
5	H	5	Total	O	0	0
			5	5		
5	I	3	Total	O	0	0
			3	3		
5	J	5	Total	O	0	0
			5	5		
5	K	2	Total	O	0	0
			2	2		
5	L	6	Total	O	0	0
			6	6		
5	M	3	Total	O	0	0
			3	3		
5	N	5	Total	O	0	0
			5	5		
5	O	1	Total	O	0	0
			1	1		

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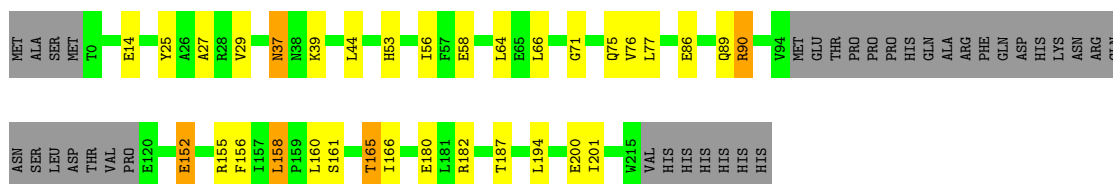
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	P	1	Total	O	0	0
			1	1		

### 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: Probable thymidylate synthase

Chain A: 




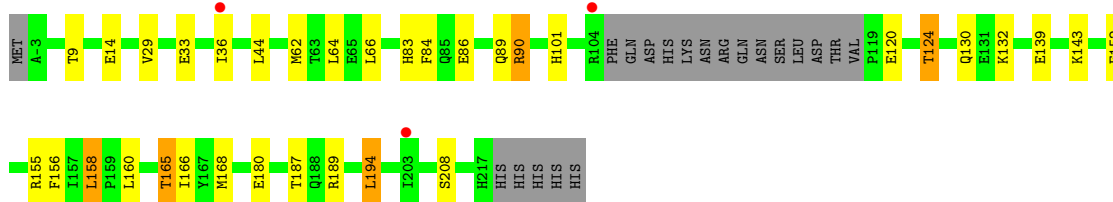
- Molecule 1: Probable thymidylate synthase

Chain B: 



- Molecule 1: Probable thymidylate synthase

Chain C: 



- Molecule 1: Probable thymidylate synthase

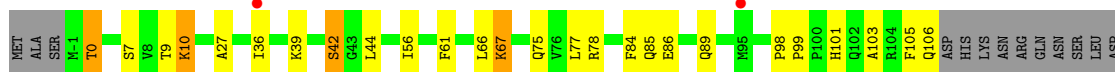
Chain D: 



● Molecule 1: Probable thymidylate synthase



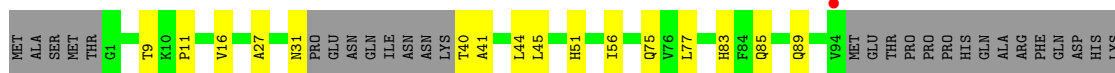
● Molecule 1: Probable thymidylate synthase



● Molecule 1: Probable thymidylate synthase

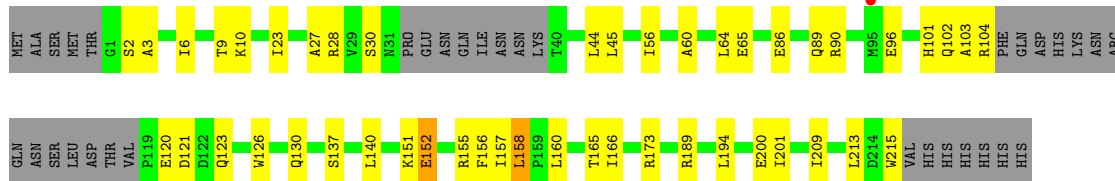


● Molecule 1: Probable thymidylate synthase



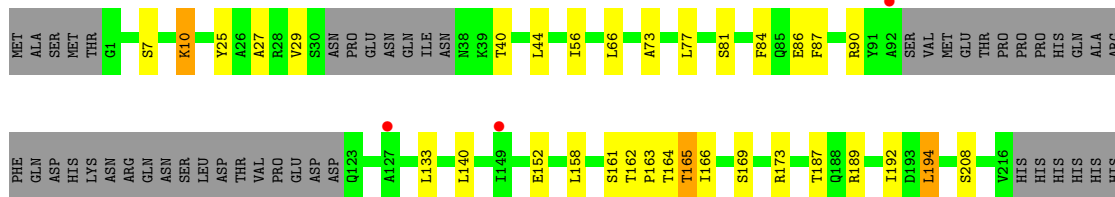
● Molecule 1: Probable thymidylate synthase

Chain I:  64% 20% 15%



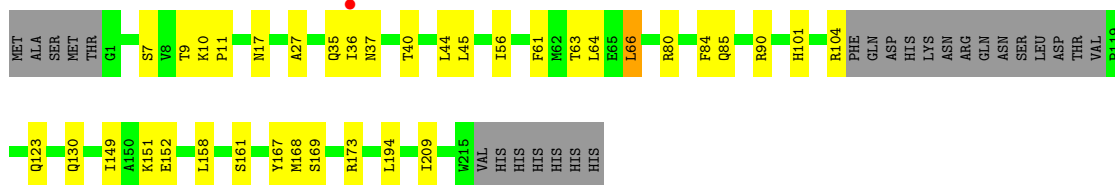
• Molecule 1: Probable thymidylate synthase

Chain J:  64% 13% 21%



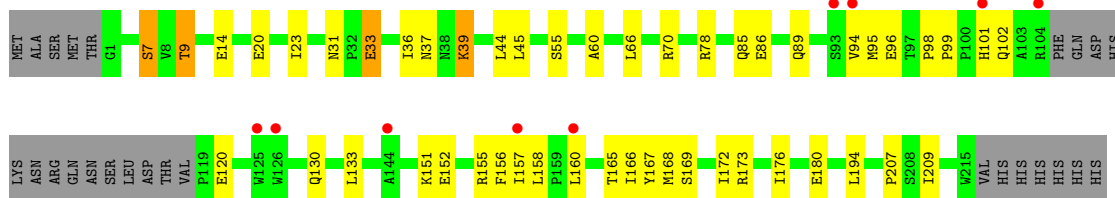
• Molecule 1: Probable thymidylate synthase

Chain K:  73% 15% 11%



• Molecule 1: Probable thymidylate synthase

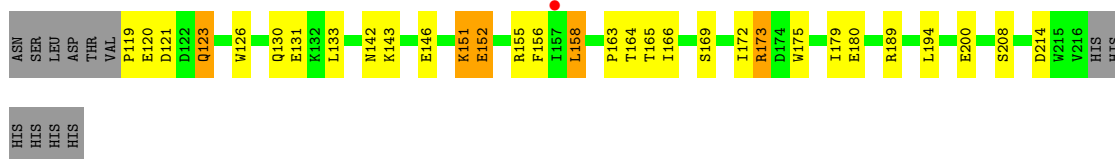
Chain L:  4% 67% 20% 11%



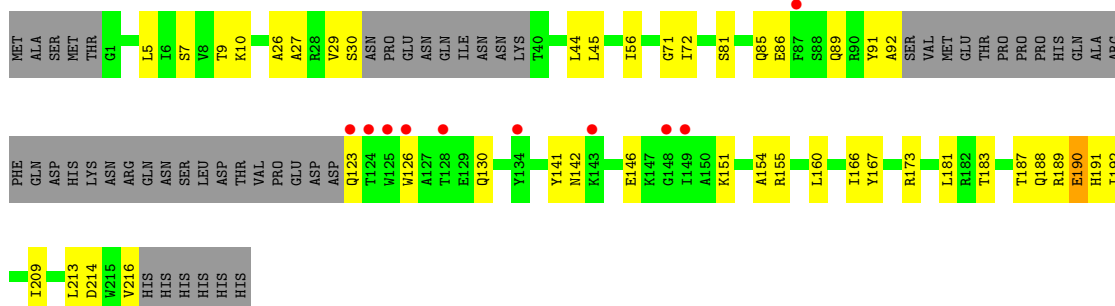
• Molecule 1: Probable thymidylate synthase

Chain M:  61% 23% 13%

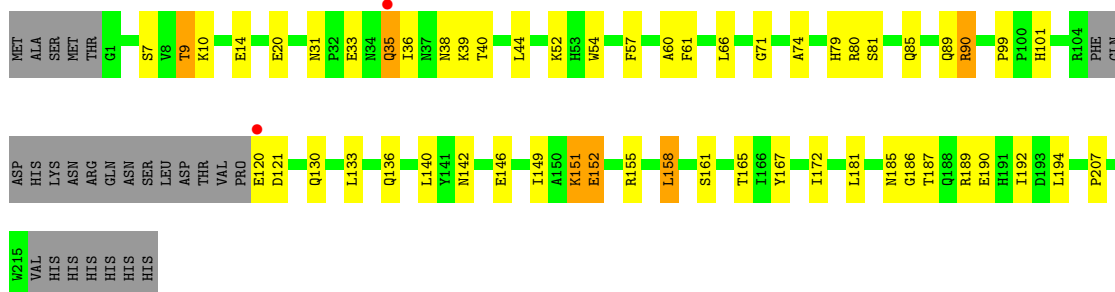




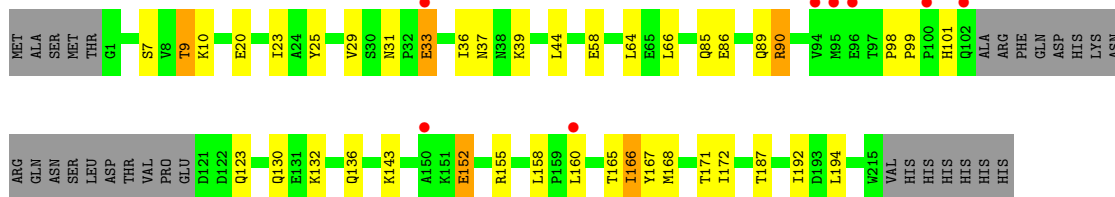
● Molecule 1: Probable thymidylate synthase



● Molecule 1: Probable thymidylate synthase



● Molecule 1: Probable thymidylate synthase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.97Å 120.58Å 128.25Å 111.65° 91.13° 90.18°	Depositor
Resolution (Å)	34.21 – 2.59 34.21 – 2.59	Depositor EDS
% Data completeness (in resolution range)	(Not available) (34.21-2.59) 92.8 (34.21-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.61Å)	Xtrriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.211 , 0.261 0.222 , 0.274	Depositor DCC
$R_{free}$ test set	5633 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.5	Xtrriage
Anisotropy	0.388	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 31.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.146 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	26503	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: FAD, DMS, 0VJ

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	0.51	0/1578	0.72	0/2134
1	B	0.51	0/1553	0.72	0/2100
1	C	0.50	0/1707	0.72	0/2311
1	D	0.50	0/1681	0.74	0/2276
1	E	0.51	0/1710	0.73	0/2314
1	F	0.53	0/1706	0.73	0/2309
1	G	0.51	0/1553	0.72	0/2100
1	H	0.51	0/1478	0.72	0/1996
1	I	0.47	0/1595	0.71	0/2157
1	J	0.47	0/1481	0.71	0/1999
1	K	0.52	0/1663	0.70	0/2251
1	L	0.48	0/1663	0.70	0/2251
1	M	0.51	0/1630	0.73	0/2204
1	N	0.48	0/1464	0.71	0/1977
1	O	0.53	0/1655	0.72	0/2240
1	P	0.49	0/1630	0.72	0/2207
All	All	0.50	0/25747	0.72	0/34826

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	A	1544	0	1533	13	0
1	B	1519	0	1519	22	0
1	C	1667	0	1652	19	0
1	D	1642	0	1627	25	0
1	E	1668	0	1657	20	0
1	F	1666	0	1652	28	0
1	G	1519	0	1519	21	0
1	H	1446	0	1448	12	0
1	I	1558	0	1546	22	0
1	J	1449	0	1456	15	0
1	K	1624	0	1610	13	0
1	L	1624	0	1610	23	0
1	M	1592	0	1584	30	1
1	N	1432	0	1437	23	0
1	O	1617	0	1602	26	1
1	P	1592	0	1578	16	0
2	A	106	0	62	0	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	E	53	0	31	1	0
2	F	106	0	62	3	0
2	H	53	0	31	1	0
2	I	106	0	62	2	0
2	J	53	0	31	3	0
2	K	53	0	31	0	0
2	M	53	0	31	1	0
2	N	53	0	31	2	0
2	O	53	0	31	1	0
2	P	53	0	31	2	0
3	A	44	0	28	0	0
3	B	22	0	14	2	0
3	D	22	0	14	1	0
3	E	22	0	14	0	0
3	F	22	0	14	0	0
3	G	22	0	14	0	0
3	H	22	0	14	0	0
3	I	22	0	14	2	0
3	J	22	0	14	1	0
3	K	22	0	14	0	0
3	L	22	0	14	0	0
3	M	22	0	14	4	0
3	N	22	0	14	4	0
3	O	22	0	14	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	22	0	14	1	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	1	0
4	E	4	0	6	2	0
4	F	4	0	6	0	0
4	G	4	0	6	0	0
4	H	4	0	6	0	0
4	I	4	0	6	0	0
4	K	4	0	6	1	0
4	M	4	0	6	3	0
4	O	4	0	6	0	0
4	P	4	0	6	0	0
5	A	11	0	0	0	0
5	B	7	0	0	0	0
5	C	2	0	0	0	0
5	D	7	0	0	0	0
5	E	8	0	0	0	0
5	F	13	0	0	0	0
5	G	13	0	0	0	0
5	H	5	0	0	0	0
5	I	3	0	0	0	0
5	J	5	0	0	0	0
5	K	2	0	0	0	0
5	L	6	0	0	0	0
5	M	3	0	0	0	0
5	N	5	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
All	All	26503	0	25828	296	1

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 296 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:F:0:THR:HG21	1:F:190:GLU:HA	1.36	1.03
1:C:101:HIS:H	1:C:130:GLN:HE22	1.04	0.98
1:C:155:ARG:HA	1:C:158:LEU:HD22	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:HIS:H	1:C:130:GLN:NE2	1.83	0.76
1:J:87:PHE:HE1	1:J:165:THR:HG23	1.48	0.76

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:0:THR:CG2	1:O:35:GLN:OE1[1_655]	2.11	0.09

## 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	187/227 (82%)	178 (95%)	7 (4%)	2 (1%)	14	30
1	B	184/227 (81%)	177 (96%)	7 (4%)	0	100	100
1	C	203/227 (89%)	194 (96%)	9 (4%)	0	100	100
1	D	199/227 (88%)	195 (98%)	4 (2%)	0	100	100
1	E	203/227 (89%)	193 (95%)	10 (5%)	0	100	100
1	F	202/227 (89%)	197 (98%)	5 (2%)	0	100	100
1	G	184/227 (81%)	179 (97%)	5 (3%)	0	100	100
1	H	173/227 (76%)	166 (96%)	7 (4%)	0	100	100
1	I	187/227 (82%)	181 (97%)	5 (3%)	1 (0%)	29	52
1	J	173/227 (76%)	170 (98%)	3 (2%)	0	100	100
1	K	197/227 (87%)	191 (97%)	5 (2%)	1 (0%)	29	52
1	L	197/227 (87%)	190 (96%)	7 (4%)	0	100	100
1	M	191/227 (84%)	186 (97%)	5 (3%)	0	100	100
1	N	171/227 (75%)	166 (97%)	4 (2%)	1 (1%)	25	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	196/227 (86%)	190 (97%)	4 (2%)	2 (1%)	15	32
1	P	193/227 (85%)	186 (96%)	7 (4%)	0	100	100
All	All	3040/3632 (84%)	2939 (97%)	94 (3%)	7 (0%)	47	71

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	PHE
1	N	214	ASP
1	O	80	ARG
1	K	80	ARG
1	O	38	ASN

### 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	165/199 (83%)	151 (92%)	14 (8%)	10	21
1	B	162/199 (81%)	142 (88%)	20 (12%)	4	9
1	C	179/199 (90%)	161 (90%)	18 (10%)	7	14
1	D	176/199 (88%)	162 (92%)	14 (8%)	12	24
1	E	179/199 (90%)	160 (89%)	19 (11%)	6	12
1	F	179/199 (90%)	160 (89%)	19 (11%)	6	12
1	G	162/199 (81%)	150 (93%)	12 (7%)	13	28
1	H	153/199 (77%)	136 (89%)	17 (11%)	6	11
1	I	166/199 (83%)	149 (90%)	17 (10%)	7	14
1	J	153/199 (77%)	138 (90%)	15 (10%)	8	15
1	K	174/199 (87%)	157 (90%)	17 (10%)	8	15
1	L	174/199 (87%)	154 (88%)	20 (12%)	5	10
1	M	170/199 (85%)	146 (86%)	24 (14%)	3	6
1	N	151/199 (76%)	140 (93%)	11 (7%)	14	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	173/199 (87%)	151 (87%)	22 (13%)	4 8
1	P	171/199 (86%)	150 (88%)	21 (12%)	4 9
All	All	2687/3184 (84%)	2407 (90%)	280 (10%)	7 13

5 of 280 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	123	GLN
1	O	9	THR
1	P	9	THR
1	F	153	CYS
1	F	120	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	89	GLN
1	P	130	GLN
1	N	85	GLN
1	O	130	GLN
1	E	85	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

45 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	0VJ	A	303	-	24,24,24	4.29	16 (66%)	31,34,34	3.54	12 (38%)
3	0VJ	B	303	-	24,24,24	5.12	16 (66%)	31,34,34	3.93	20 (64%)
4	DMS	B	302	-	3,3,3	0.96	0	3,3,3	1.31	0
3	0VJ	N	302	-	24,24,24	4.83	18 (75%)	31,34,34	3.44	12 (38%)
3	0VJ	K	301	-	24,24,24	4.79	18 (75%)	31,34,34	3.60	13 (41%)
4	DMS	O	303	-	3,3,3	0.69	0	3,3,3	0.18	0
3	0VJ	H	301	-	24,24,24	4.55	18 (75%)	31,34,34	2.99	12 (38%)
3	0VJ	I	304	-	24,24,24	4.41	16 (66%)	31,34,34	3.52	13 (41%)
4	DMS	A	304	-	3,3,3	1.04	0	3,3,3	1.06	0
2	FAD	H	302	-	53,58,58	1.43	8 (15%)	68,89,89	1.33	10 (14%)
2	FAD	I	302	-	53,58,58	1.72	13 (24%)	68,89,89	1.62	12 (17%)
3	0VJ	G	301	-	24,24,24	4.70	16 (66%)	31,34,34	3.29	10 (32%)
2	FAD	E	301	-	53,58,58	1.71	14 (26%)	68,89,89	1.62	12 (17%)
2	FAD	F	301	-	53,58,58	1.90	16 (30%)	68,89,89	1.61	21 (30%)
4	DMS	E	303	-	3,3,3	0.67	0	3,3,3	1.34	0
2	FAD	F	302	-	53,58,58	1.72	13 (24%)	68,89,89	1.62	12 (17%)
3	0VJ	M	303	-	24,24,24	4.67	18 (75%)	31,34,34	3.36	13 (41%)
3	0VJ	A	305	-	24,24,24	4.53	16 (66%)	31,34,34	3.37	14 (45%)
3	0VJ	F	304	-	24,24,24	4.47	16 (66%)	31,34,34	3.43	13 (41%)
2	FAD	P	301	-	53,58,58	1.72	13 (24%)	68,89,89	1.62	12 (17%)
4	DMS	D	302	-	3,3,3	0.96	0	3,3,3	1.08	0
2	FAD	A	302	-	53,58,58	1.72	14 (26%)	68,89,89	1.62	12 (17%)
4	DMS	C	302	-	3,3,3	0.79	0	3,3,3	0.98	0
4	DMS	F	303	-	3,3,3	0.78	0	3,3,3	0.94	0
4	DMS	H	303	-	3,3,3	1.07	0	3,3,3	0.92	0
3	0VJ	E	302	-	24,24,24	4.76	18 (75%)	31,34,34	2.94	12 (38%)
4	DMS	I	303	-	3,3,3	0.85	0	3,3,3	0.78	0
3	0VJ	D	301	-	24,24,24	4.55	16 (66%)	31,34,34	3.40	12 (38%)
4	DMS	M	302	-	3,3,3	0.72	0	3,3,3	0.46	0
2	FAD	K	302	-	53,58,58	1.45	12 (22%)	68,89,89	1.31	7 (10%)
2	FAD	J	301	-	53,58,58	1.84	13 (24%)	68,89,89	1.69	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	0VJ	O	301	-	24,24,24	4.74	16 (66%)	31,34,34	3.78	14 (45%)
2	FAD	N	301	-	53,58,58	1.70	15 (28%)	68,89,89	1.75	16 (23%)
2	FAD	O	302	-	53,58,58	1.43	8 (15%)	68,89,89	1.54	16 (23%)
2	FAD	M	301	-	53,58,58	1.71	13 (24%)	68,89,89	1.62	12 (17%)
4	DMS	P	303	-	3,3,3	0.89	0	3,3,3	0.54	0
4	DMS	G	302	-	3,3,3	1.07	0	3,3,3	0.83	0
2	FAD	C	301	-	53,58,58	1.68	13 (24%)	68,89,89	1.52	12 (17%)
2	FAD	I	301	-	53,58,58	1.72	13 (24%)	68,89,89	1.63	12 (17%)
3	0VJ	L	301	-	24,24,24	4.88	18 (75%)	31,34,34	3.13	14 (45%)
3	0VJ	J	302	-	24,24,24	4.95	18 (75%)	31,34,34	3.62	9 (29%)
4	DMS	K	303	-	3,3,3	0.80	0	3,3,3	0.89	0
2	FAD	A	301	-	53,58,58	1.71	13 (24%)	68,89,89	1.62	12 (17%)
2	FAD	B	301	-	53,58,58	1.65	10 (18%)	68,89,89	1.51	12 (17%)
3	0VJ	P	302	-	24,24,24	4.51	17 (70%)	31,34,34	3.22	10 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	0VJ	A	303	-	-	0/6/26/26	0/3/3/3
3	0VJ	B	303	-	-	2/6/26/26	0/3/3/3
3	0VJ	N	302	-	-	2/6/26/26	0/3/3/3
3	0VJ	K	301	-	-	0/6/26/26	0/3/3/3
3	0VJ	H	301	-	-	0/6/26/26	0/3/3/3
3	0VJ	I	304	-	-	0/6/26/26	0/3/3/3
2	FAD	H	302	-	-	6/30/50/50	0/6/6/6
2	FAD	I	302	-	-	3/30/50/50	0/6/6/6
3	0VJ	G	301	-	-	0/6/26/26	0/3/3/3
2	FAD	E	301	-	-	3/30/50/50	0/6/6/6
2	FAD	F	301	-	-	7/30/50/50	0/6/6/6
2	FAD	F	302	-	-	3/30/50/50	0/6/6/6
3	0VJ	M	303	-	-	0/6/26/26	0/3/3/3
3	0VJ	A	305	-	-	2/6/26/26	0/3/3/3
3	0VJ	F	304	-	-	0/6/26/26	0/3/3/3
2	FAD	P	301	-	-	3/30/50/50	0/6/6/6
2	FAD	A	302	-	-	3/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	0VJ	E	302	-	-	0/6/26/26	0/3/3/3
3	0VJ	D	301	-	-	2/6/26/26	0/3/3/3
2	FAD	K	302	-	-	5/30/50/50	0/6/6/6
2	FAD	J	301	-	-	9/30/50/50	0/6/6/6
3	0VJ	O	301	-	-	0/6/26/26	0/3/3/3
2	FAD	N	301	-	-	7/30/50/50	0/6/6/6
2	FAD	O	302	-	-	8/30/50/50	0/6/6/6
2	FAD	M	301	-	-	3/30/50/50	0/6/6/6
2	FAD	C	301	-	-	5/30/50/50	0/6/6/6
2	FAD	I	301	-	-	3/30/50/50	0/6/6/6
3	0VJ	L	301	-	-	0/6/26/26	0/3/3/3
3	0VJ	J	302	-	-	0/6/26/26	0/3/3/3
2	FAD	A	301	-	-	3/30/50/50	0/6/6/6
2	FAD	B	301	-	-	8/30/50/50	0/6/6/6
3	0VJ	P	302	-	-	0/6/26/26	0/3/3/3

The worst 5 of 472 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	0VJ	C03-C04	9.87	1.55	1.39
3	O	301	0VJ	C02-C01	9.82	1.64	1.38
3	E	302	0VJ	C02-C01	9.73	1.63	1.38
3	B	303	0VJ	C17-C12	9.73	1.59	1.38
3	O	301	0VJ	C17-C12	9.69	1.59	1.38

The worst 5 of 406 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	301	0VJ	C11-C12-C13	-12.77	102.61	120.89
3	I	304	0VJ	C11-C12-C13	-12.71	102.69	120.89
3	J	302	0VJ	C11-C12-C13	-12.49	103.02	120.89
3	B	303	0VJ	C11-C12-C13	-12.45	103.07	120.89
3	A	303	0VJ	C11-C12-C13	-12.18	103.46	120.89

There are no chirality outliers.

5 of 87 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	FAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	C	301	FAD	C1'-C2'-C3'-C4'
2	H	302	FAD	P-O3P-PA-O5B
2	H	302	FAD	C1'-C2'-C3'-C4'
2	J	301	FAD	C5B-O5B-PA-O1A

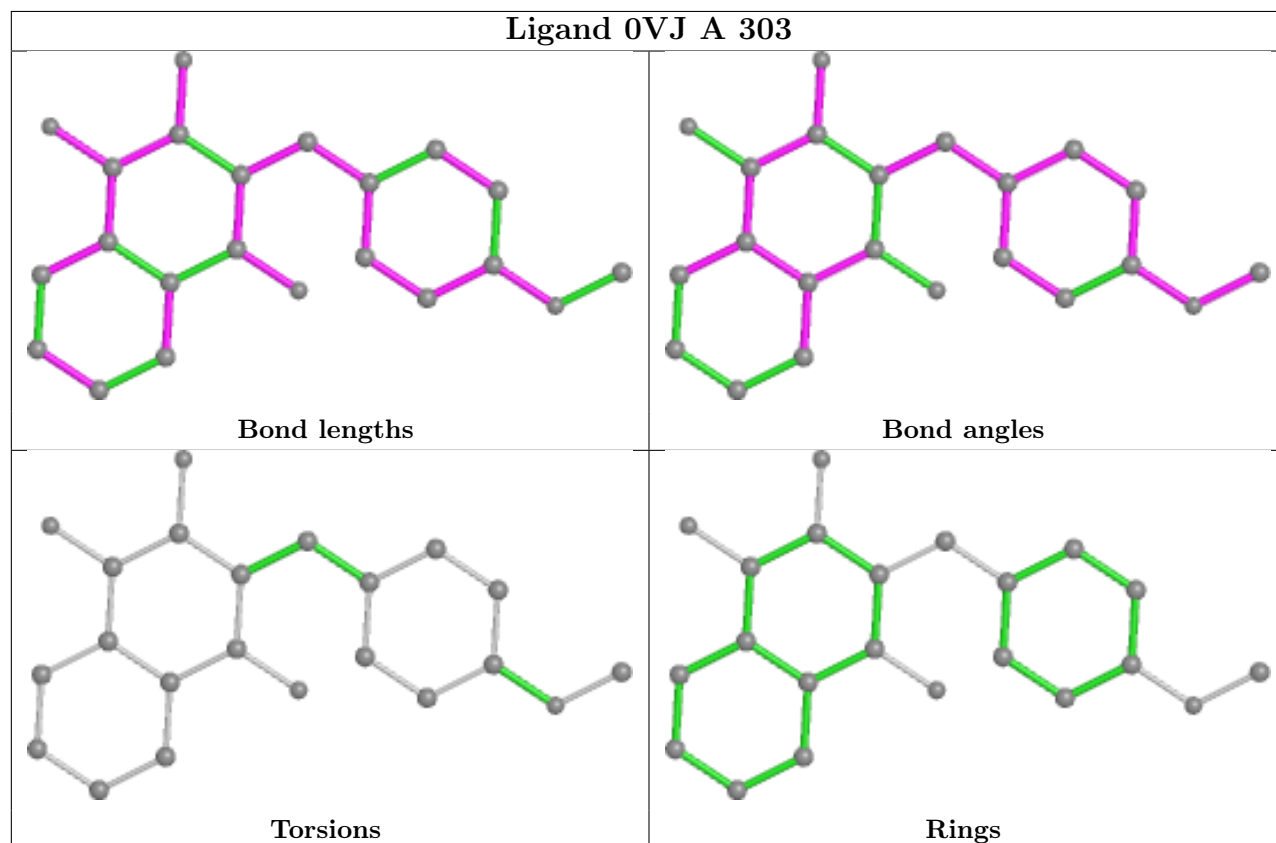
There are no ring outliers.

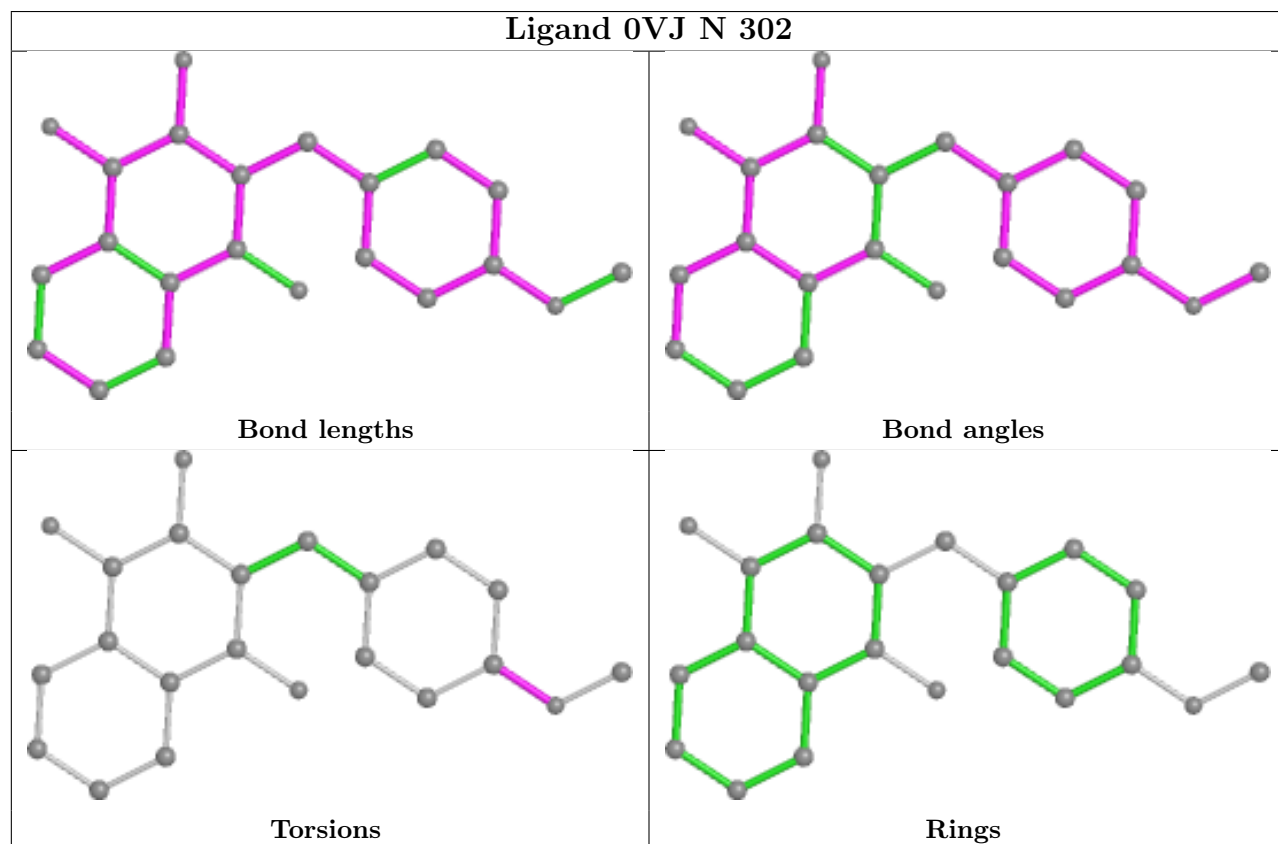
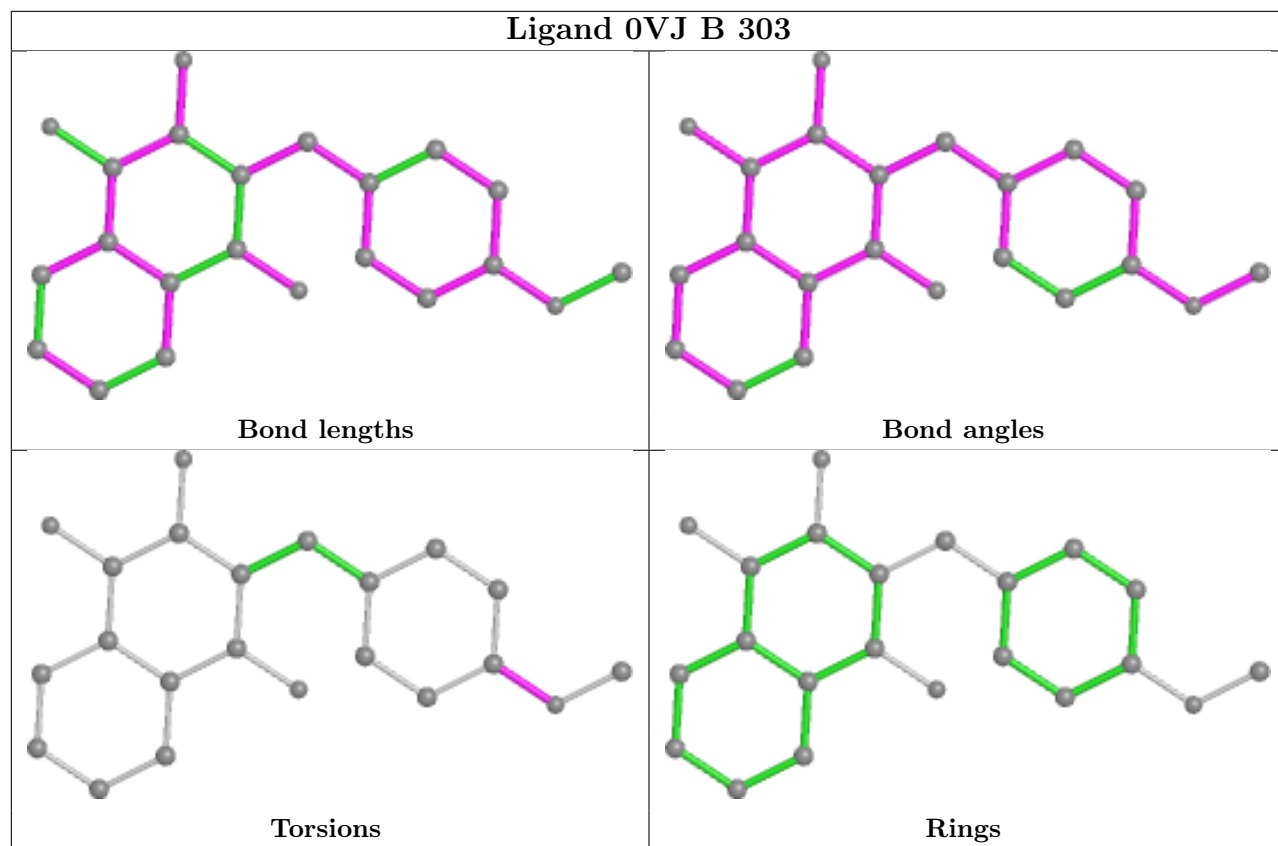
25 monomers are involved in 41 short contacts:

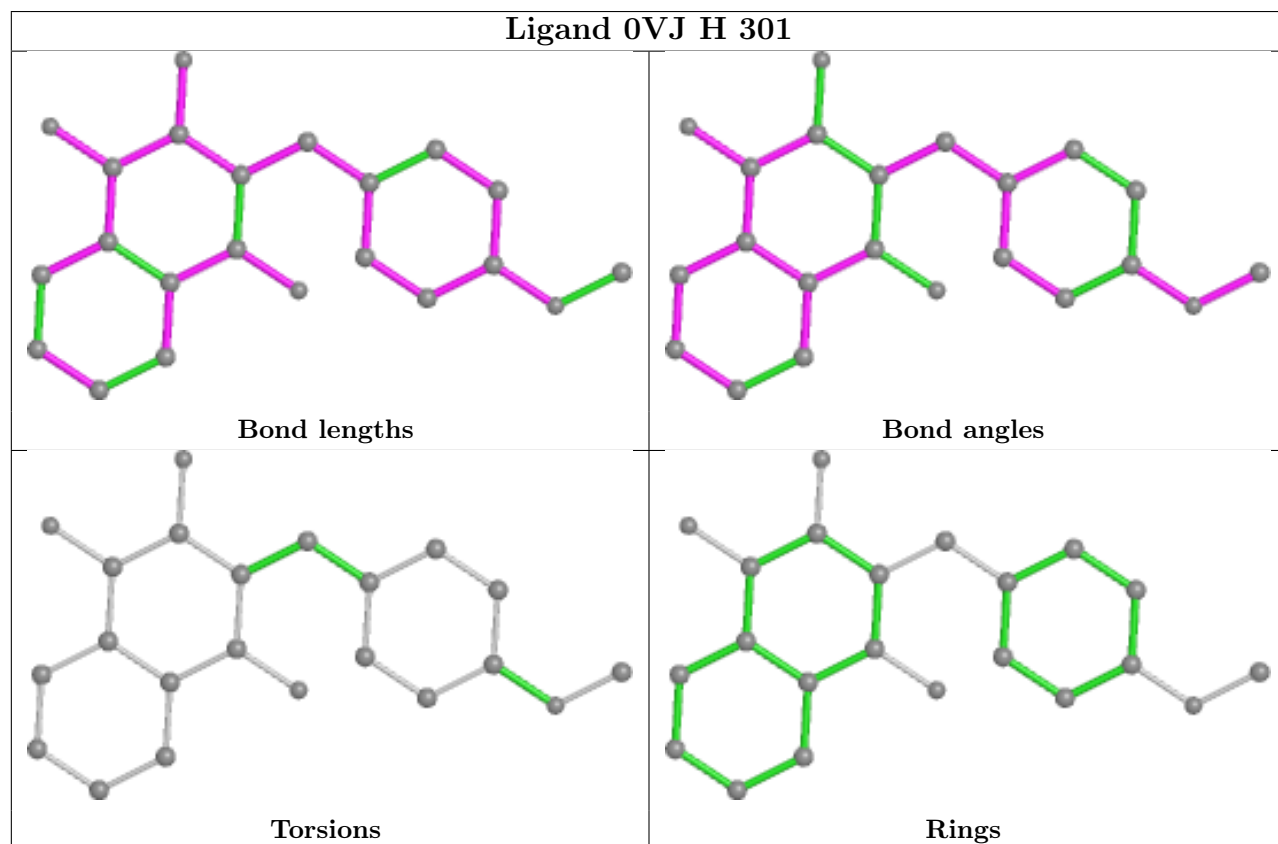
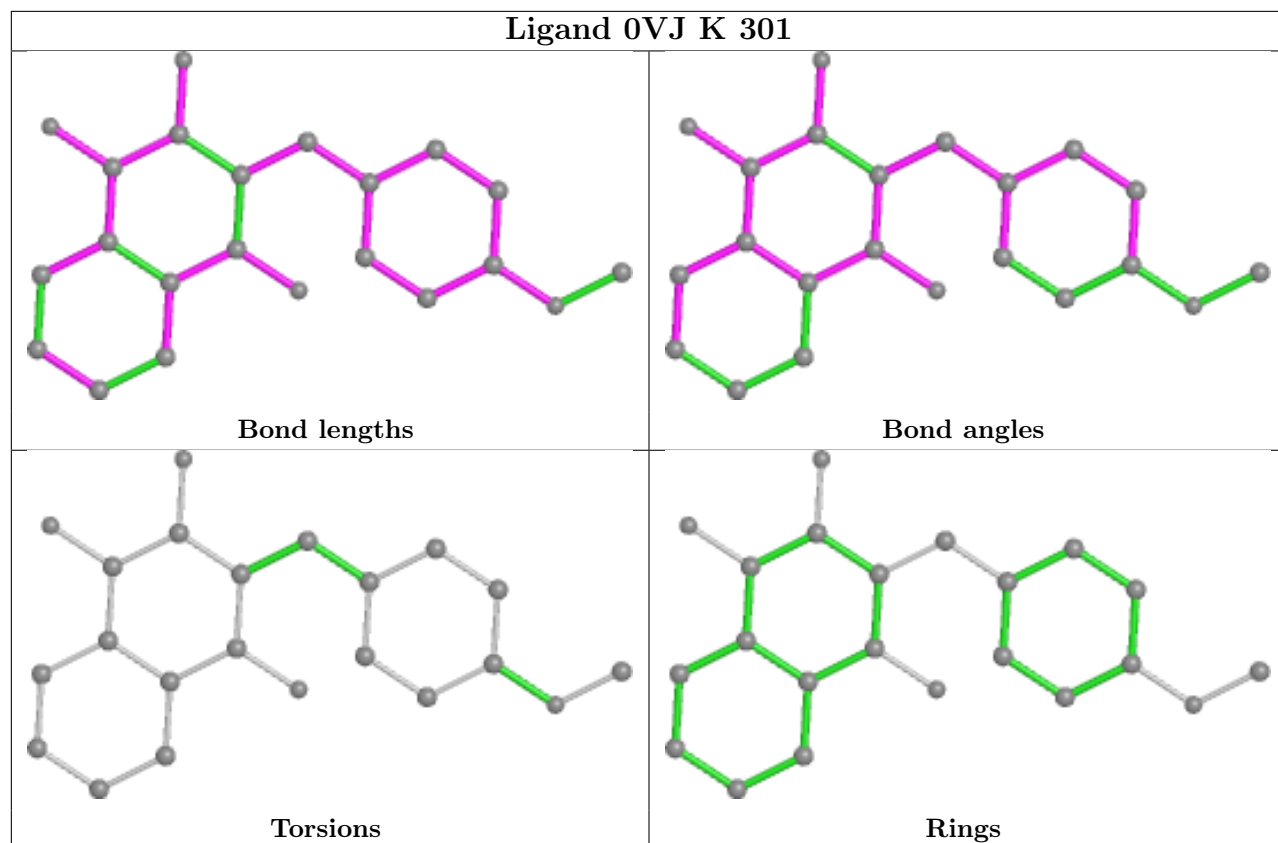
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	303	0VJ	2	0
3	N	302	0VJ	4	0
3	I	304	0VJ	2	0
2	H	302	FAD	1	0
2	I	302	FAD	2	0
2	E	301	FAD	1	0
2	F	301	FAD	1	0
4	E	303	DMS	2	0
2	F	302	FAD	2	0
3	M	303	0VJ	4	0
2	P	301	FAD	2	0
4	D	302	DMS	1	0
3	D	301	0VJ	1	0
4	M	302	DMS	3	0
2	J	301	FAD	3	0
3	O	301	0VJ	3	0
2	N	301	FAD	2	0
2	O	302	FAD	1	0
2	M	301	FAD	1	0
2	C	301	FAD	1	0
2	I	301	FAD	1	0
3	J	302	0VJ	1	0
4	K	303	DMS	1	0
2	B	301	FAD	1	0
3	P	302	0VJ	1	0

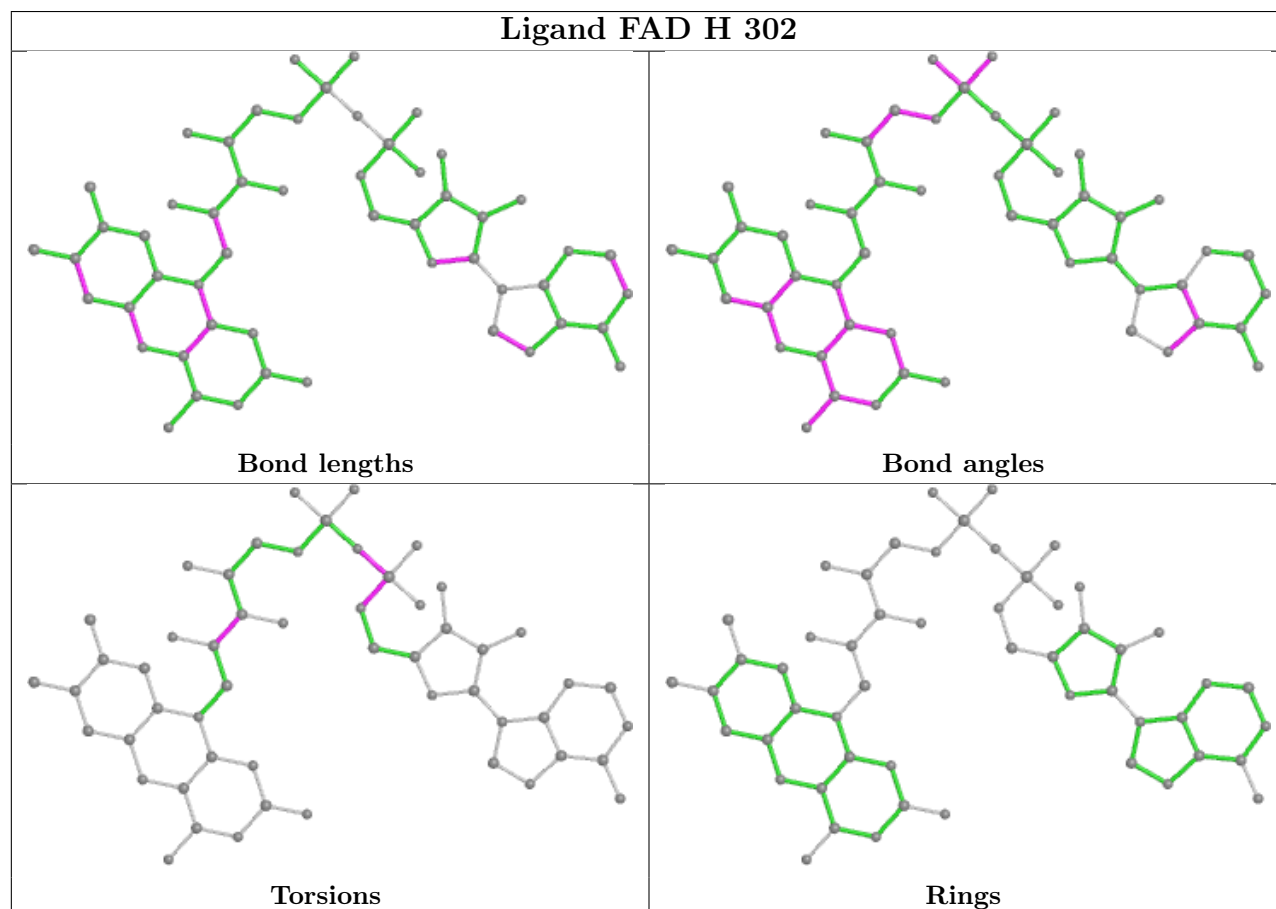
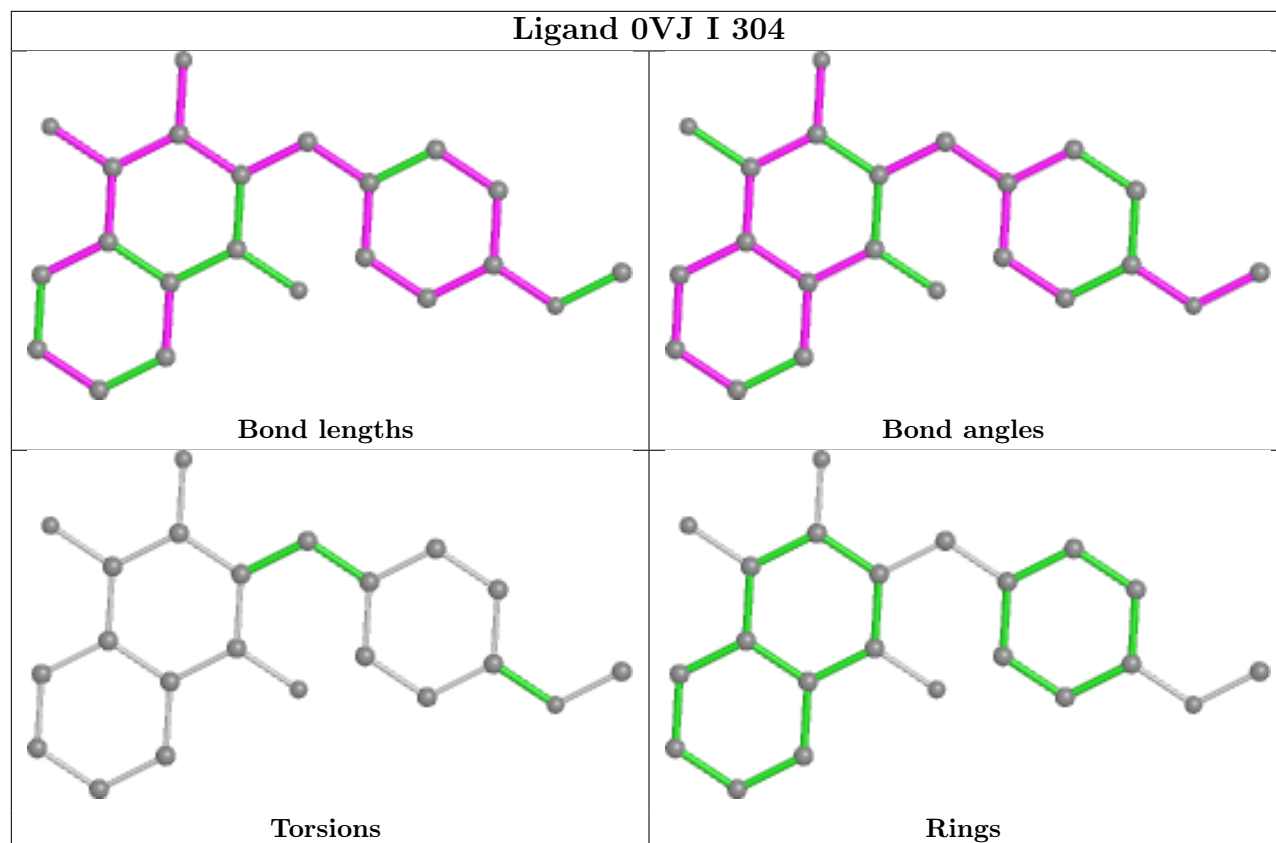
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

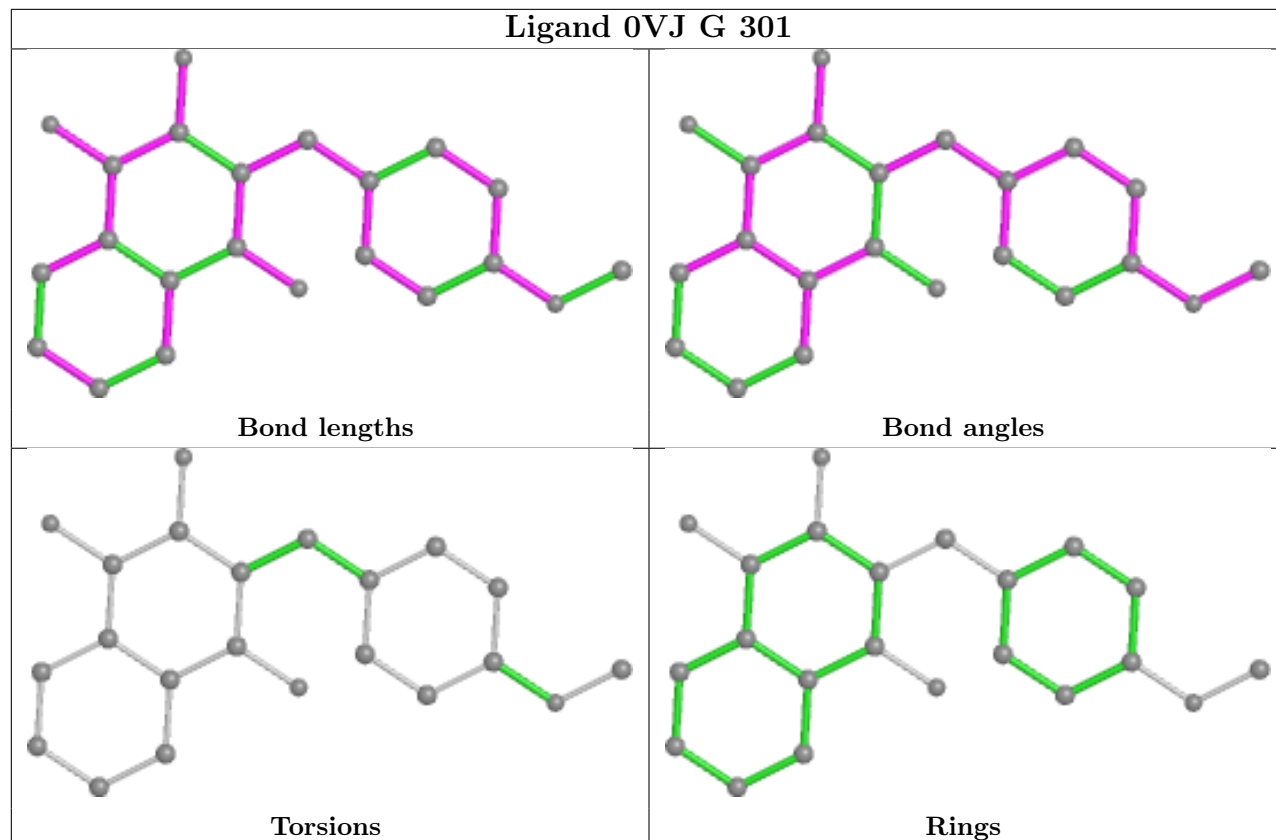
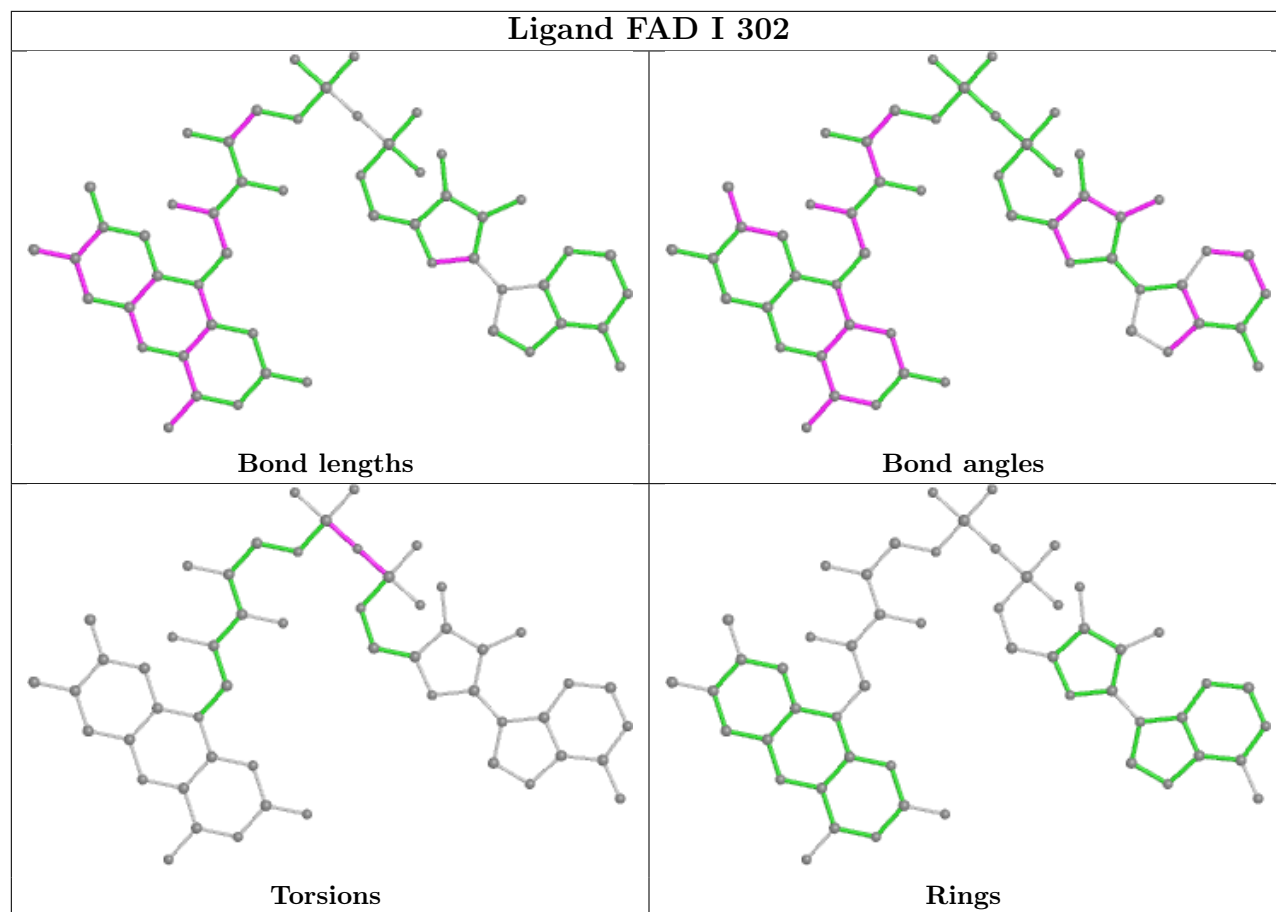
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

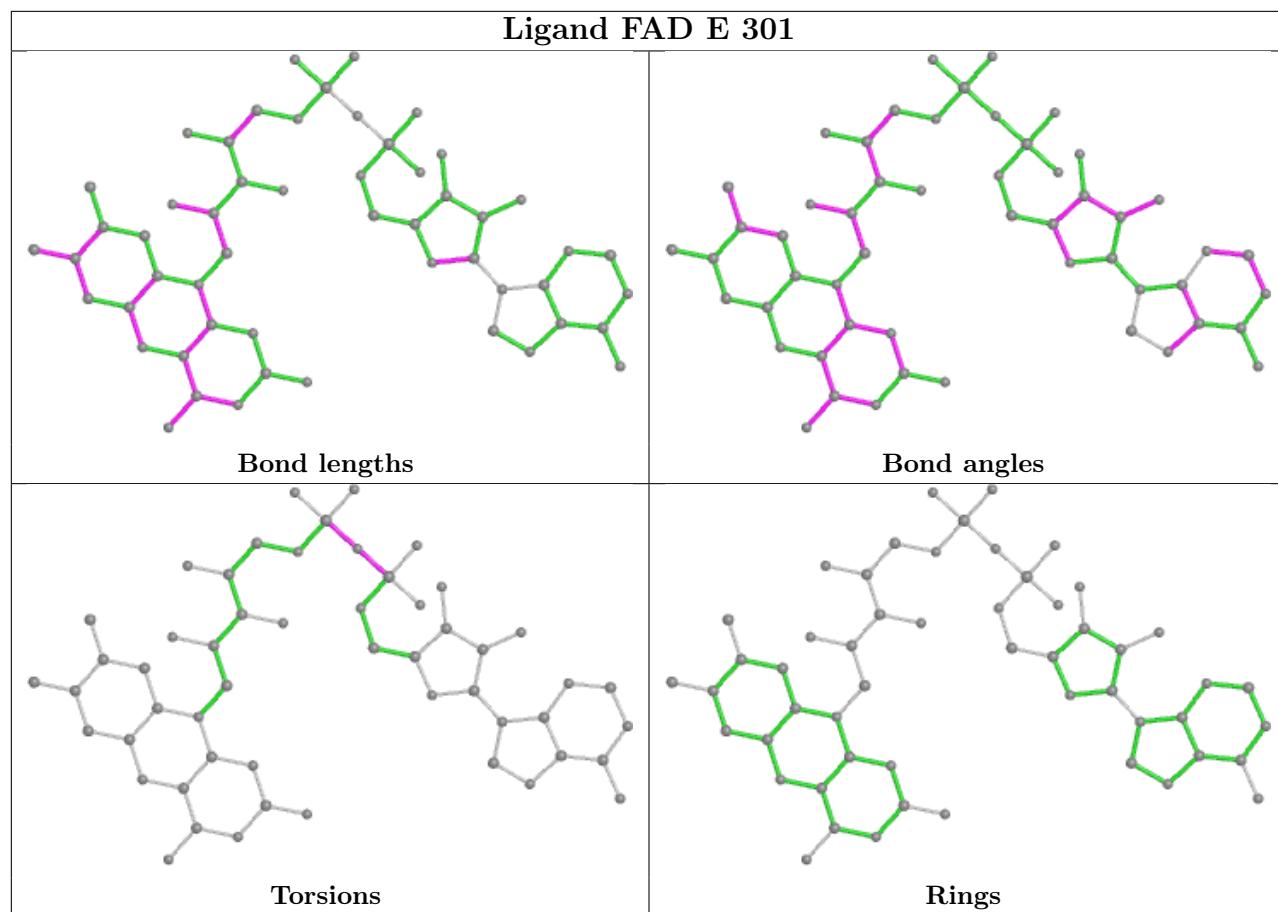


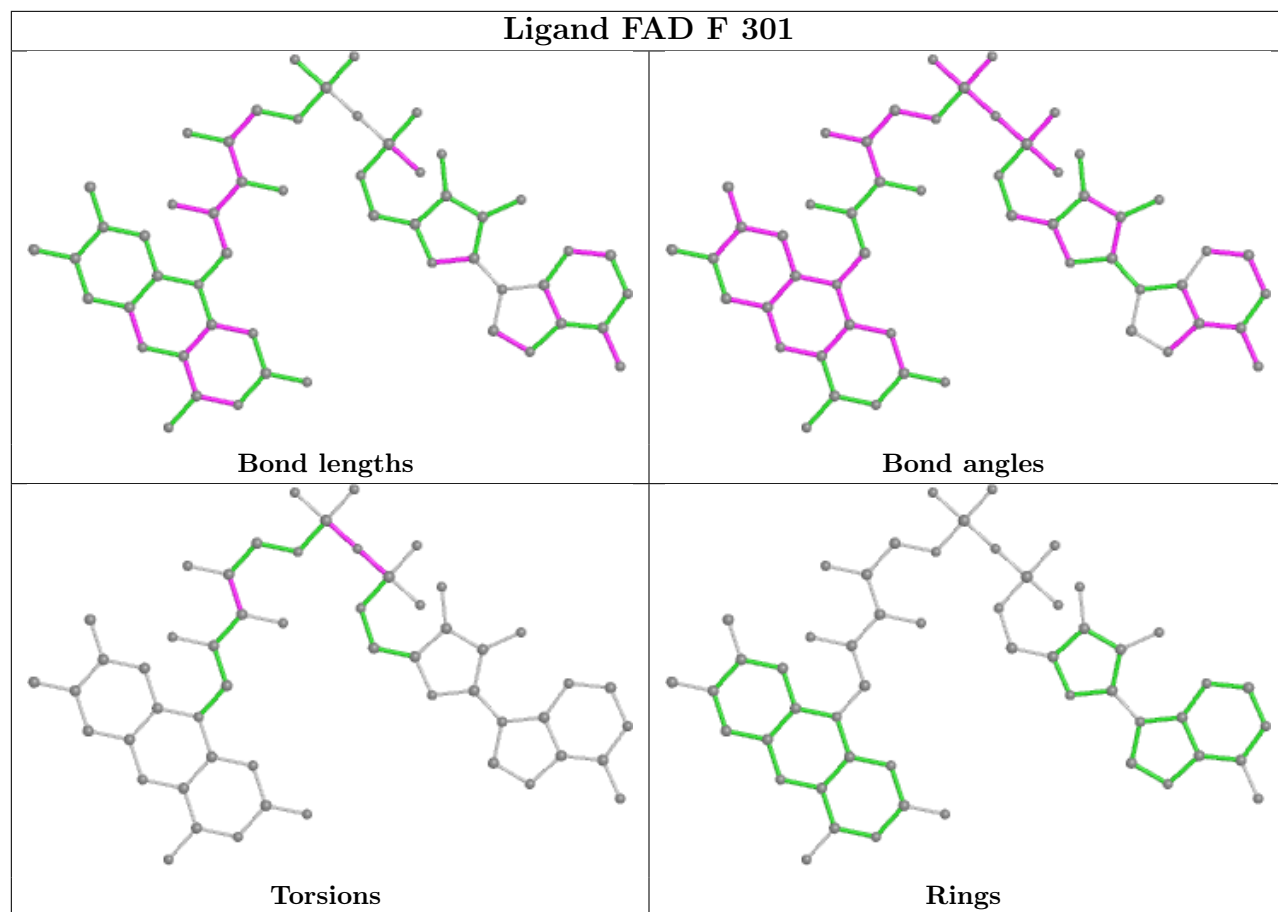




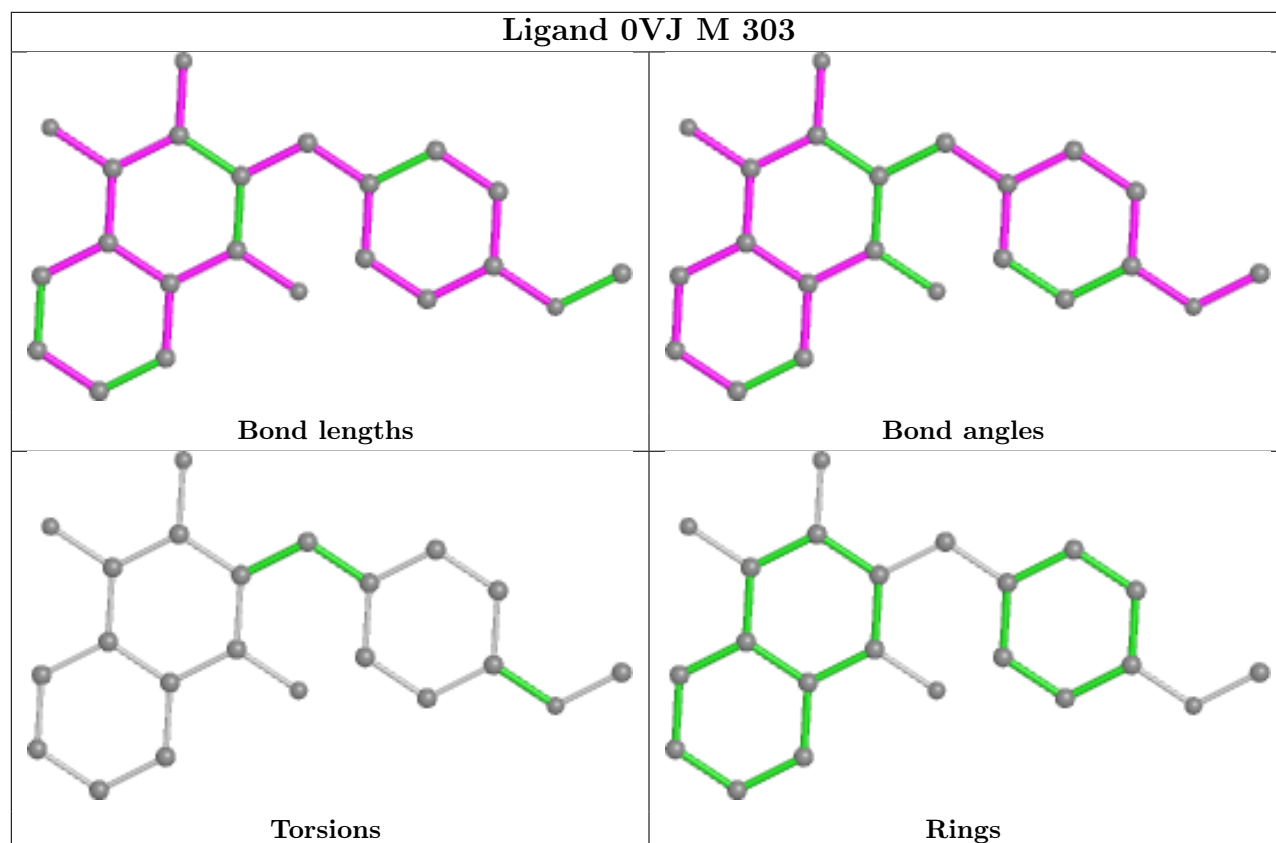
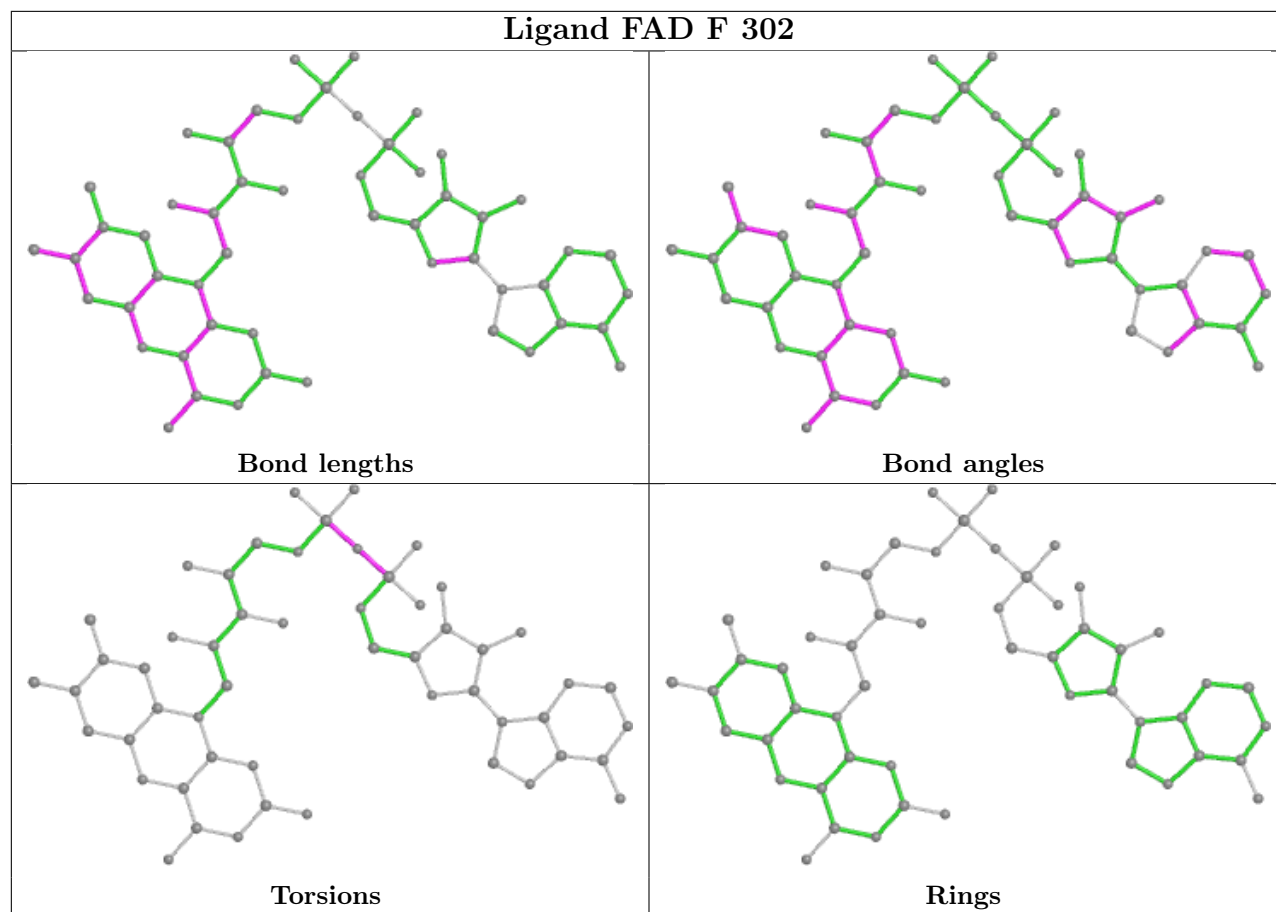


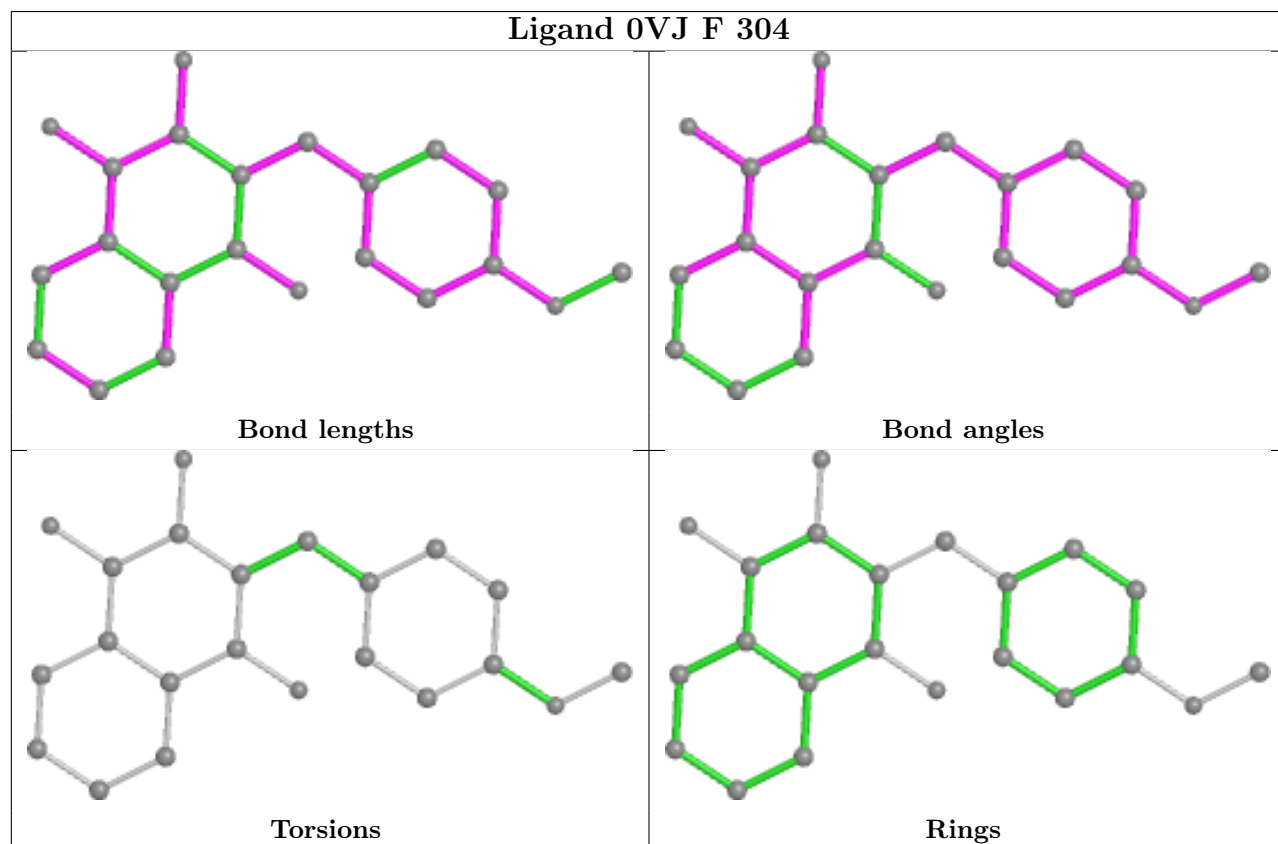
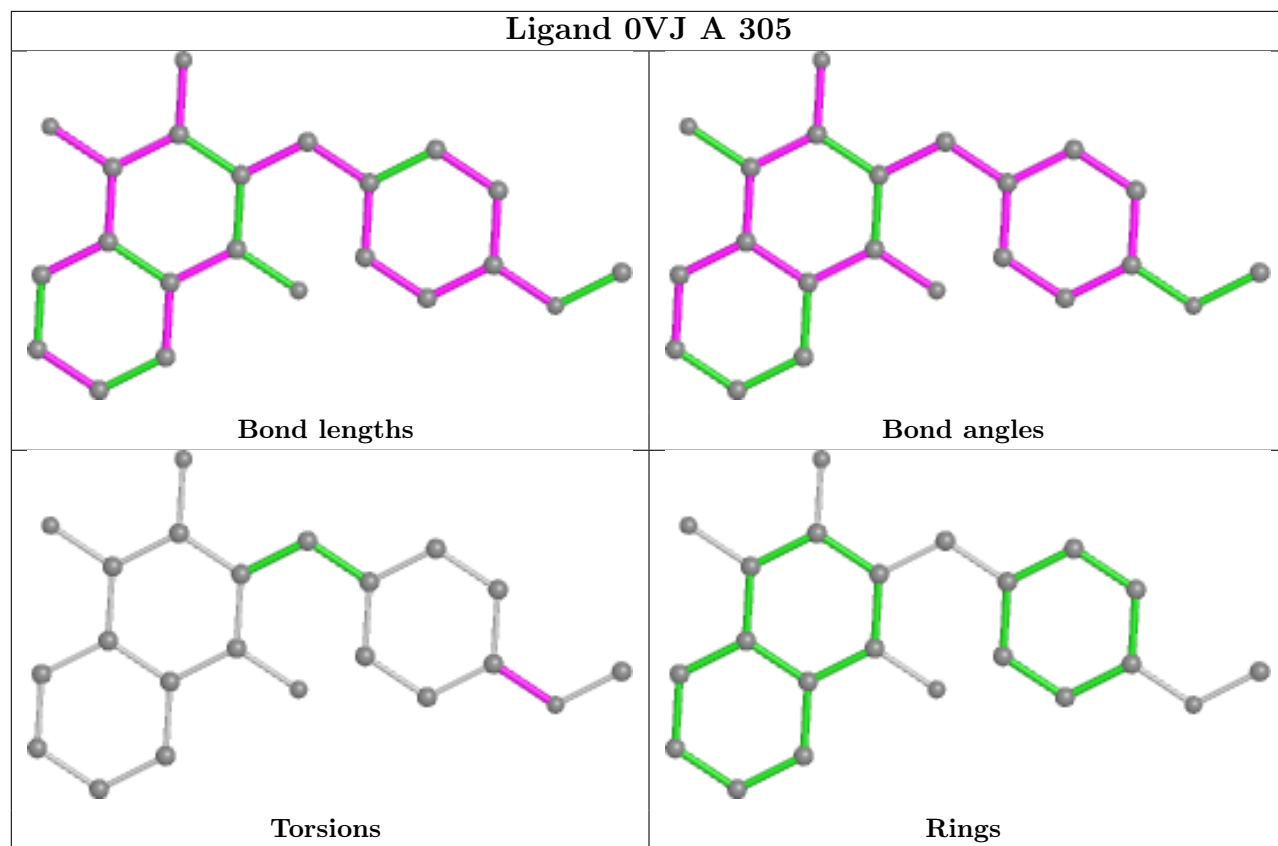


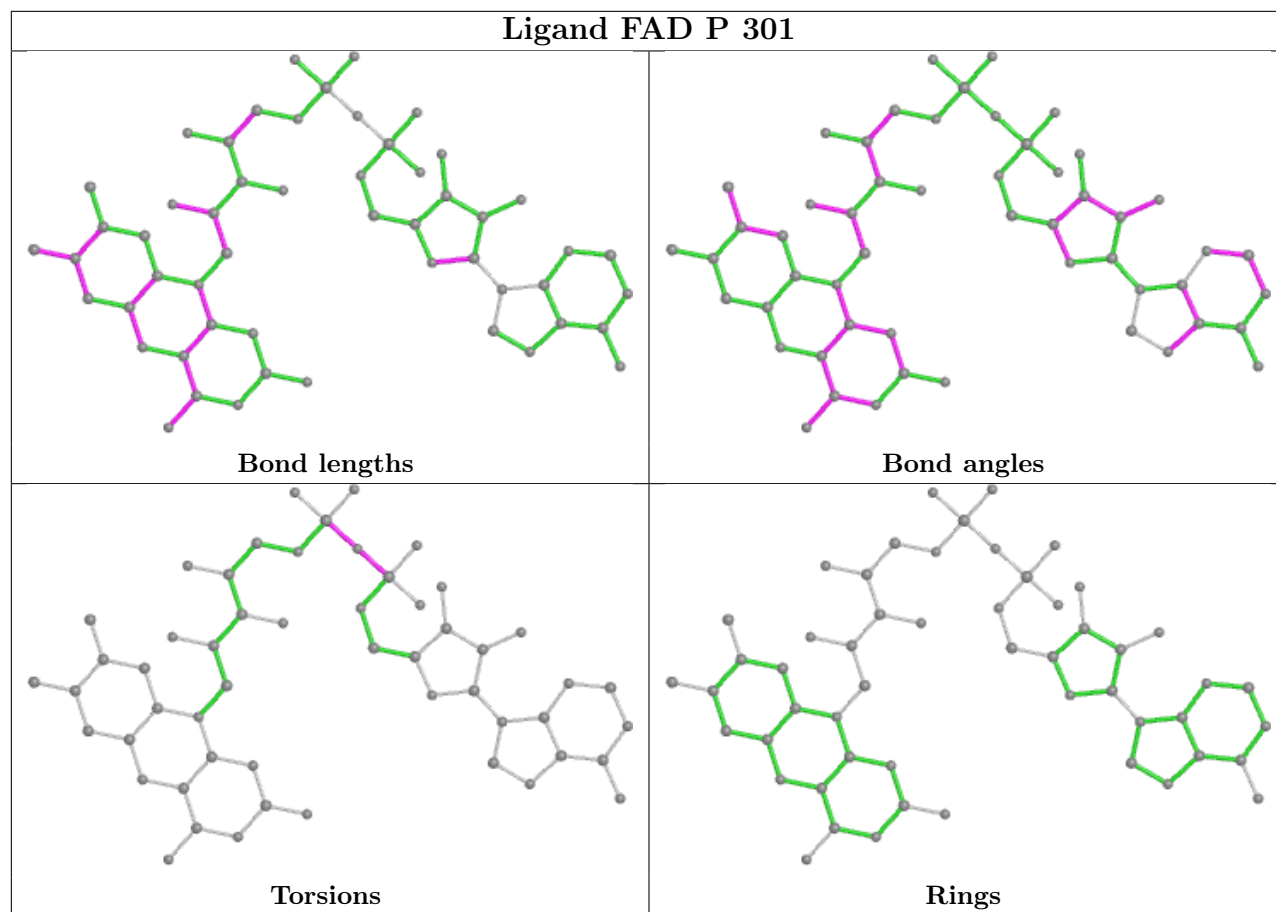


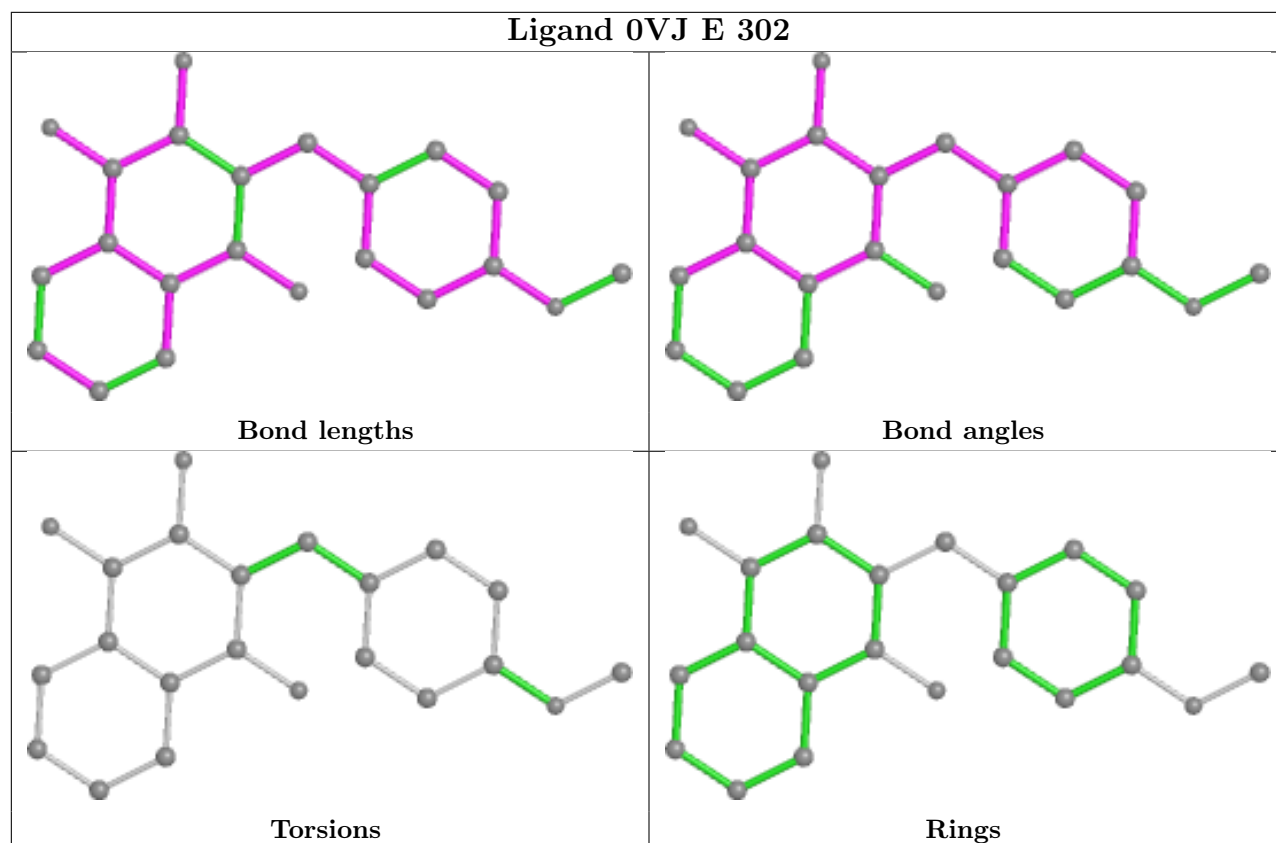
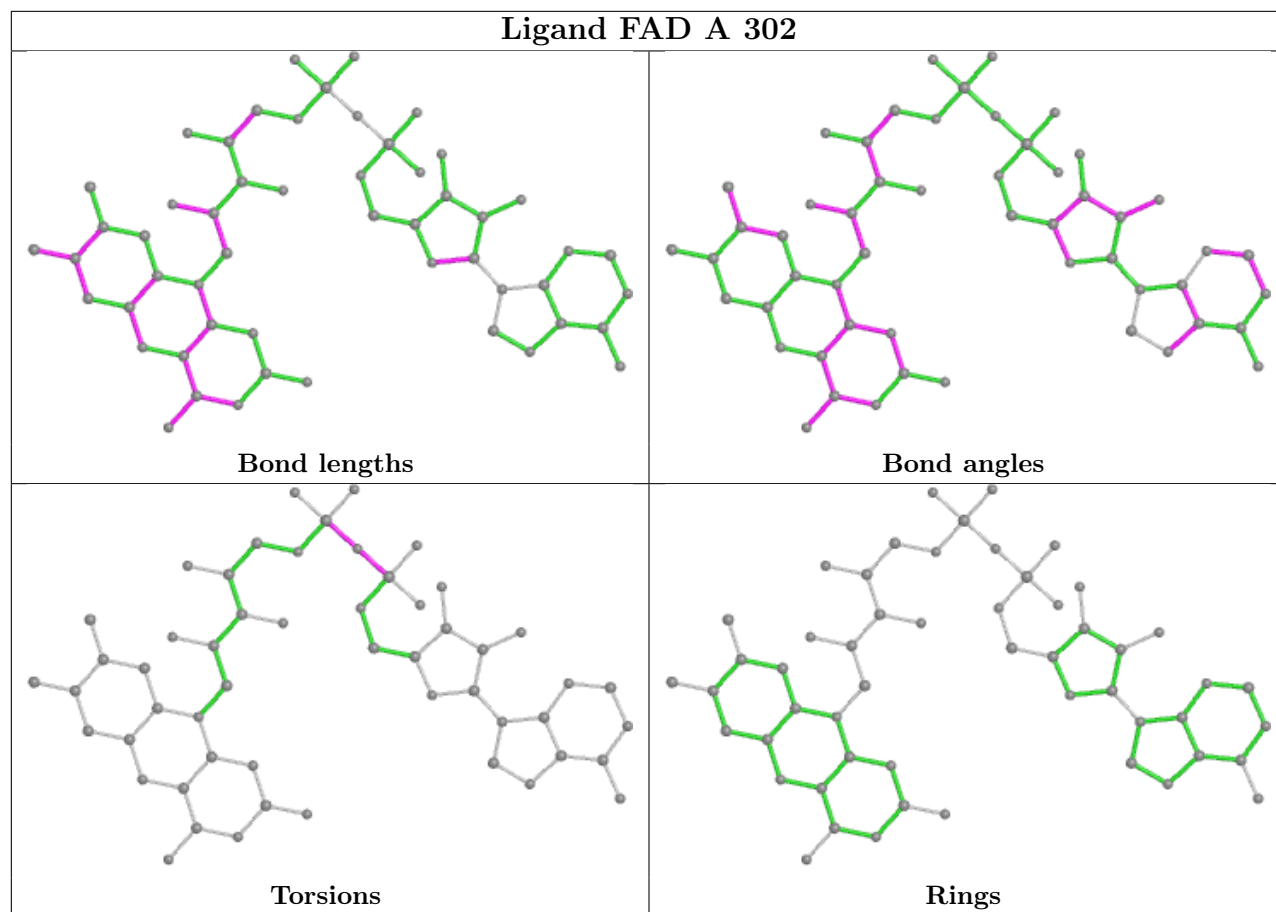


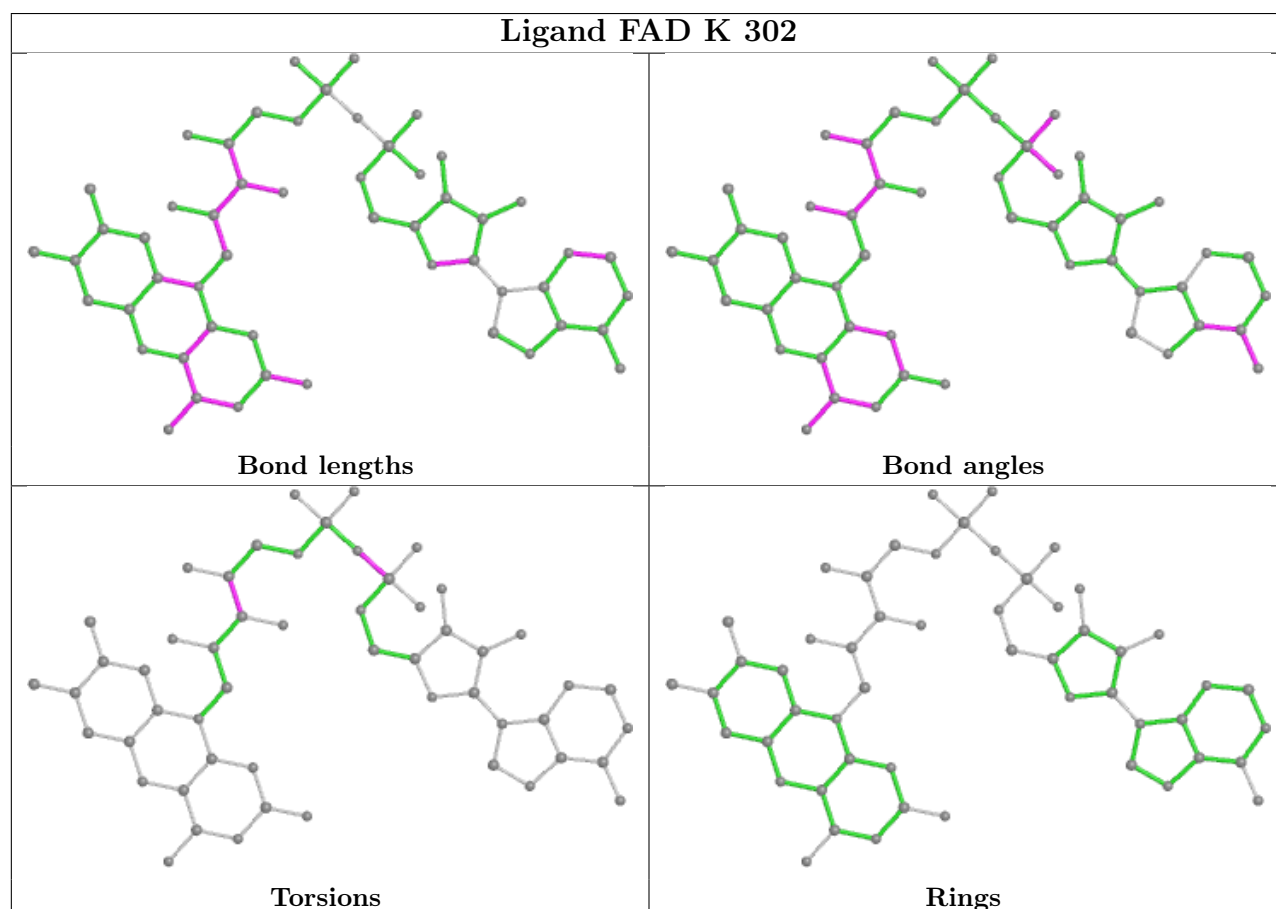
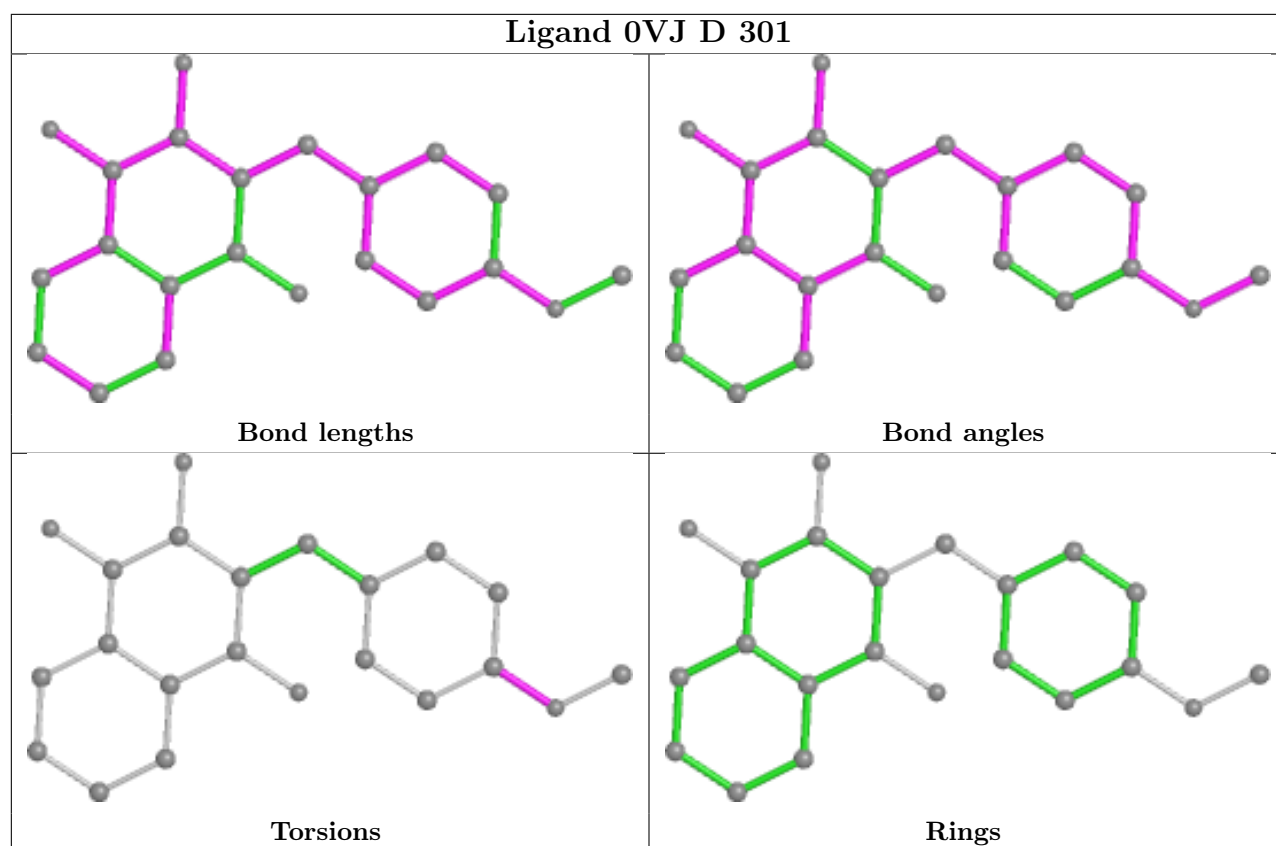


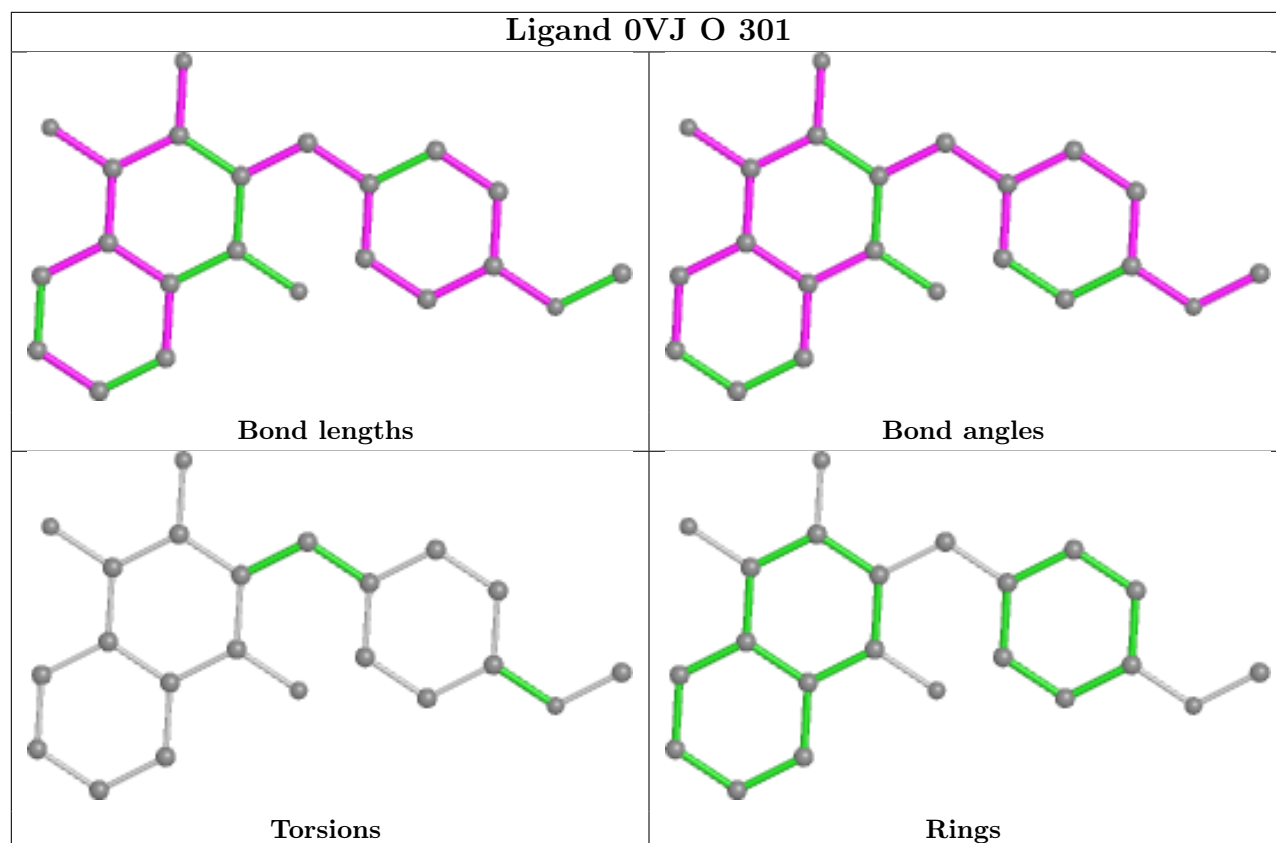
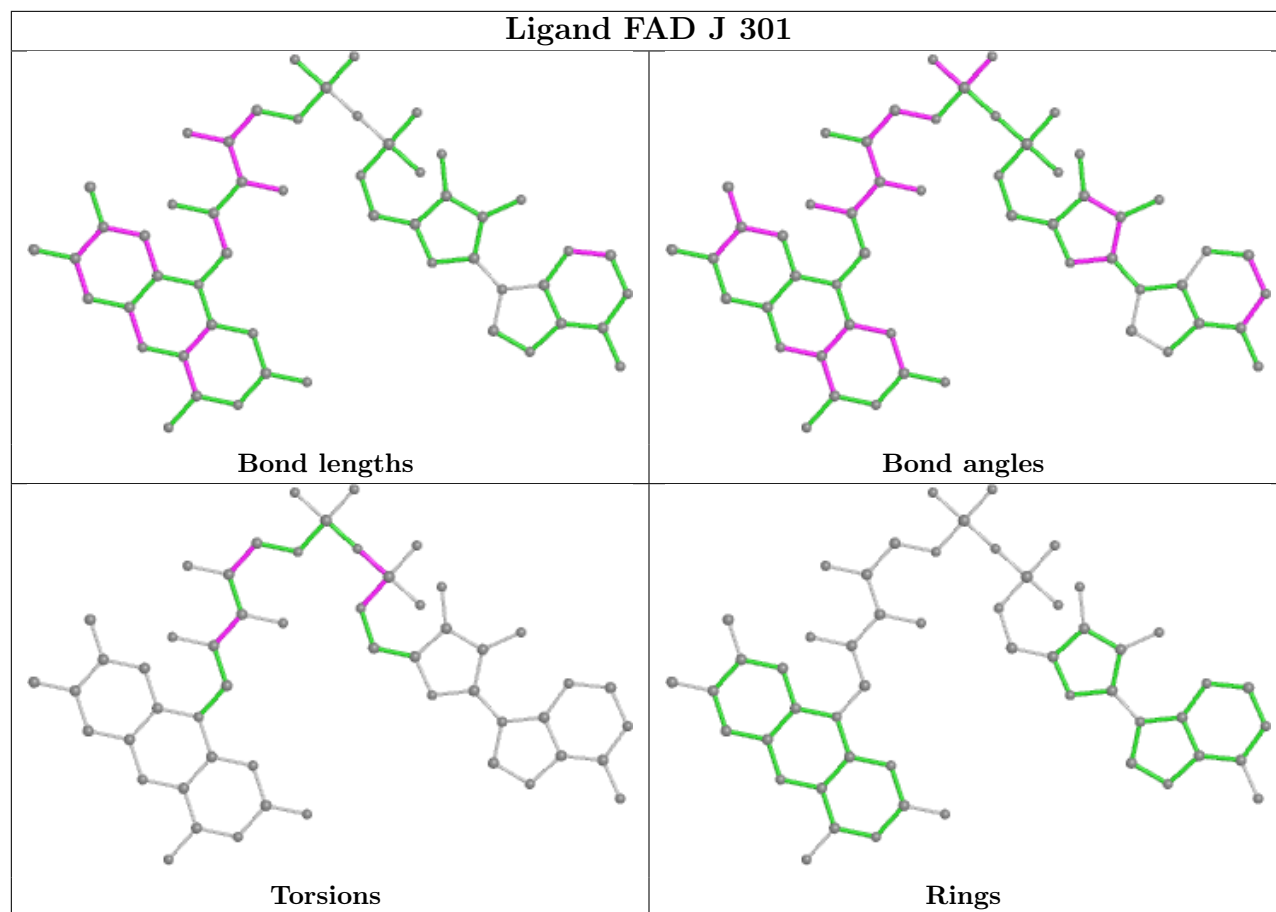


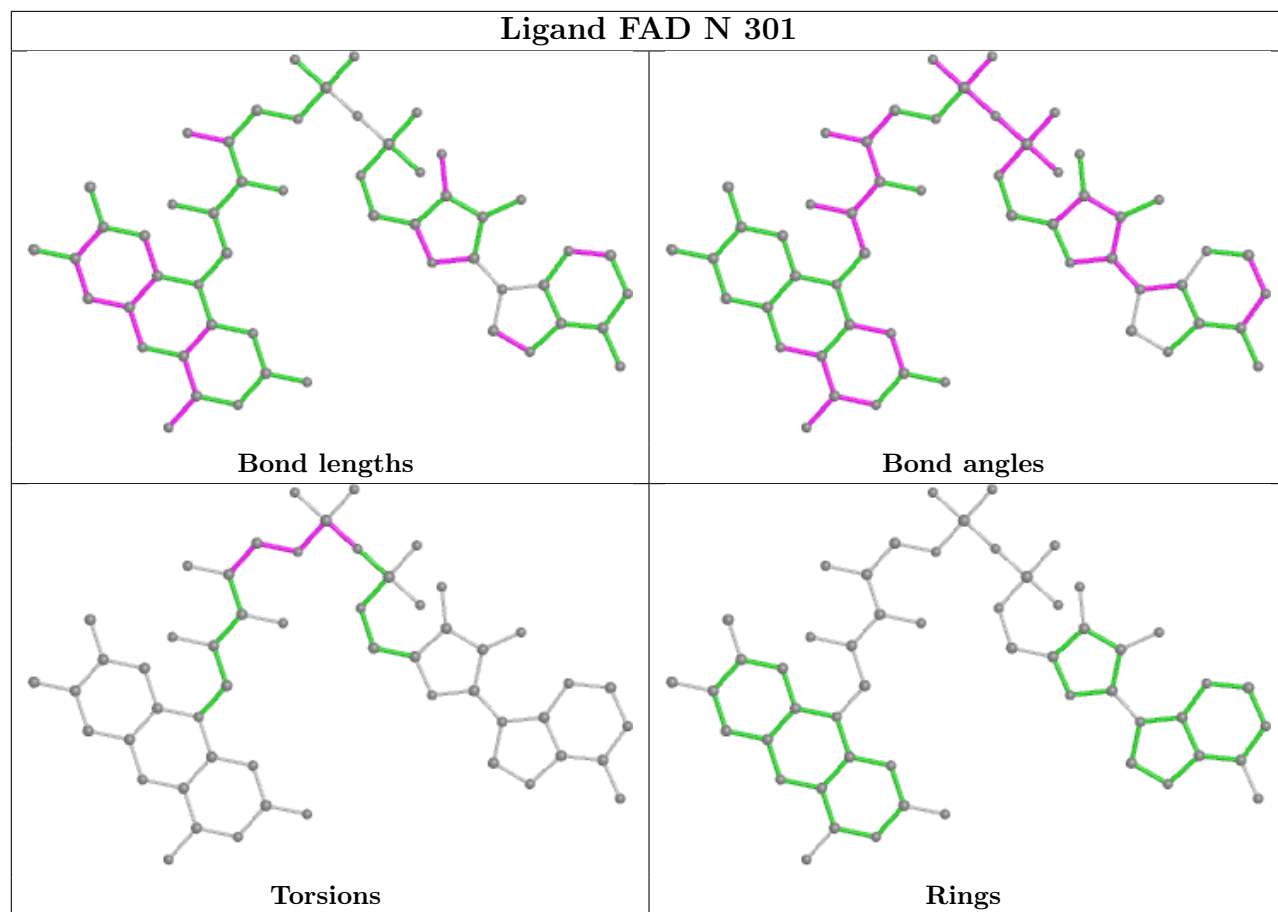


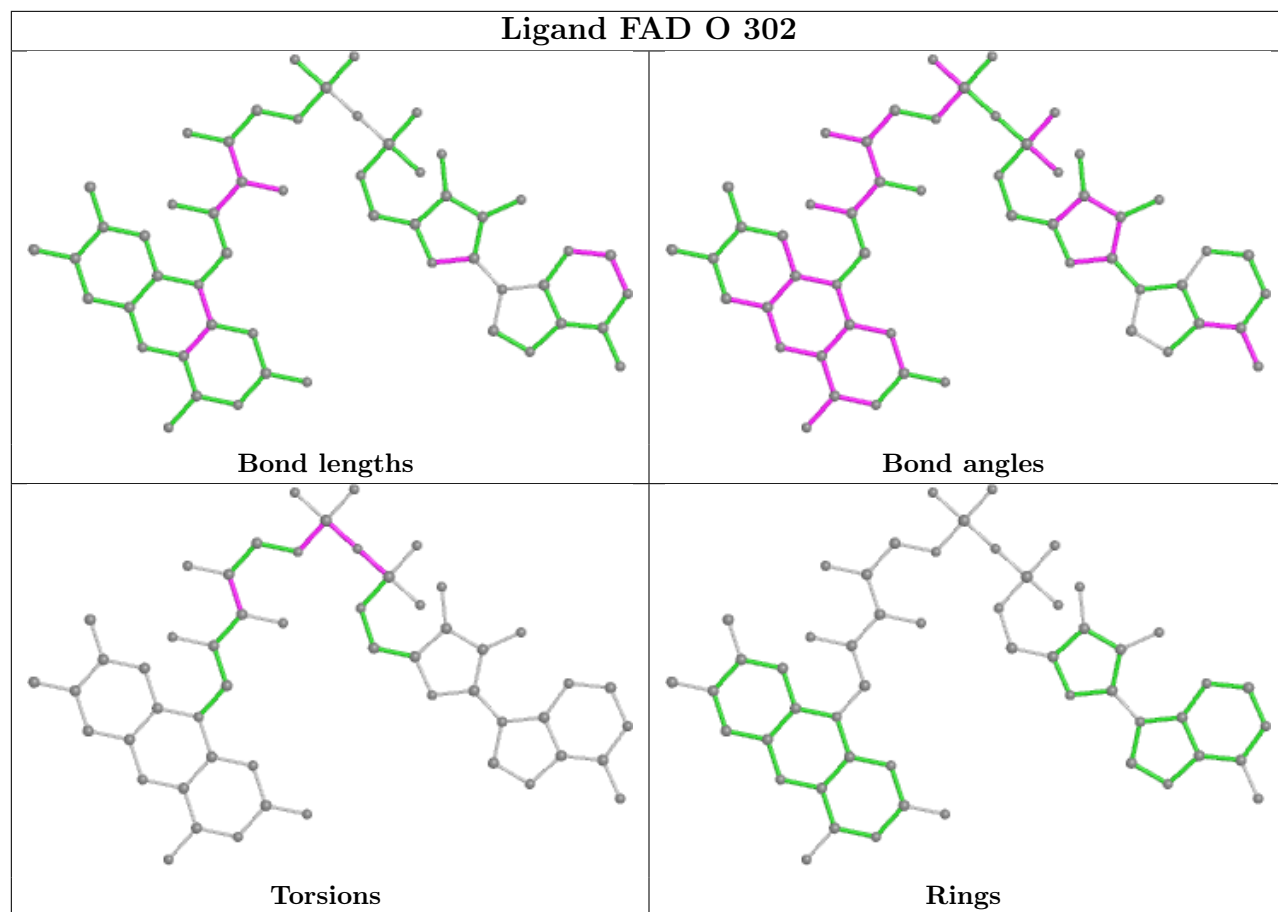




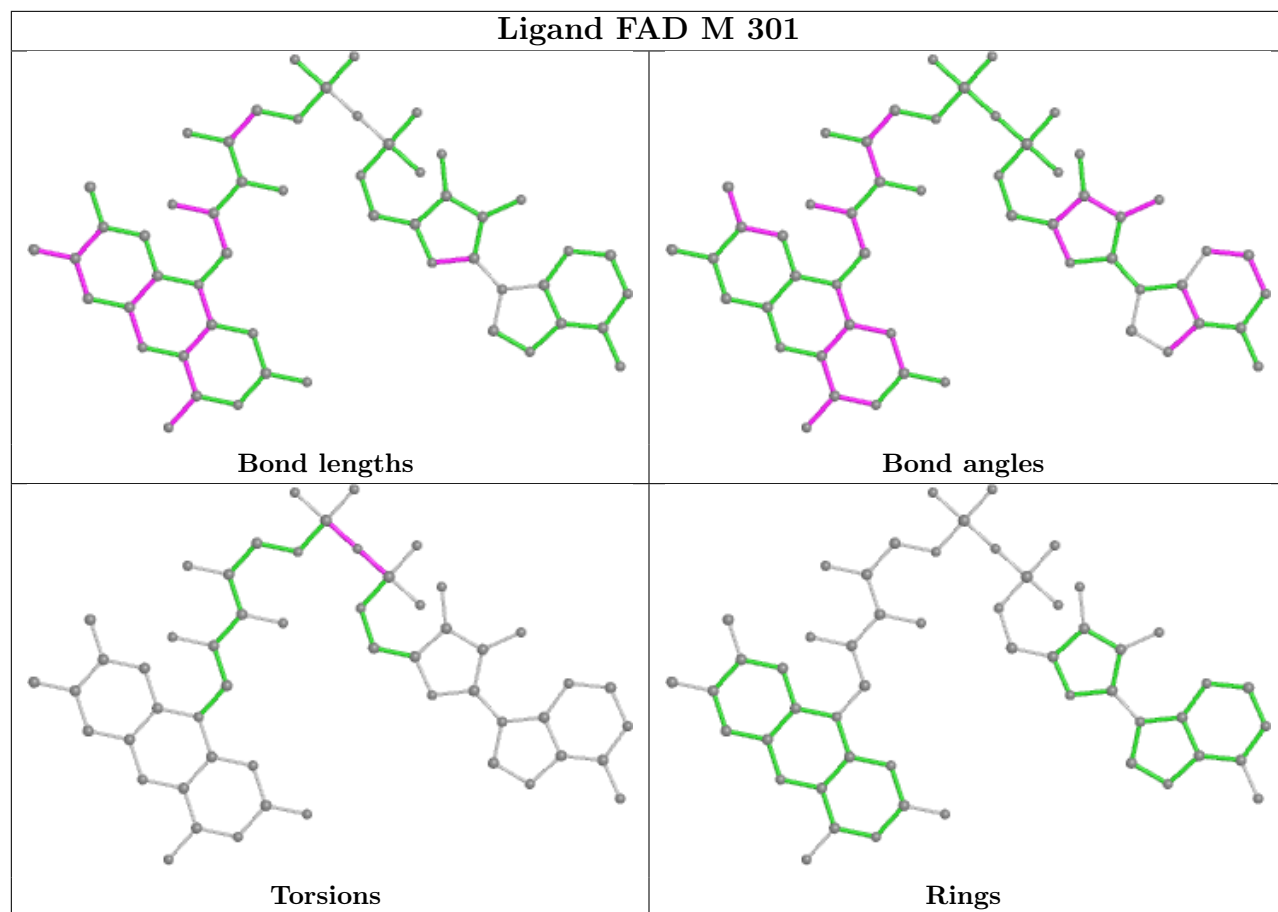


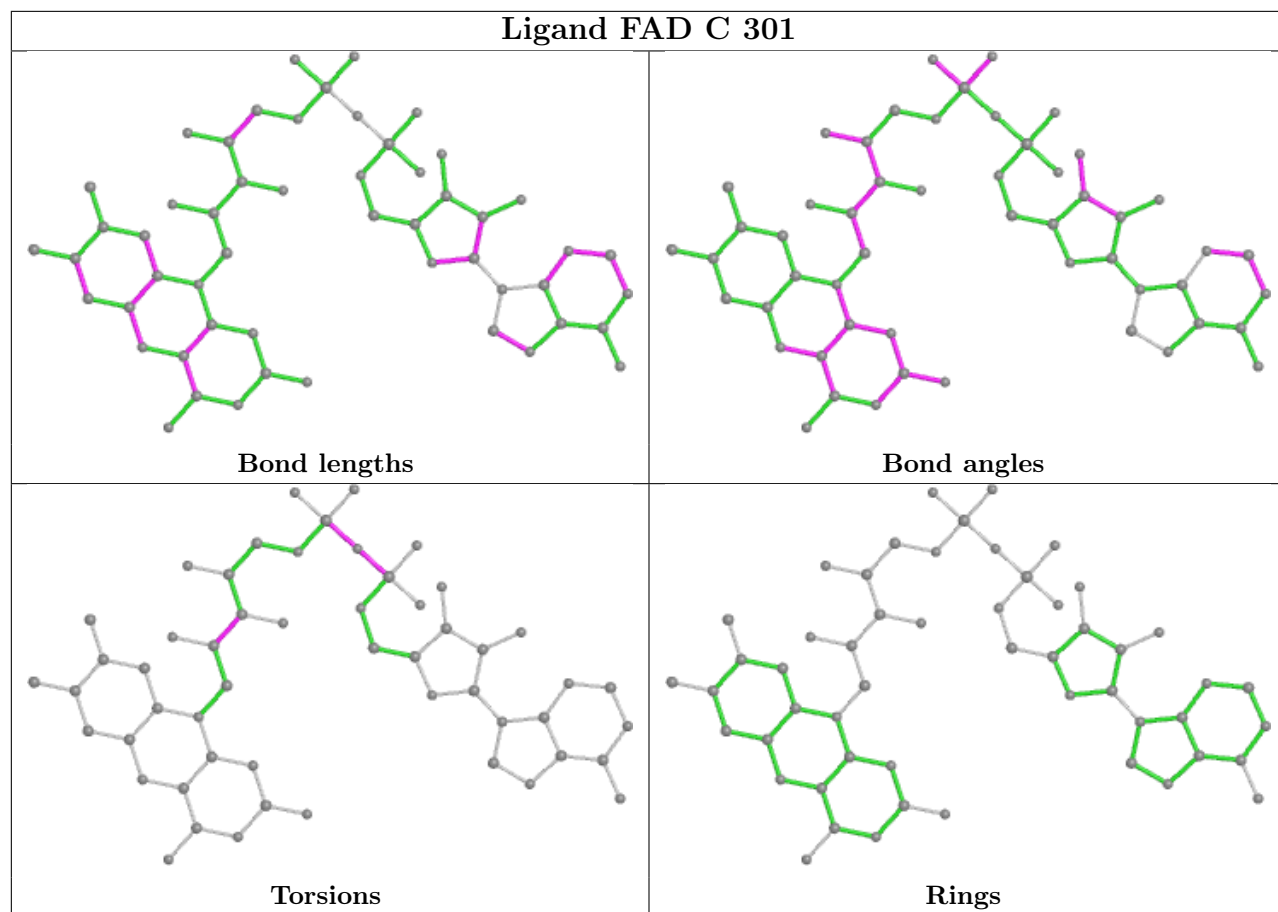


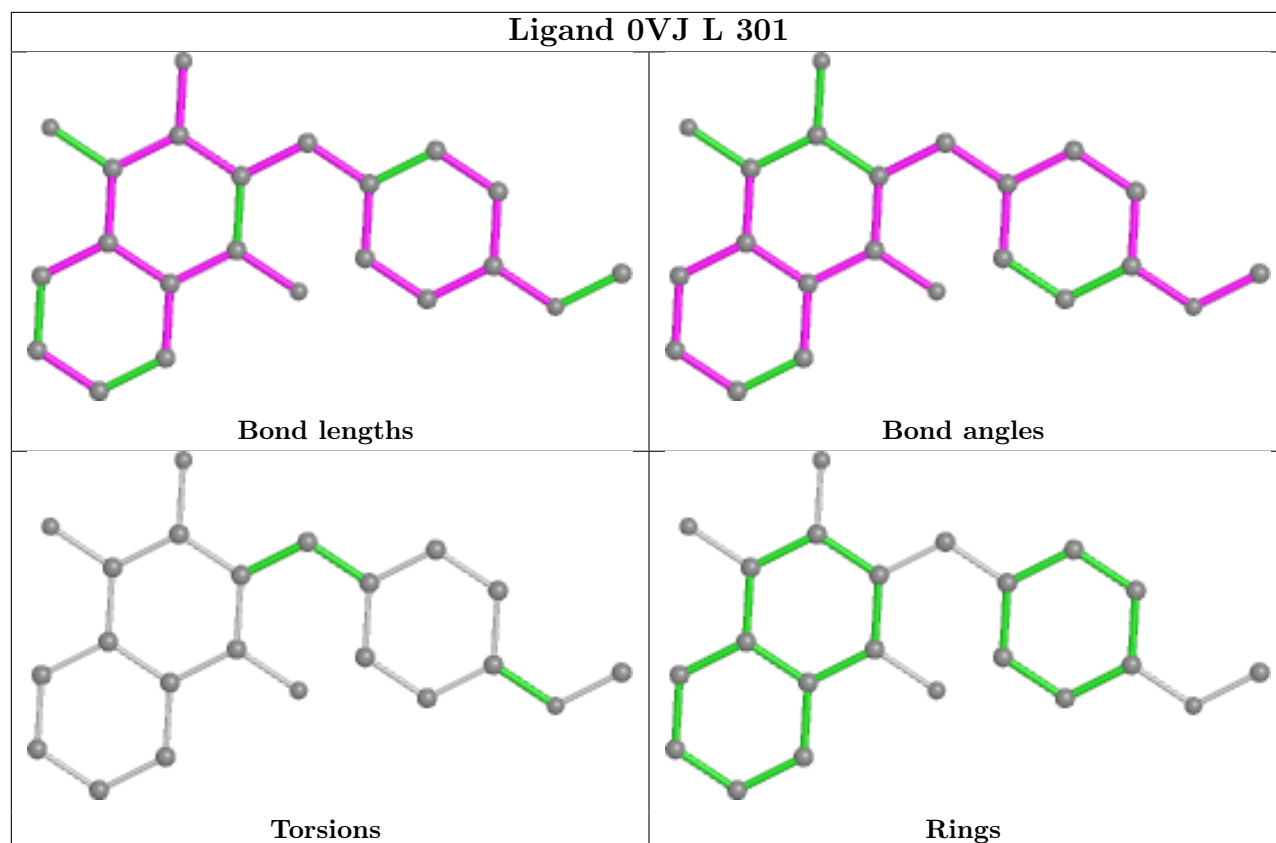
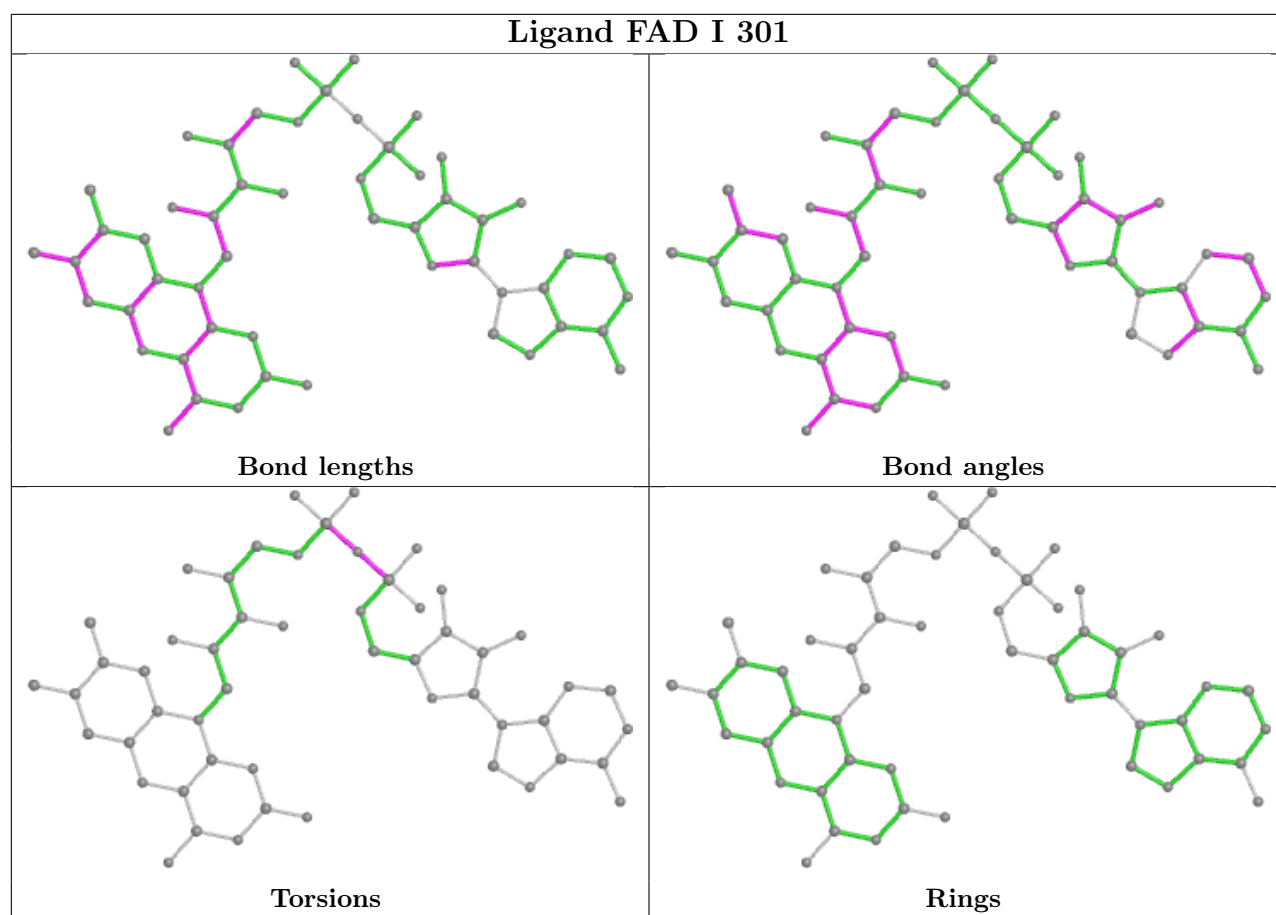


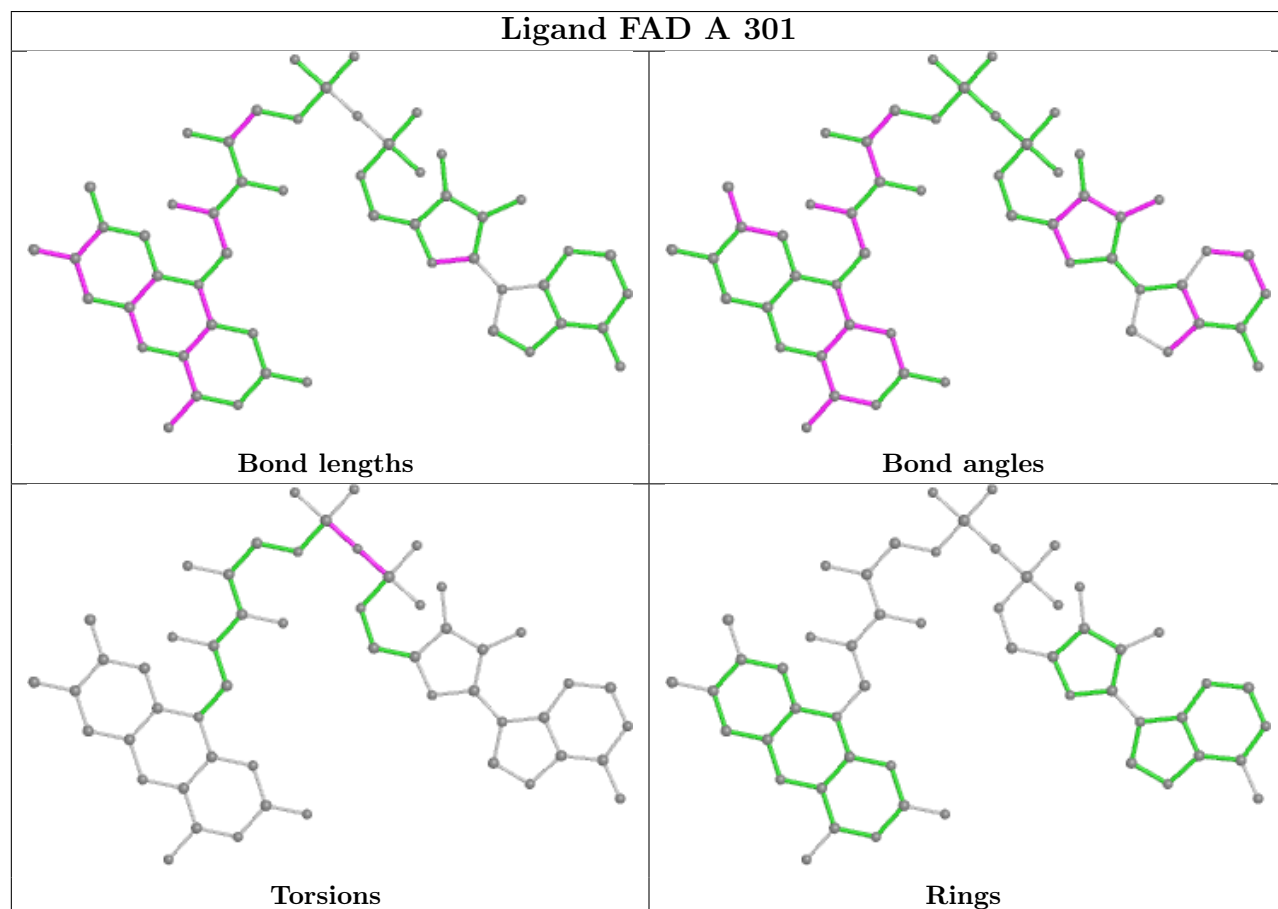
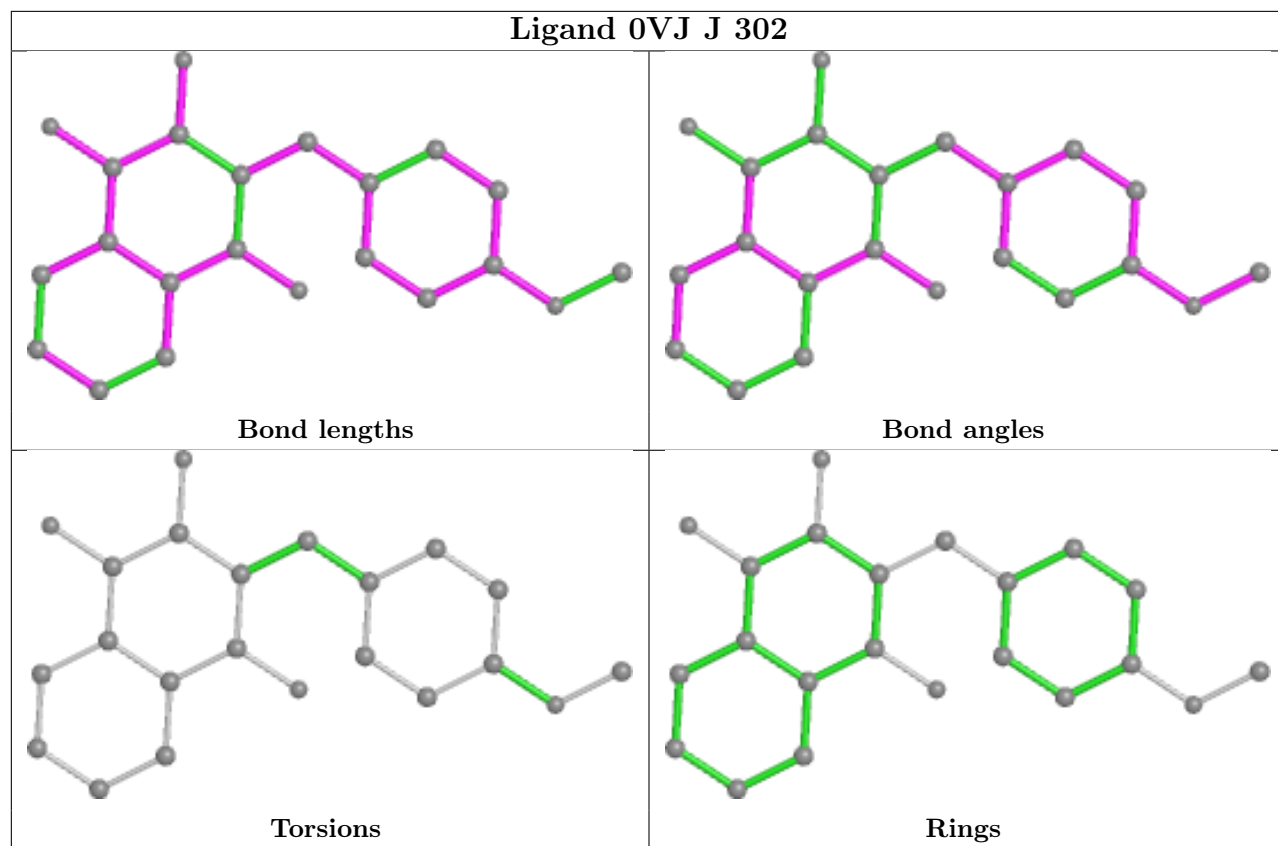


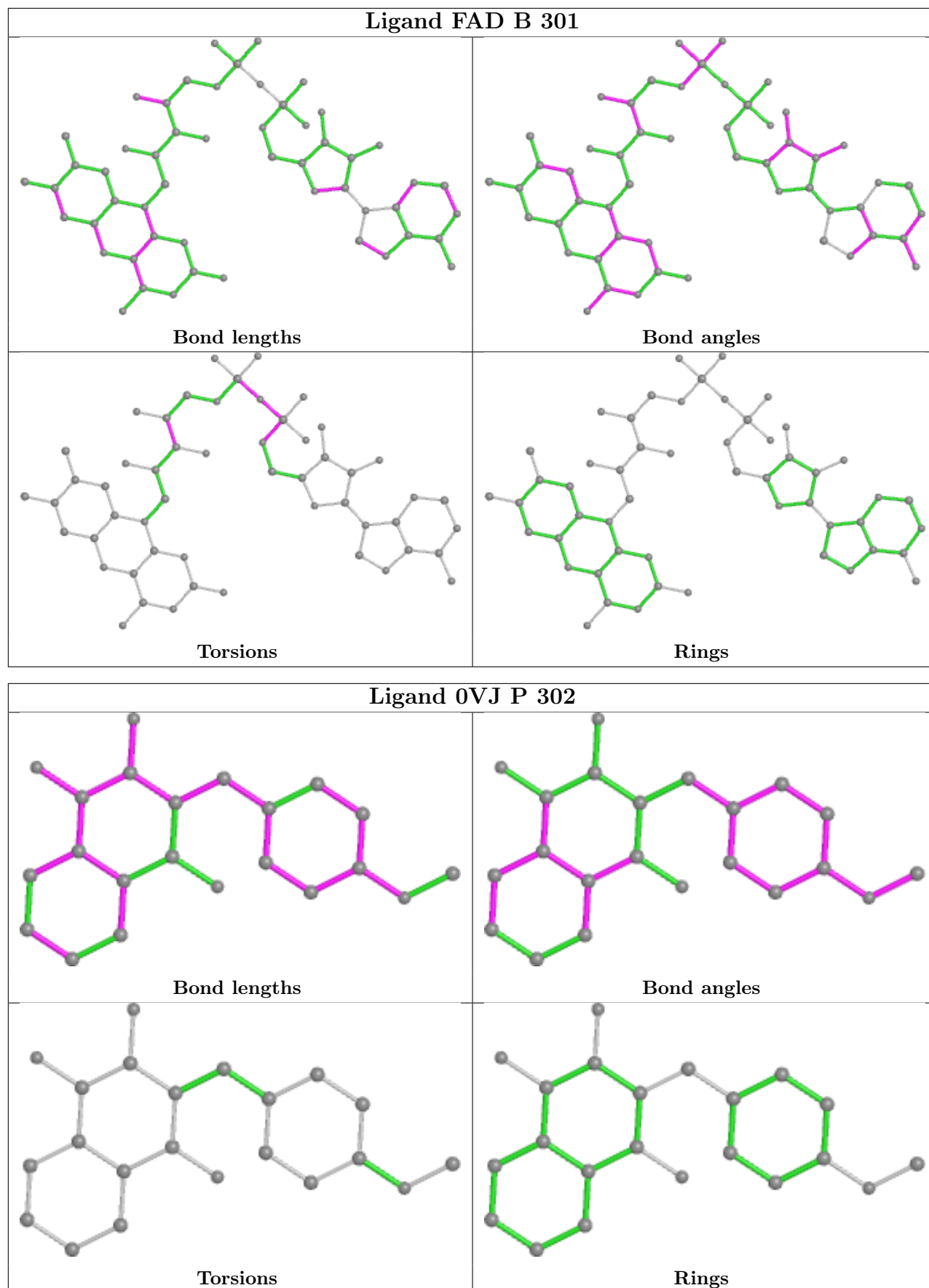












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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, 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	191/227 (84%)	-0.08	0 <b>100</b> <b>100</b>	27, 46, 77, 94	0
1	B	188/227 (82%)	0.02	2 (1%) 80 78	28, 50, 89, 119	0
1	C	207/227 (91%)	0.02	3 (1%) 75 71	27, 51, 91, 104	0
1	D	203/227 (89%)	-0.09	2 (0%) 82 80	28, 45, 71, 90	0
1	E	206/227 (90%)	-0.08	2 (0%) 82 80	26, 49, 86, 107	0
1	F	206/227 (90%)	-0.05	3 (1%) 73 70	24, 44, 74, 111	0
1	G	188/227 (82%)	-0.12	0 <b>100</b> <b>100</b>	27, 46, 71, 99	0
1	H	179/227 (78%)	-0.03	3 (1%) 70 66	30, 48, 72, 108	0
1	I	193/227 (85%)	-0.13	1 (0%) 91 89	23, 49, 74, 91	0
1	J	179/227 (78%)	0.18	3 (1%) 70 66	32, 57, 91, 101	0
1	K	201/227 (88%)	-0.04	1 (0%) 91 89	32, 51, 90, 110	0
1	L	201/227 (88%)	0.17	9 (4%) 33 26	31, 54, 99, 130	0
1	M	197/227 (86%)	-0.07	2 (1%) 82 80	29, 51, 78, 92	0
1	N	177/227 (77%)	0.24	10 (5%) 24 19	29, 58, 102, 138	0
1	O	200/227 (88%)	0.02	2 (1%) 82 80	34, 53, 93, 119	0
1	P	197/227 (86%)	0.22	8 (4%) 37 30	29, 60, 101, 120	0
All	All	3113/3632 (85%)	0.01	51 (1%) 72 68	23, 51, 89, 138	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	104	ARG	5.6
1	F	95	MET	5.4
1	N	125	TRP	4.6
1	J	149	ILE	3.9
1	N	126	TRP	3.8

## 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
4	DMS	P	303	4/4	0.90	0.17	78,87,87,91	0
4	DMS	G	302	4/4	0.93	0.25	70,70,71,76	0
3	0VJ	N	302	22/22	0.93	0.17	59,65,70,71	0
3	0VJ	I	304	22/22	0.94	0.18	38,44,48,49	0
3	0VJ	J	302	22/22	0.94	0.16	51,55,59,60	0
2	FAD	I	302	53/53	0.94	0.15	33,34,35,37	0
3	0VJ	P	302	22/22	0.94	0.18	44,47,53,57	0
4	DMS	A	304	4/4	0.94	0.40	63,70,74,74	0
3	0VJ	A	305	22/22	0.94	0.18	35,40,44,48	0
3	0VJ	F	304	22/22	0.94	0.19	52,58,61,62	0
3	0VJ	L	301	22/22	0.95	0.17	39,42,48,51	0
2	FAD	P	301	53/53	0.95	0.14	33,34,35,37	0
2	FAD	I	301	53/53	0.95	0.15	33,34,35,37	0
2	FAD	E	301	53/53	0.95	0.15	33,34,35,37	0
2	FAD	M	301	53/53	0.95	0.17	33,34,35,37	0
2	FAD	N	301	53/53	0.95	0.13	44,45,47,48	0
3	0VJ	H	301	22/22	0.96	0.14	27,33,39,39	0
2	FAD	F	302	53/53	0.96	0.16	33,34,35,37	0
3	0VJ	A	303	22/22	0.96	0.18	34,39,43,47	0
3	0VJ	K	301	22/22	0.96	0.15	21,26,34,35	0
2	FAD	J	301	53/53	0.96	0.13	42,44,46,48	0
3	0VJ	M	303	22/22	0.96	0.17	33,43,52,53	0
3	0VJ	B	303	22/22	0.96	0.14	24,27,36,40	0
3	0VJ	D	301	22/22	0.96	0.14	45,50,56,56	0
3	0VJ	E	302	22/22	0.96	0.15	32,39,43,44	0
2	FAD	O	302	53/53	0.96	0.14	40,41,43,44	0
4	DMS	H	303	4/4	0.96	0.20	60,62,63,69	0

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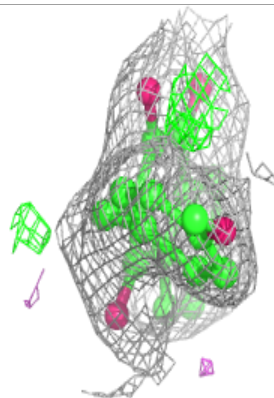
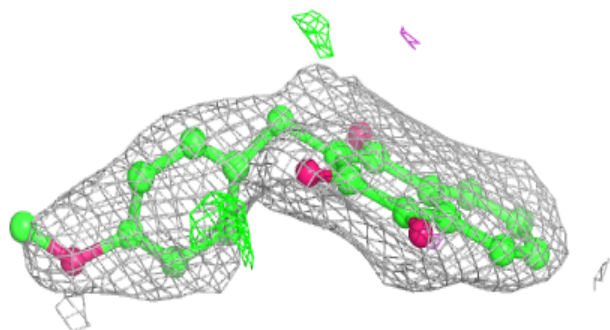
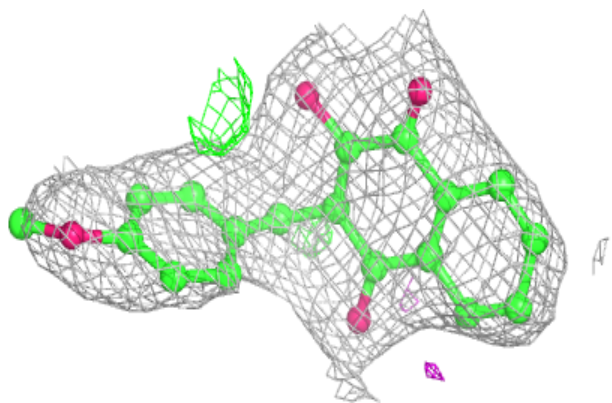
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	0VJ	G	301	22/22	0.96	0.17	30,39,47,47	0
2	FAD	H	302	53/53	0.97	0.15	45,46,47,49	0
2	FAD	K	302	53/53	0.97	0.14	37,38,40,40	0
4	DMS	C	302	4/4	0.97	0.23	63,64,65,65	0
4	DMS	D	302	4/4	0.97	0.13	63,63,67,74	0
4	DMS	E	303	4/4	0.97	0.18	57,64,68,70	0
4	DMS	F	303	4/4	0.97	0.12	60,63,67,74	0
2	FAD	A	302	53/53	0.97	0.16	33,34,35,37	0
2	FAD	B	301	53/53	0.97	0.13	40,41,43,44	0
4	DMS	M	302	4/4	0.97	0.21	80,87,87,88	0
3	0VJ	O	301	22/22	0.97	0.15	18,27,33,36	0
2	FAD	C	301	53/53	0.98	0.13	33,34,36,38	0
2	FAD	A	301	53/53	0.98	0.14	33,34,35,37	0
4	DMS	I	303	4/4	0.98	0.20	81,84,87,89	0
4	DMS	K	303	4/4	0.98	0.19	54,54,60,61	0
2	FAD	F	301	53/53	0.98	0.14	28,29,30,32	0
4	DMS	O	303	4/4	0.98	0.16	53,56,60,63	0
4	DMS	B	302	4/4	0.98	0.25	44,46,55,55	0

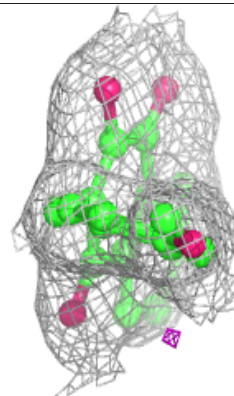
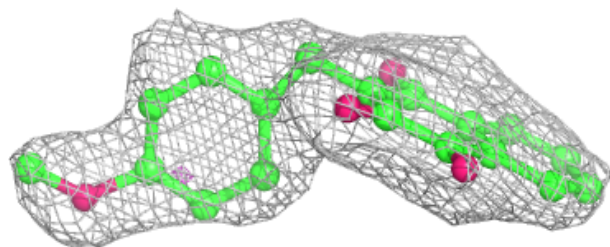
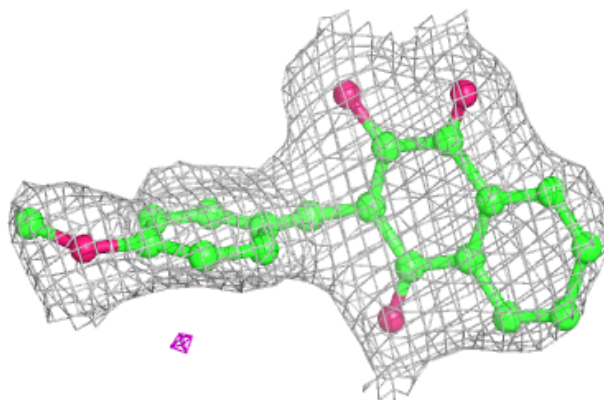
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 0VJ N 302:**

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

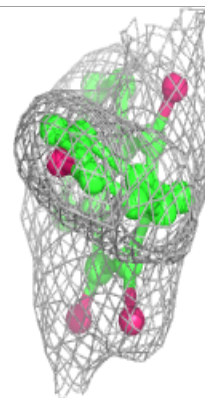
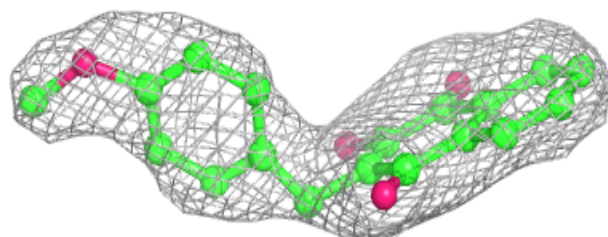
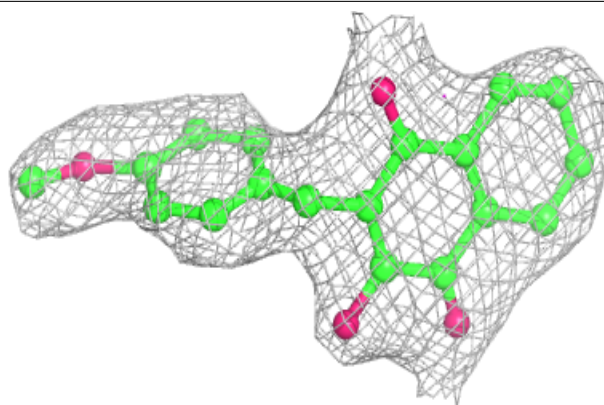
**Electron density around 0VJ I 304:**

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

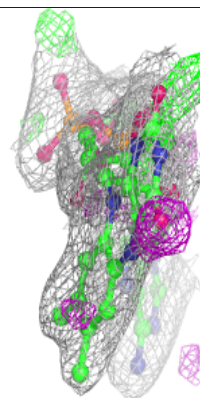
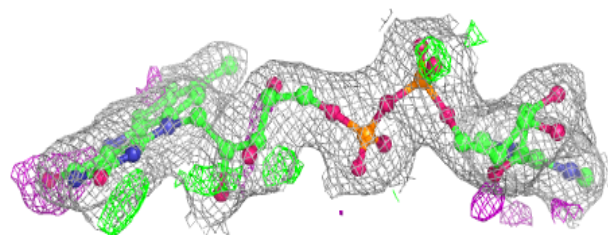
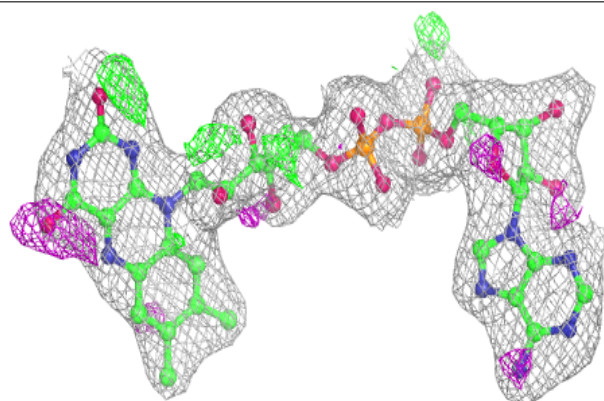


**Electron density around 0VJ J 302:**

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

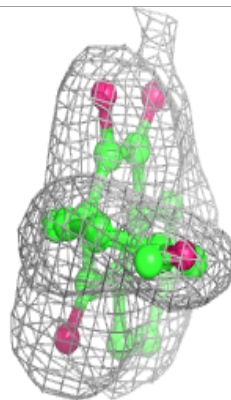
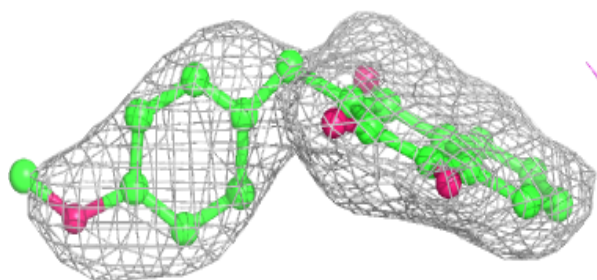
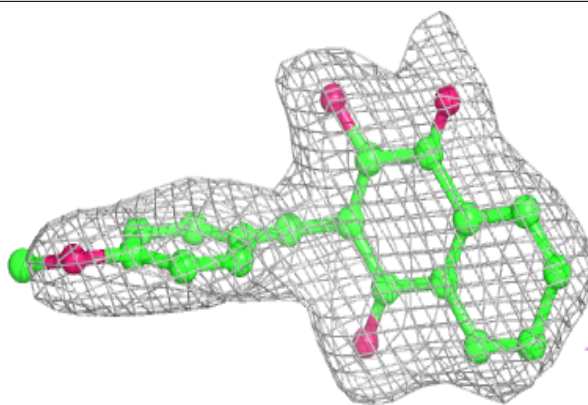
**Electron density around FAD I 302:**

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

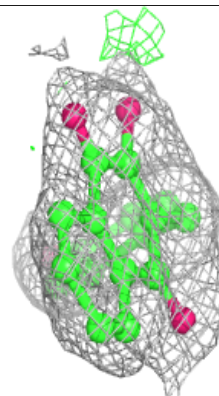
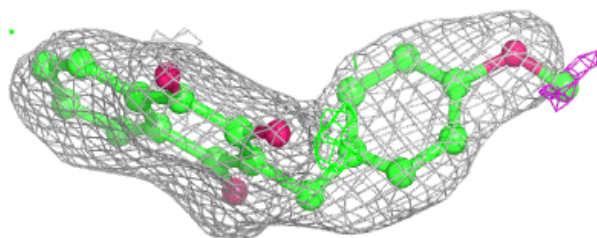
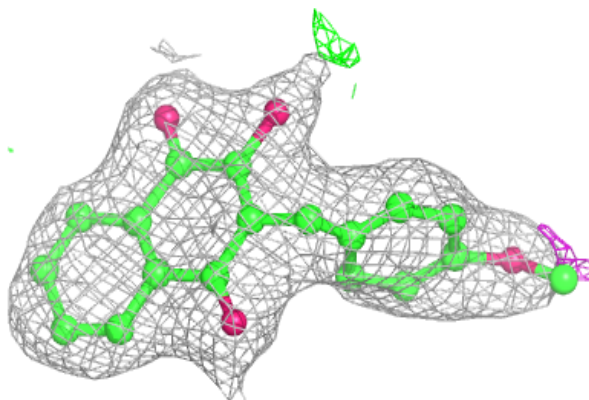


**Electron density around 0VJ P 302:**

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

**Electron density around 0VJ A 305:**

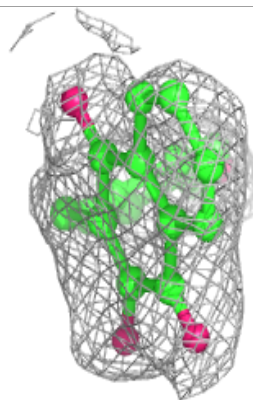
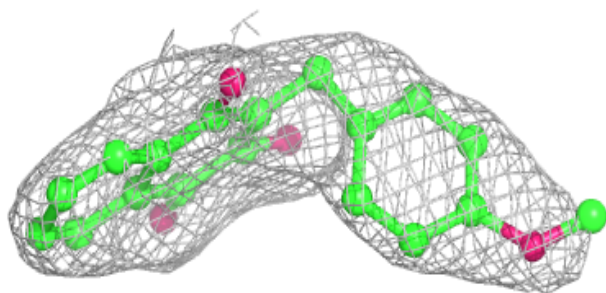
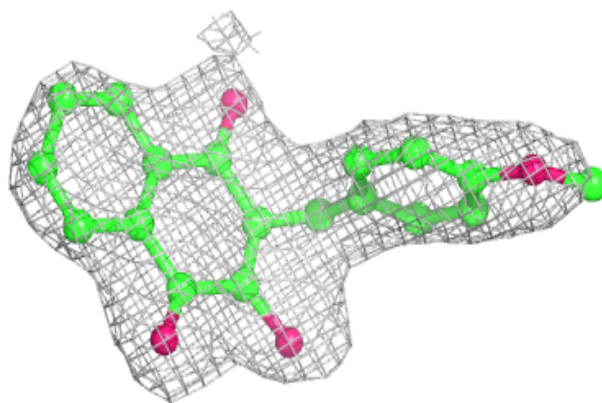
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



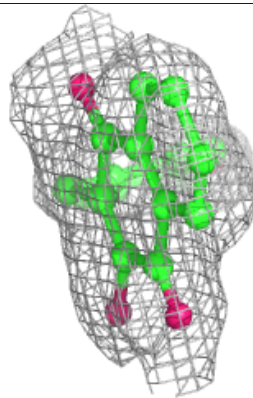
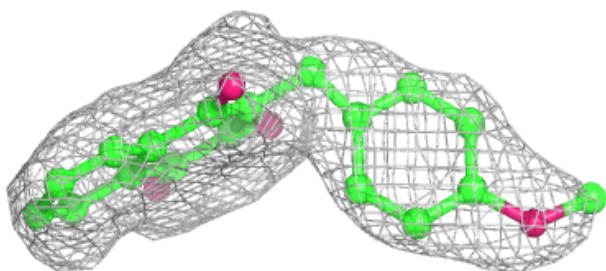
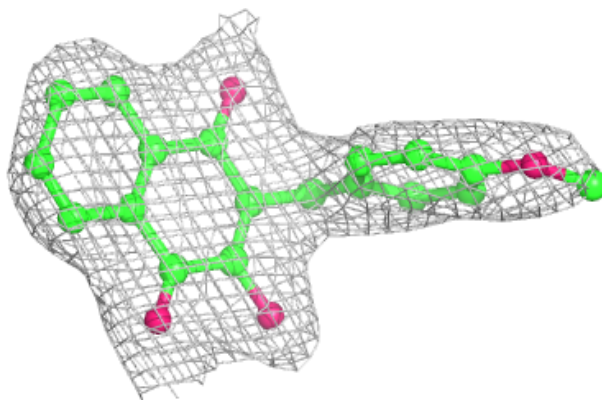


**Electron density around 0VJ F 304:**

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

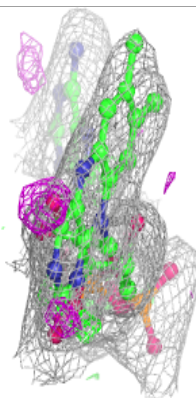
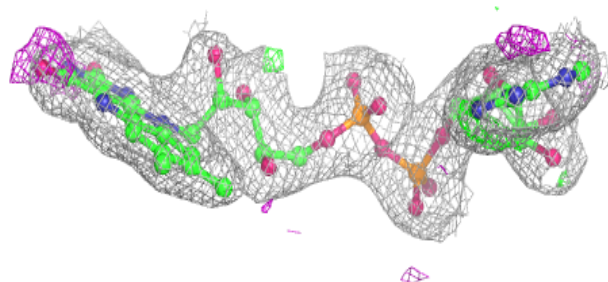
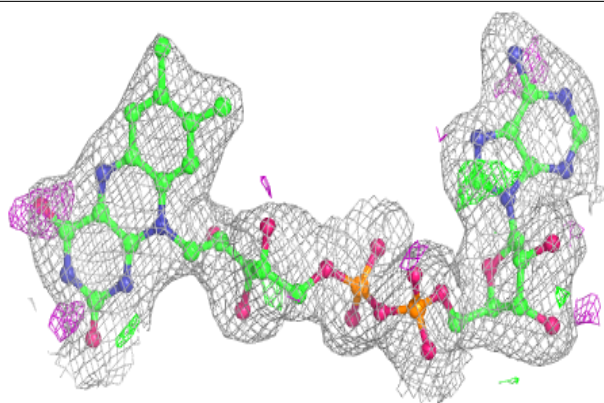
**Electron density around 0VJ L 301:**

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

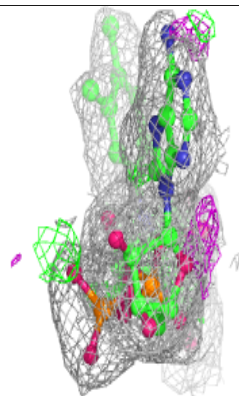
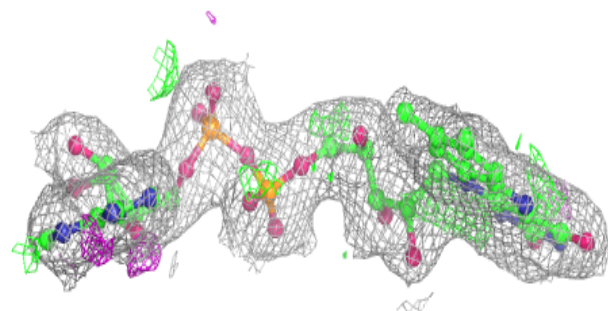
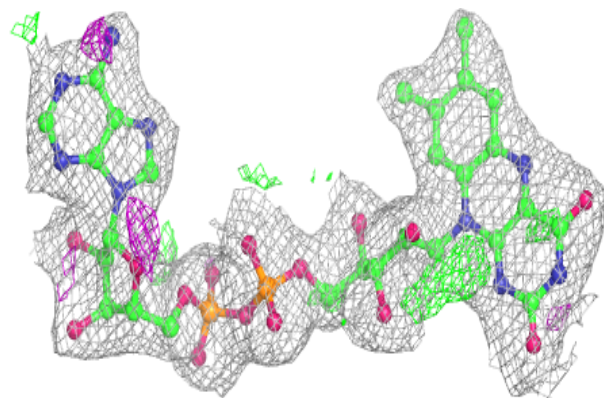


**Electron density around FAD P 301:**

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

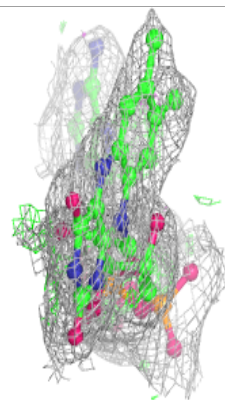
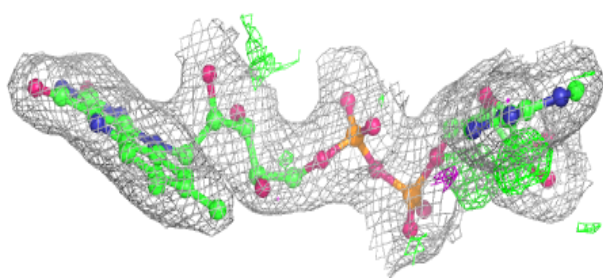
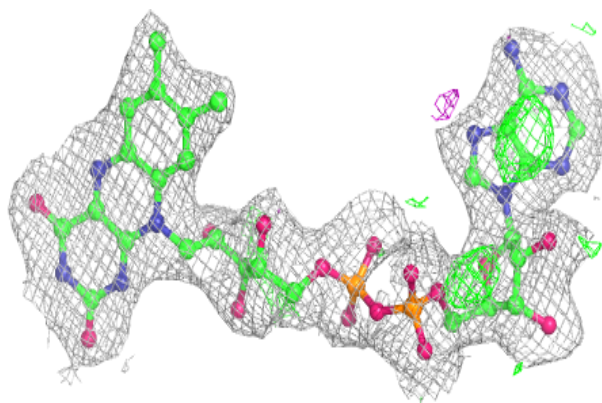
**Electron density around FAD I 301:**

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

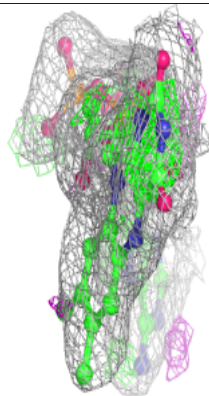
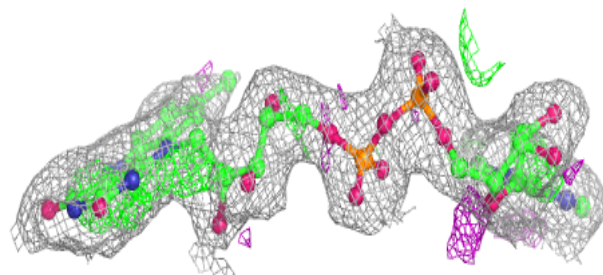
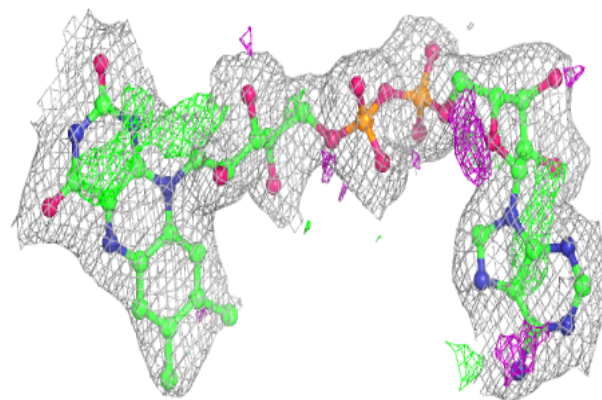


**Electron density around FAD E 301:**

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

**Electron density around FAD M 301:**

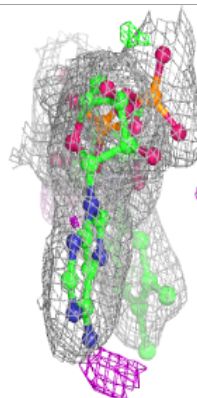
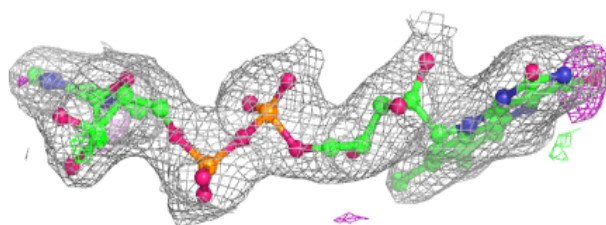
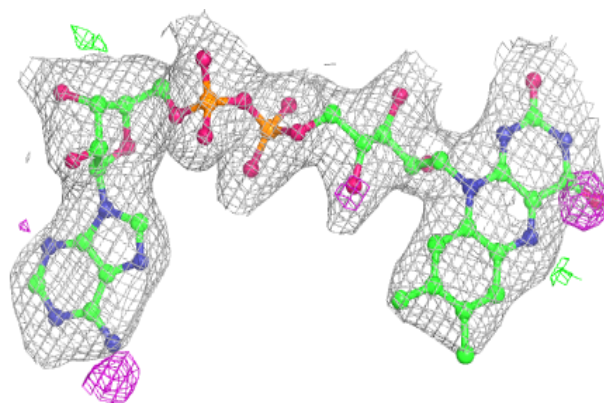
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



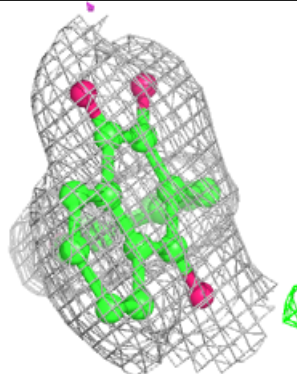
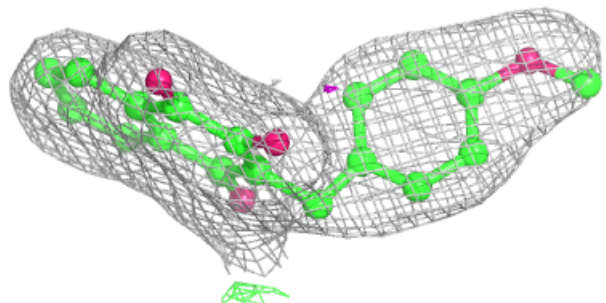
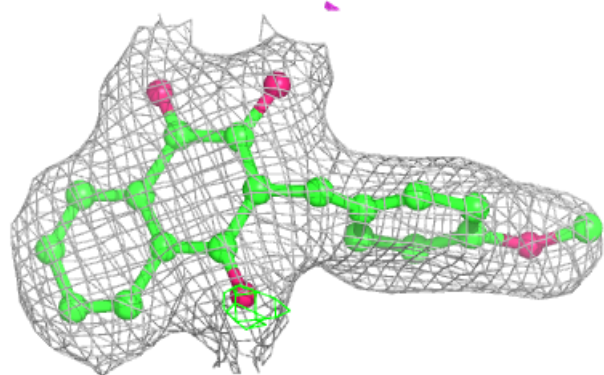


**Electron density around FAD N 301:**

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

**Electron density around 0VJ H 301:**

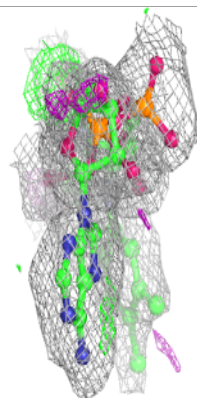
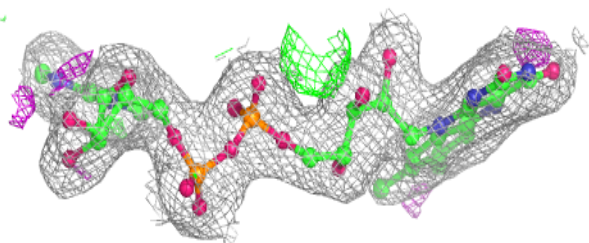
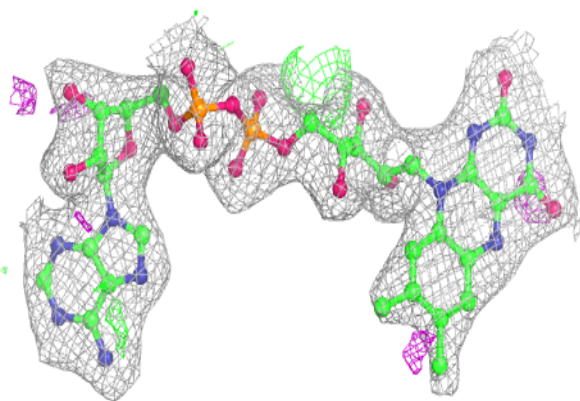
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



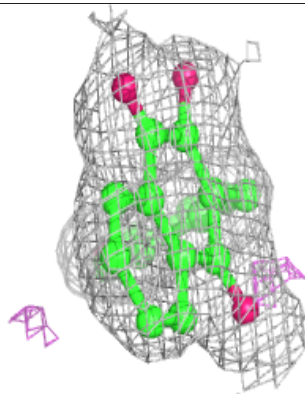
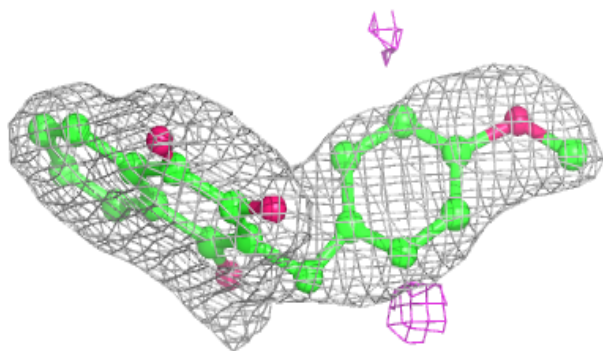
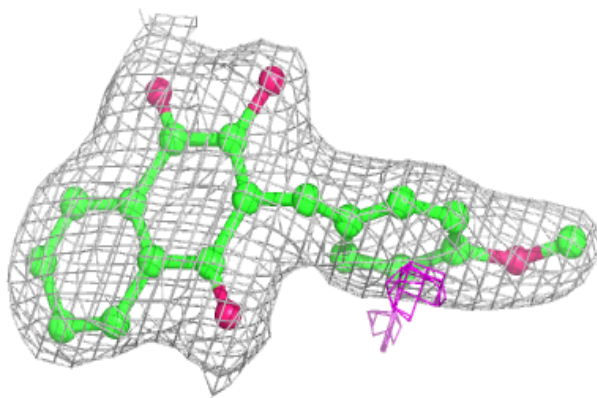


**Electron density around FAD F 302:**

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

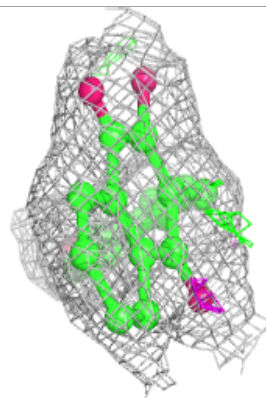
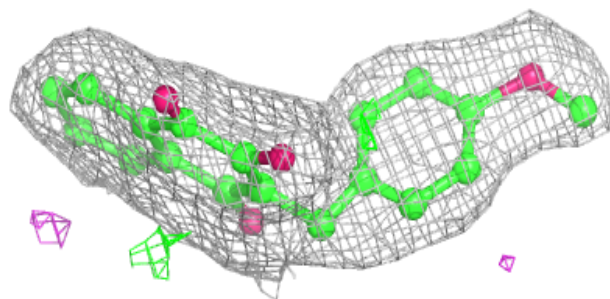
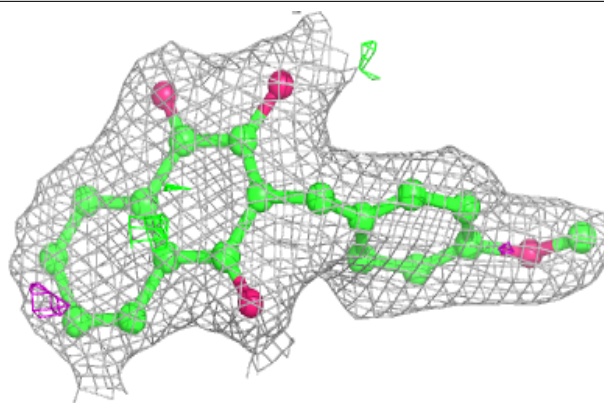
**Electron density around 0VJ A 303:**

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

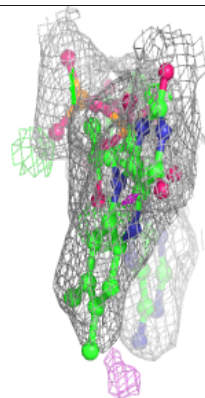
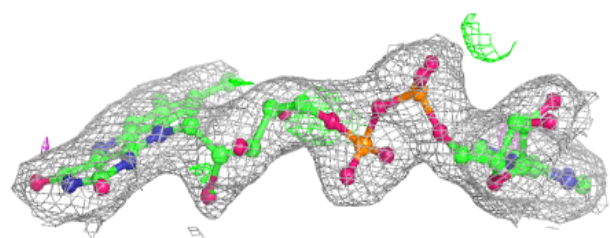
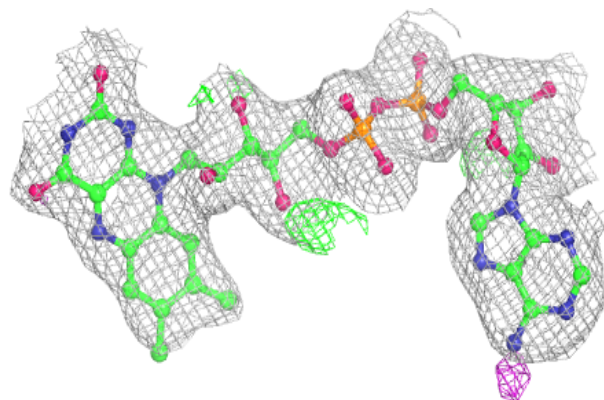


**Electron density around 0VJ K 301:**

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

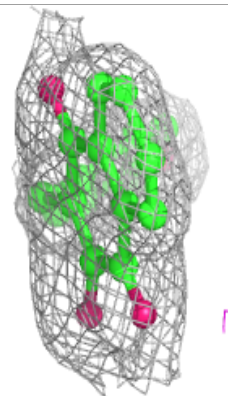
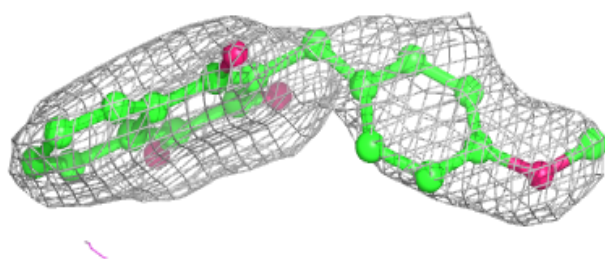
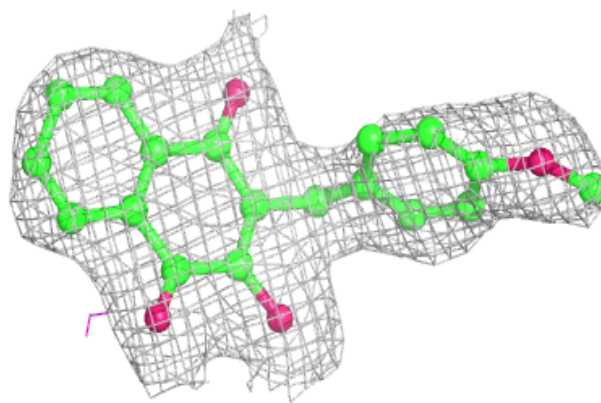
**Electron density around FAD J 301:**

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

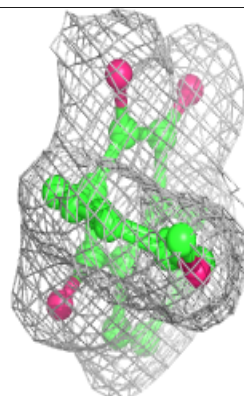
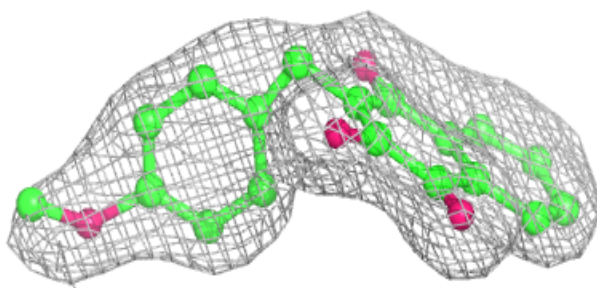
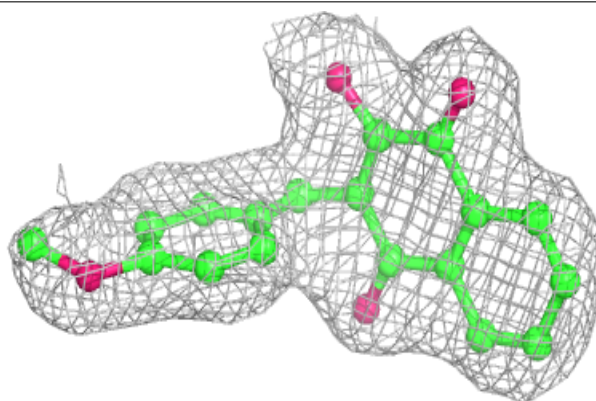


**Electron density around 0VJ M 303:**

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

**Electron density around 0VJ B 303:**

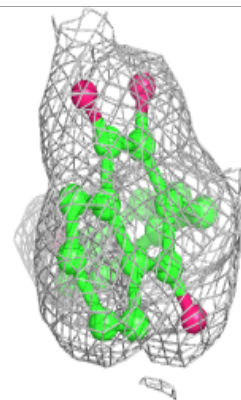
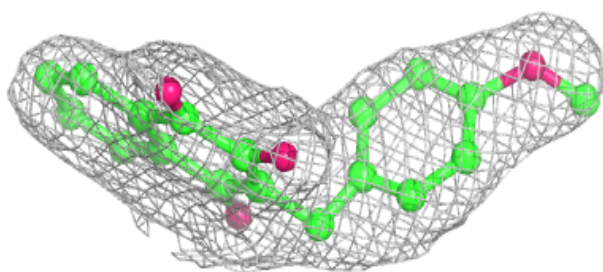
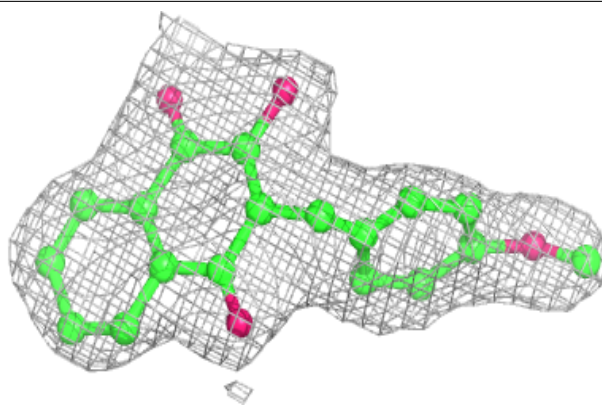
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



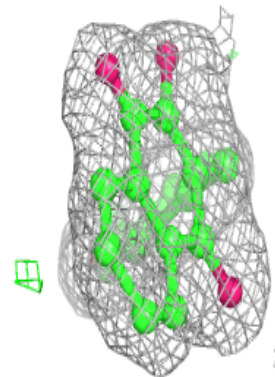
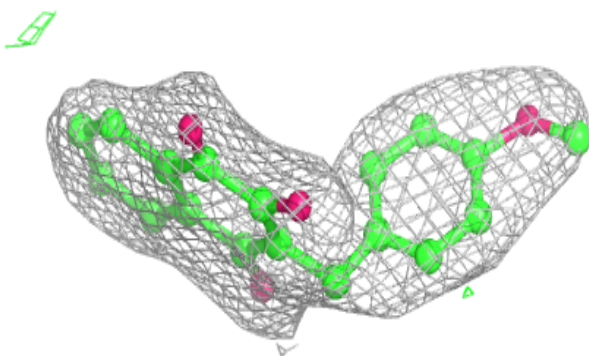
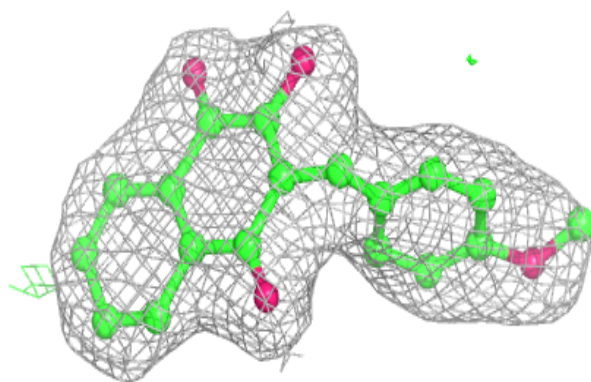


**Electron density around 0VJ D 301:**

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

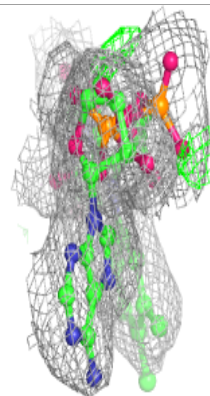
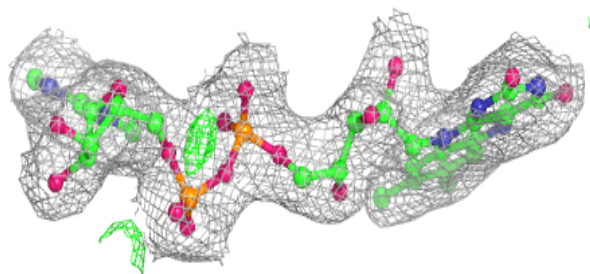
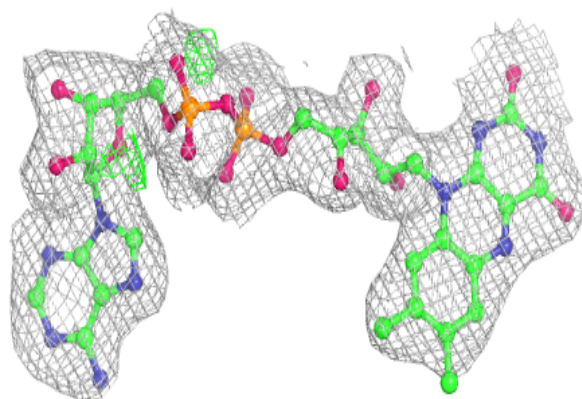
**Electron density around 0VJ E 302:**

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

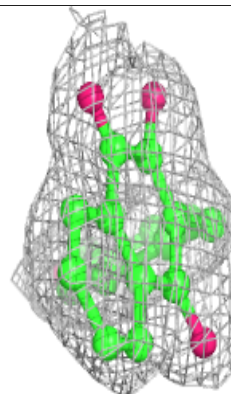
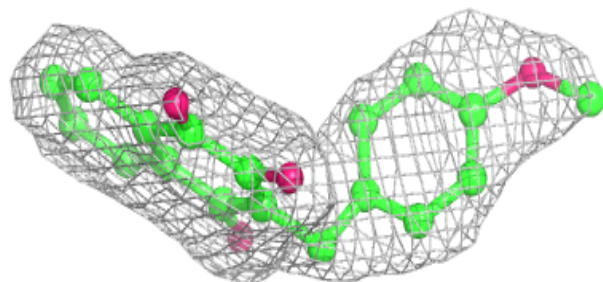
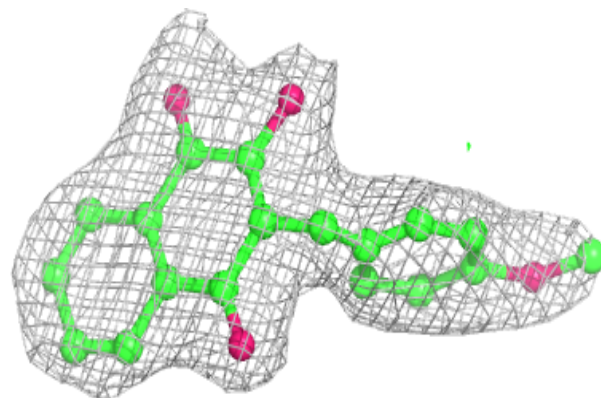


**Electron density around FAD O 302:**

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

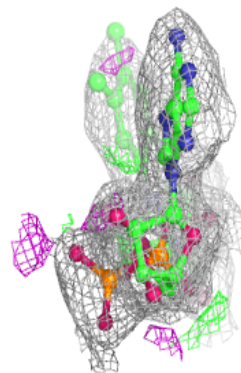
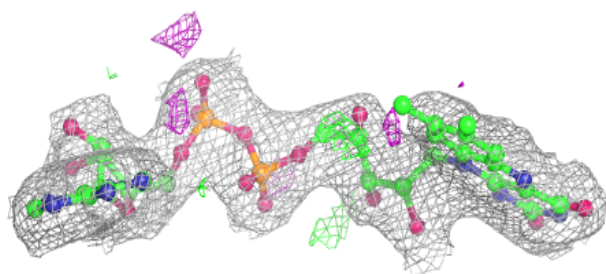
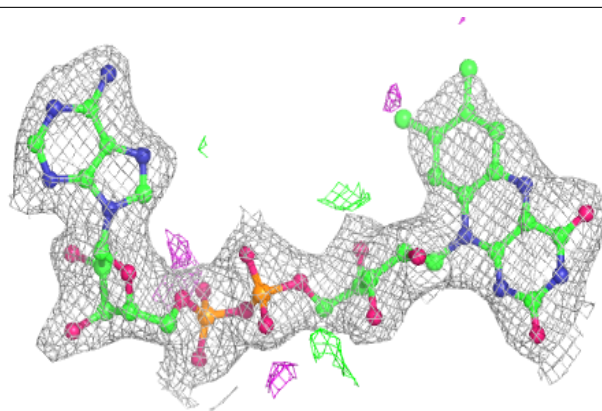
**Electron density around 0VJ G 301:**

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

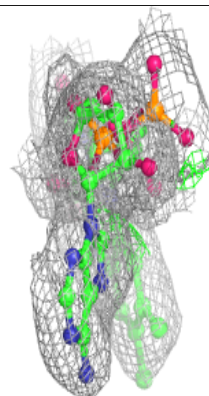
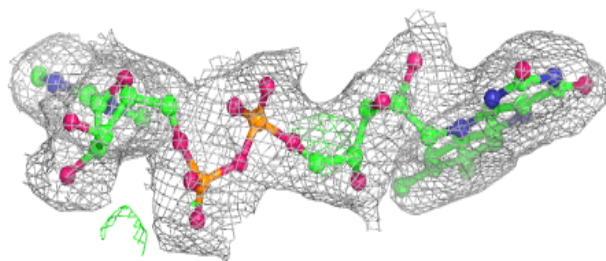
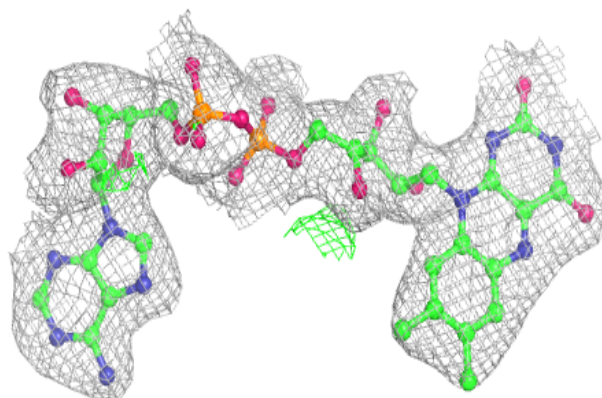


**Electron density around FAD H 302:**

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

**Electron density around FAD K 302:**

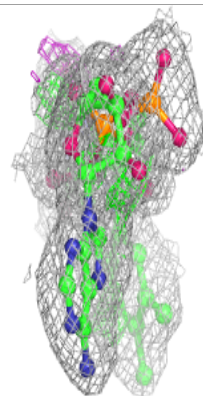
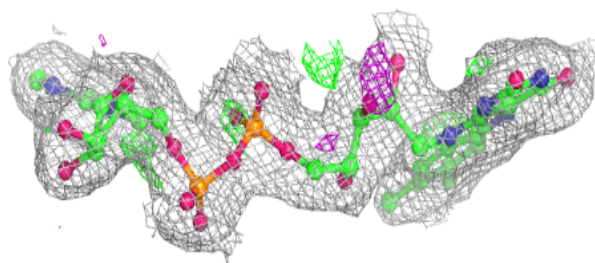
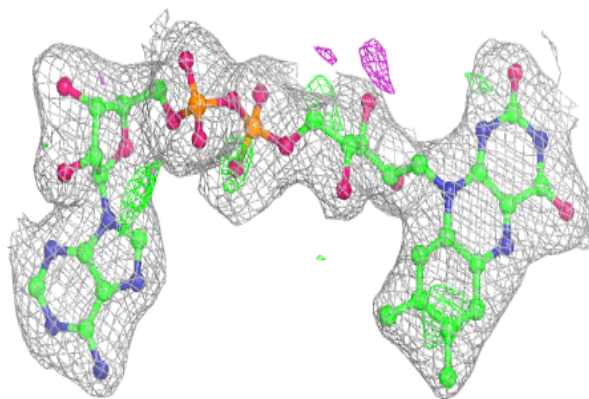
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



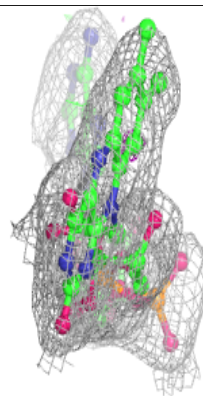
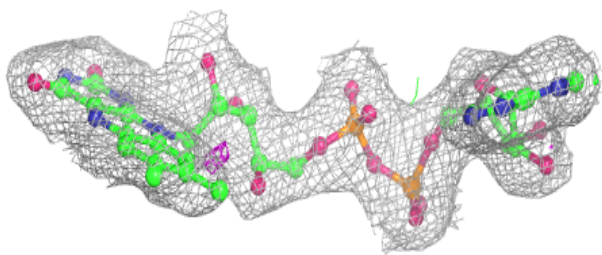
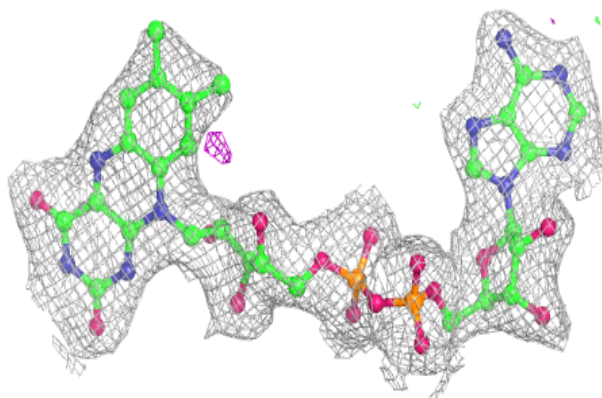


**Electron density around FAD A 302:**

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

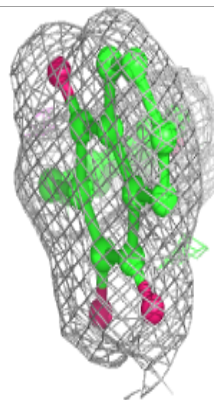
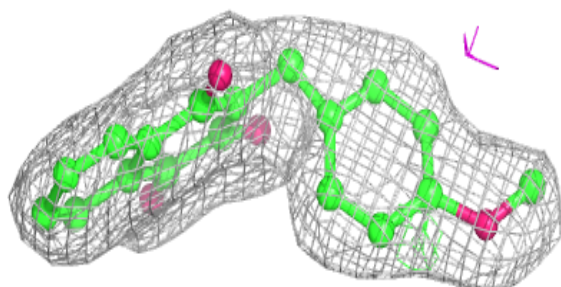
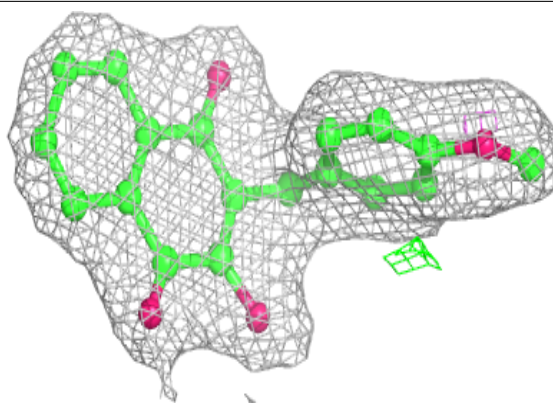
**Electron density around FAD B 301:**

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

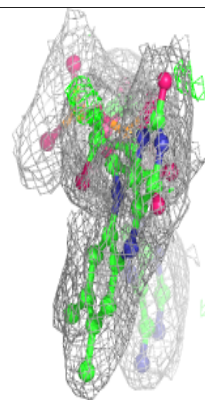
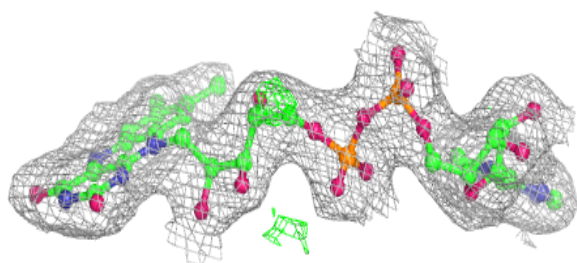
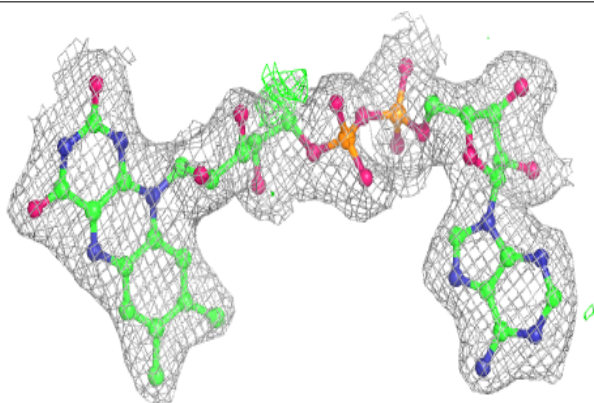


**Electron density around 0VJ O 301:**

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

**Electron density around FAD C 301:**

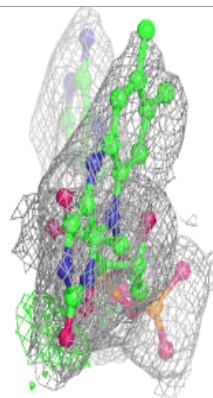
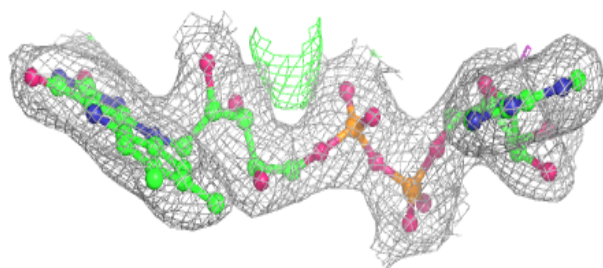
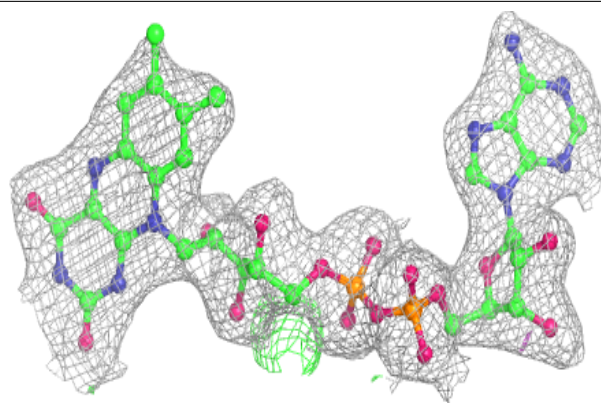
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



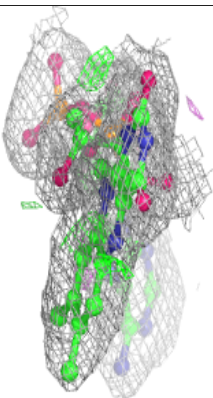
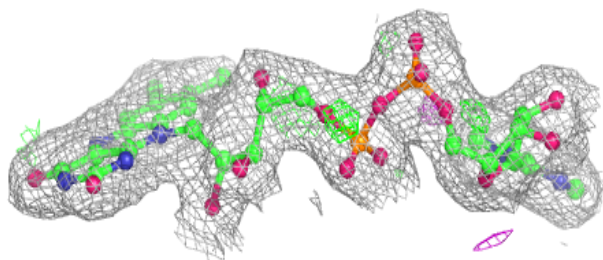
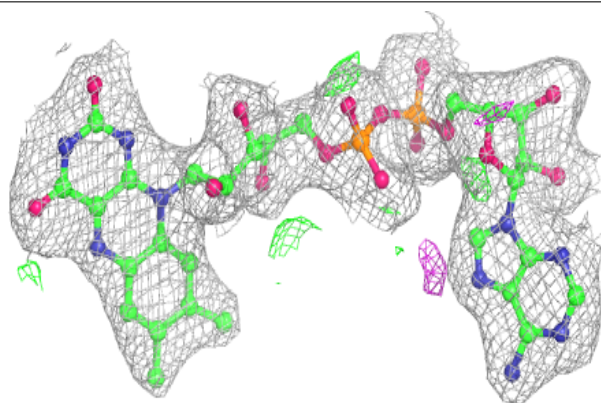


**Electron density around FAD A 301:**

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

**Electron density around FAD 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.