



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 06:21 AM UTC

PDB ID : 4FZB / pdb_00004fzb
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.; Myllylkalio, 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

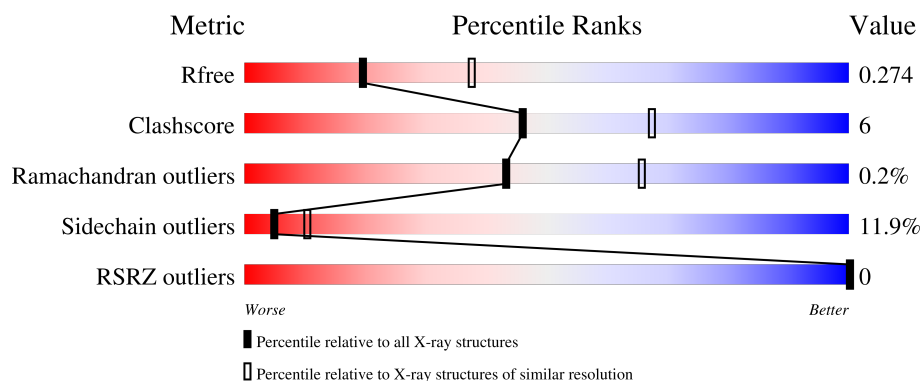
1 Overall quality at a glance ⓘ

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 ≥ 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	
1	B	227	
1	C	227	
1	D	227	

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Mol	Chain	Length	Quality of chain
1	E	227	
1	F	227	
1	G	227	
1	H	227	
1	I	227	
1	J	227	
1	K	227	
1	L	227	
1	M	227	
1	N	227	
1	O	227	
1	P	227	

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	A	305	-	X	-	-
3	0VJ	B	303	-	X	-	-
4	DMS	M	302	-	-	X	-

2 Entry composition

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

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
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L	221	HIS	-	expression tag	UNP O41156
L	222	HIS	-	expression tag	UNP O41156
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M	-3	ALA	-	expression tag	UNP O41156
M	-2	SER	-	expression tag	UNP O41156
M	-1	MET	-	expression tag	UNP O41156
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M	1	GLY	-	expression tag	UNP O41156
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M	222	HIS	-	expression tag	UNP O41156
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N	-3	ALA	-	expression tag	UNP O41156
N	-2	SER	-	expression tag	UNP O41156
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N	0	THR	-	expression tag	UNP O41156
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N	222	HIS	-	expression tag	UNP O41156

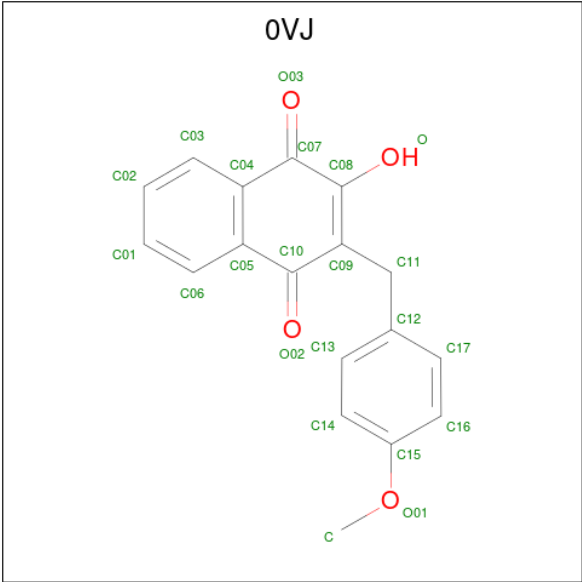
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Chain	Residue	Modelled	Actual	Comment	Reference
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O	-1	MET	-	expression tag	UNP O41156
O	0	THR	-	expression tag	UNP O41156
O	1	GLY	-	expression tag	UNP O41156
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O	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
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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

- # FAD

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

- Molecule 3 is 2-hydroxy-3-(4-methoxybenzyl)naphthalene-1,4-dione (CCD ID: 0VJ) (formula: C₁₈H₁₄O₄).



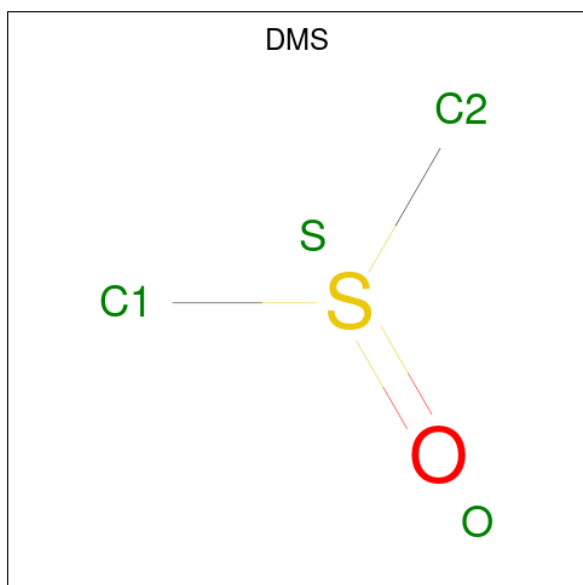
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	18	4		
3	A	1	Total	C	O	0	0
			22	18	4		
3	B	1	Total	C	O	0	0
			22	18	4		
3	D	1	Total	C	O	0	0
			22	18	4		
3	E	1	Total	C	O	0	0
			22	18	4		
3	F	1	Total	C	O	0	0
			22	18	4		
3	G	1	Total	C	O	0	0
			22	18	4		
3	H	1	Total	C	O	0	0
			22	18	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 (CCD ID: DMS) (formula: C₂H₆OS).



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 4	C 2	O 1	S 1	0	0
4	M	1	Total 4	C 2	O 1	S 1	0	0
4	O	1	Total 4	C 2	O 1	S 1	0	0
4	P	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 5 is water.

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

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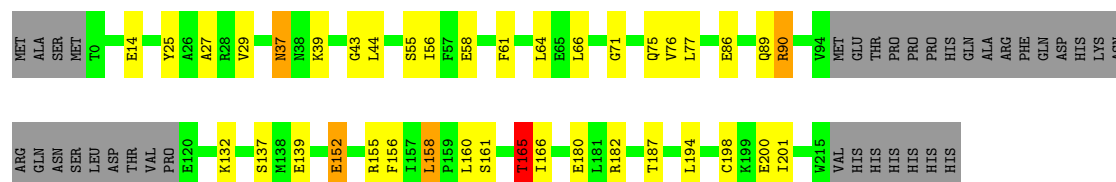
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	1	Total	O	0	0
			1	1		

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.

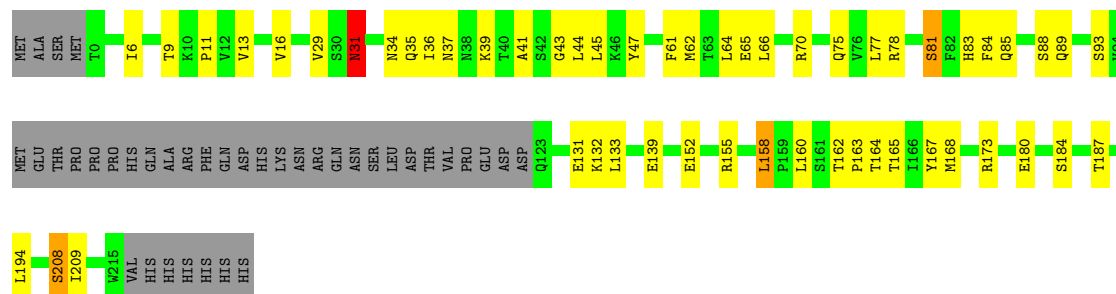
• Molecule 1: Probable thymidylate synthase

Chain A: 



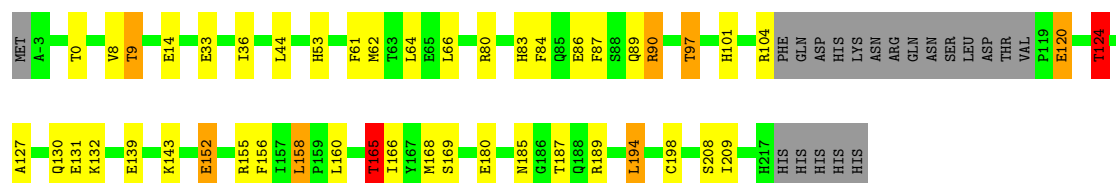
• Molecule 1: Probable thymidylate synthase

Chain B: 



• Molecule 1: Probable thymidylate synthase

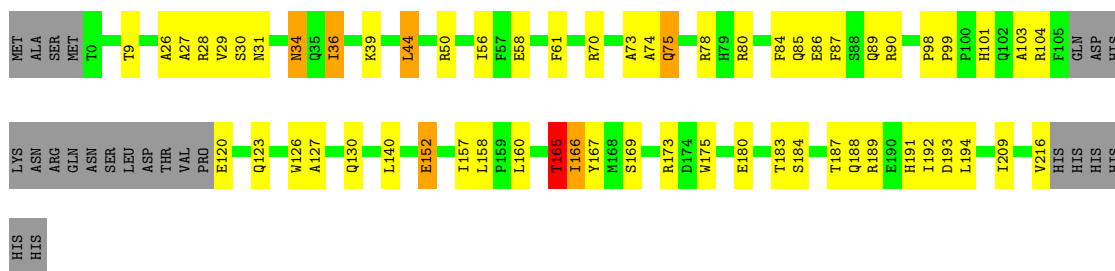
Chain C: 



• Molecule 1: Probable thymidylate synthase

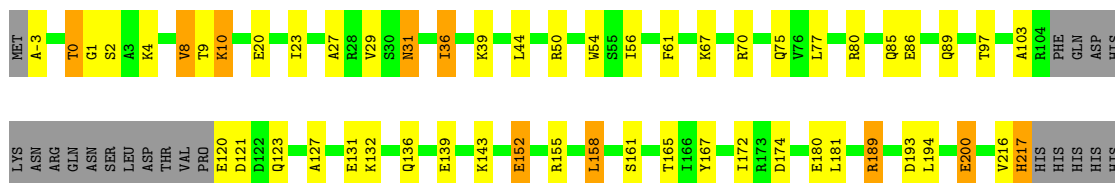
Chain D: 





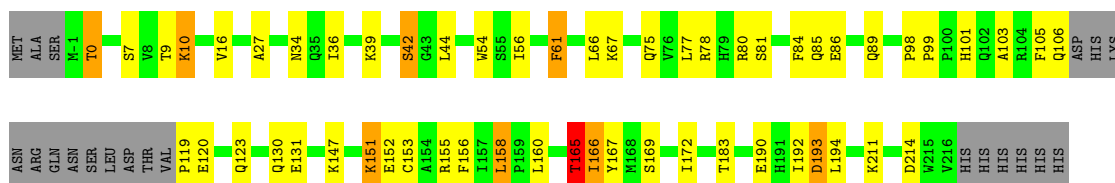
- Molecule 1: Probable thymidylate synthase

Chain E: 67% 20% 9%



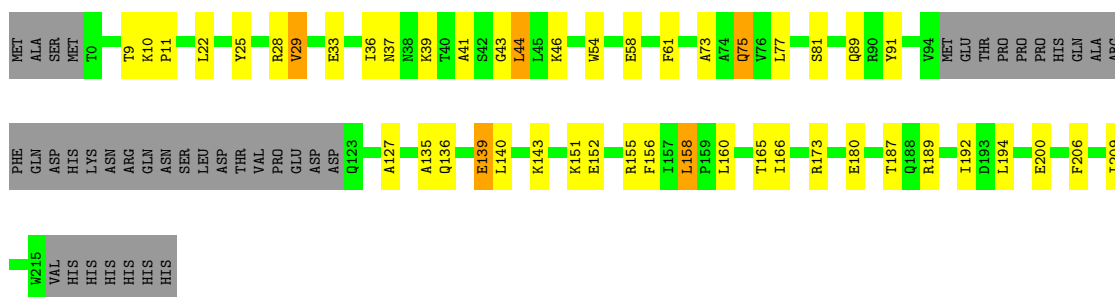
- Molecule 1: Probable thymidylate synthase

Chain F: 66% 21% 9%



- Molecule 1: Probable thymidylate synthase

Chain G: 62% 19% 17%



- Molecule 1: Probable thymidylate synthase

Chain H: 63% 15% 21%









4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 87.3 (34.21-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.61Å)	Xtriage
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 (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.146 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26503	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

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

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	0.86	0/1578	1.45	7/2134 (0.3%)
1	B	0.86	0/1553	1.43	8/2100 (0.4%)
1	C	0.87	0/1707	1.47	17/2311 (0.7%)
1	D	0.86	0/1681	1.48	24/2276 (1.1%)
1	E	0.88	0/1710	1.51	25/2314 (1.1%)
1	F	0.89	0/1706	1.47	16/2309 (0.7%)
1	G	0.86	0/1553	1.46	15/2100 (0.7%)
1	H	0.87	0/1478	1.45	9/1996 (0.5%)
1	I	0.79	0/1595	1.47	12/2157 (0.6%)
1	J	0.79	0/1481	1.44	6/1999 (0.3%)
1	K	0.88	0/1663	1.45	5/2251 (0.2%)
1	L	0.85	0/1663	1.49	14/2251 (0.6%)
1	M	0.86	0/1630	1.50	18/2204 (0.8%)
1	N	0.84	0/1464	1.48	10/1977 (0.5%)
1	O	0.92	0/1655	1.45	10/2240 (0.4%)
1	P	0.86	0/1630	1.55	20/2207 (0.9%)
All	All	0.86	0/25747	1.47	216/34826 (0.6%)

There are no bond length outliers.

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	61	PHE	CA-CB-CG	9.11	122.91	113.80
1	M	165	THR	CB-CA-C	9.06	124.64	110.14
1	F	165	THR	CB-CA-C	8.88	124.02	110.62
1	A	165	THR	CB-CA-C	8.52	123.77	110.14
1	H	61	PHE	CA-CB-CG	8.13	121.93	113.80

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	23	0
1	C	1667	0	1652	20	0
1	D	1642	0	1627	26	0
1	E	1668	0	1657	19	0
1	F	1666	0	1652	28	0
1	G	1519	0	1519	21	0
1	H	1446	0	1448	13	0
1	I	1558	0	1546	23	0
1	J	1449	0	1456	16	0
1	K	1624	0	1610	14	0
1	L	1624	0	1610	23	0
1	M	1592	0	1584	31	1
1	N	1432	0	1437	24	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	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	2	0
4	D	4	0	6	1	0
4	E	4	0	6	1	0
4	F	4	0	6	0	0
4	G	4	0	6	0	0
4	H	4	0	6	1	0
4	I	4	0	6	2	0
4	K	4	0	6	2	0
4	M	4	0	6	4	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	305	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 305 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:M:85:GLN:HG3	4:M:302:DMS:H23	1.61	0.83
1:C:155:ARG:HA	1:C:158:LEU:HD22	1.64	0.79
1:C:101:HIS:H	1:C:130:GLN:NE2	1.83	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	11	25
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%)	24	46
1	J	173/227 (76%)	170 (98%)	3 (2%)	0	100	100
1	K	197/227 (87%)	191 (97%)	5 (2%)	1 (0%)	24	46
1	L	197/227 (87%)	190 (96%)	7 (4%)	0	100	100
1	M	191/227 (84%)	186 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	171/227 (75%)	166 (97%)	4 (2%)	1 (1%)	21	42
1	O	196/227 (86%)	190 (97%)	4 (2%)	2 (1%)	12	28
1	P	193/227 (85%)	186 (96%)	7 (4%)	0	100	100
All	All	3040/3632 (84%)	2939 (97%)	94 (3%)	7 (0%)	43	66

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 ⓘ

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%)	149 (90%)	16 (10%)	8	17
1	B	162/199 (81%)	141 (87%)	21 (13%)	4	8
1	C	179/199 (90%)	154 (86%)	25 (14%)	3	6
1	D	176/199 (88%)	159 (90%)	17 (10%)	8	17
1	E	179/199 (90%)	157 (88%)	22 (12%)	4	9
1	F	179/199 (90%)	159 (89%)	20 (11%)	6	12
1	G	162/199 (81%)	147 (91%)	15 (9%)	8	18
1	H	153/199 (77%)	134 (88%)	19 (12%)	4	9
1	I	166/199 (83%)	146 (88%)	20 (12%)	5	10
1	J	153/199 (77%)	133 (87%)	20 (13%)	4	8
1	K	174/199 (87%)	155 (89%)	19 (11%)	6	13
1	L	174/199 (87%)	153 (88%)	21 (12%)	5	10
1	M	170/199 (85%)	143 (84%)	27 (16%)	2	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	151/199 (76%)	140 (93%)	11 (7%)	13	29
1	O	173/199 (87%)	152 (88%)	21 (12%)	5	10
1	P	171/199 (86%)	145 (85%)	26 (15%)	3	5
All	All	2687/3184 (84%)	2367 (88%)	320 (12%)	5	10

5 of 320 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	169	SER
1	O	151	LYS
1	M	29	VAL
1	M	200	GLU
1	P	39	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	130	GLN
1	M	31	ASN
1	K	17	ASN
1	L	85	GLN
1	M	130	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
2	FAD	F	301	-	58,58,58	1.88	16 (27%)	85,89,89	1.79	28 (32%)
3	0VJ	O	301	-	24,24,24	5.12	16 (66%)	33,34,34	4.74	17 (51%)
3	0VJ	I	304	-	24,24,24	4.74	16 (66%)	33,34,34	4.80	15 (45%)
3	0VJ	J	302	-	24,24,24	5.33	18 (75%)	33,34,34	4.59	13 (39%)
4	DMS	G	302	-	3,3,3	1.10	0	3,3,3	0.85	0
2	FAD	M	301	-	58,58,58	1.69	13 (22%)	85,89,89	1.46	16 (18%)
2	FAD	C	301	-	58,58,58	1.53	10 (17%)	85,89,89	1.55	18 (21%)
2	FAD	I	301	-	58,58,58	1.70	13 (22%)	85,89,89	1.46	16 (18%)
4	DMS	M	302	-	3,3,3	0.74	0	3,3,3	0.48	0
3	0VJ	P	302	-	24,24,24	4.87	18 (75%)	33,34,34	3.83	12 (36%)
3	0VJ	H	301	-	24,24,24	4.88	18 (75%)	33,34,34	3.72	15 (45%)
3	0VJ	D	301	-	24,24,24	4.87	17 (70%)	33,34,34	4.61	14 (42%)
2	FAD	J	301	-	58,58,58	1.80	15 (25%)	85,89,89	1.73	20 (23%)
2	FAD	A	302	-	58,58,58	1.69	13 (22%)	85,89,89	1.46	16 (18%)
4	DMS	P	303	-	3,3,3	0.91	0	3,3,3	0.55	0
3	0VJ	E	302	-	24,24,24	5.13	19 (79%)	33,34,34	3.67	15 (45%)
4	DMS	B	302	-	3,3,3	0.98	0	3,3,3	1.33	1 (33%)
4	DMS	C	302	-	3,3,3	0.81	0	3,3,3	1.00	0
4	DMS	I	303	-	3,3,3	0.88	0	3,3,3	0.81	0
2	FAD	K	302	-	58,58,58	1.35	12 (20%)	85,89,89	1.27	10 (11%)
4	DMS	K	303	-	3,3,3	0.82	0	3,3,3	0.91	0
3	0VJ	B	303	-	24,24,24	5.44	16 (66%)	33,34,34	4.76	22 (66%)
4	DMS	A	304	-	3,3,3	1.07	0	3,3,3	1.08	0
2	FAD	N	301	-	58,58,58	1.55	14 (24%)	85,89,89	1.70	20 (23%)
4	DMS	F	303	-	3,3,3	0.80	0	3,3,3	0.97	0
4	DMS	O	303	-	3,3,3	0.71	0	3,3,3	0.18	0
2	FAD	H	302	-	58,58,58	1.36	8 (13%)	85,89,89	1.34	12 (14%)
2	FAD	F	302	-	58,58,58	1.70	14 (24%)	85,89,89	1.46	16 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	E	303	-	3,3,3	0.69	0	3,3,3	1.38	0
4	DMS	H	303	-	3,3,3	1.10	0	3,3,3	0.94	0
3	0VJ	A	305	-	24,24,24	4.85	16 (66%)	33,34,34	4.88	17 (51%)
3	0VJ	A	303	-	24,24,24	4.58	17 (70%)	33,34,34	5.28	15 (45%)
2	FAD	O	302	-	58,58,58	1.32	8 (13%)	85,89,89	1.43	16 (18%)
2	FAD	I	302	-	58,58,58	1.70	13 (22%)	85,89,89	1.46	16 (18%)
3	0VJ	G	301	-	24,24,24	5.01	17 (70%)	33,34,34	4.38	12 (36%)
3	0VJ	L	301	-	24,24,24	5.27	18 (75%)	33,34,34	3.77	16 (48%)
3	0VJ	M	303	-	24,24,24	5.01	19 (79%)	33,34,34	4.63	15 (45%)
2	FAD	E	301	-	58,58,58	1.70	14 (24%)	85,89,89	1.46	16 (18%)
2	FAD	A	301	-	58,58,58	1.70	13 (22%)	85,89,89	1.46	16 (18%)
2	FAD	B	301	-	58,58,58	1.46	12 (20%)	85,89,89	1.55	19 (22%)
4	DMS	D	302	-	3,3,3	0.98	0	3,3,3	1.10	0
2	FAD	P	301	-	58,58,58	1.70	14 (24%)	85,89,89	1.46	15 (17%)
3	0VJ	F	304	-	24,24,24	4.79	16 (66%)	33,34,34	4.64	15 (45%)
3	0VJ	N	302	-	24,24,24	5.19	18 (75%)	33,34,34	4.83	14 (42%)
3	0VJ	K	301	-	24,24,24	5.12	18 (75%)	33,34,34	4.55	15 (45%)

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	FAD	F	301	-	-	7/34/50/50	0/6/6/6
3	0VJ	O	301	-	-	0/6/26/26	0/3/3/3
3	0VJ	I	304	-	-	0/6/26/26	0/3/3/3
3	0VJ	J	302	-	-	0/6/26/26	0/3/3/3
2	FAD	M	301	-	-	3/34/50/50	0/6/6/6
2	FAD	C	301	-	-	5/34/50/50	0/6/6/6
2	FAD	I	301	-	-	3/34/50/50	0/6/6/6
3	0VJ	P	302	-	-	0/6/26/26	0/3/3/3
3	0VJ	H	301	-	-	0/6/26/26	0/3/3/3
3	0VJ	D	301	-	-	2/6/26/26	0/3/3/3
2	FAD	J	301	-	-	10/34/50/50	0/6/6/6
2	FAD	A	302	-	-	3/34/50/50	0/6/6/6
3	0VJ	E	302	-	-	0/6/26/26	0/3/3/3
2	FAD	K	302	-	-	5/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	0VJ	B	303	-	-	2/6/26/26	0/3/3/3
2	FAD	N	301	-	-	7/34/50/50	0/6/6/6
2	FAD	H	302	-	-	6/34/50/50	0/6/6/6
2	FAD	F	302	-	-	3/34/50/50	0/6/6/6
3	0VJ	A	305	-	-	2/6/26/26	0/3/3/3
3	0VJ	A	303	-	-	0/6/26/26	0/3/3/3
2	FAD	O	302	-	-	9/34/50/50	0/6/6/6
2	FAD	I	302	-	-	3/34/50/50	0/6/6/6
3	0VJ	G	301	-	-	0/6/26/26	0/3/3/3
3	0VJ	L	301	-	-	0/6/26/26	0/3/3/3
3	0VJ	M	303	-	-	0/6/26/26	0/3/3/3
2	FAD	E	301	-	-	3/34/50/50	0/6/6/6
2	FAD	A	301	-	-	3/34/50/50	0/6/6/6
2	FAD	B	301	-	-	8/34/50/50	0/6/6/6
2	FAD	P	301	-	-	3/34/50/50	0/6/6/6
3	0VJ	F	304	-	-	0/6/26/26	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

The worst 5 of 479 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	301	0VJ	C02-C01	11.74	1.64	1.38
3	E	302	0VJ	C02-C01	11.64	1.63	1.38
3	L	301	0VJ	C02-C01	11.52	1.63	1.38
3	P	302	0VJ	C02-C01	11.38	1.63	1.38
3	J	302	0VJ	C02-C01	11.14	1.62	1.38

The worst 5 of 513 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	0VJ	C09-C08-C07	-16.79	116.39	123.17
3	N	302	0VJ	C09-C08-C07	-16.61	116.46	123.17
3	A	303	0VJ	C08-C09-C10	16.11	127.33	119.30
3	D	301	0VJ	C09-C08-C07	-15.75	116.81	123.17
3	A	305	0VJ	C09-C08-C07	-15.61	116.86	123.17

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

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

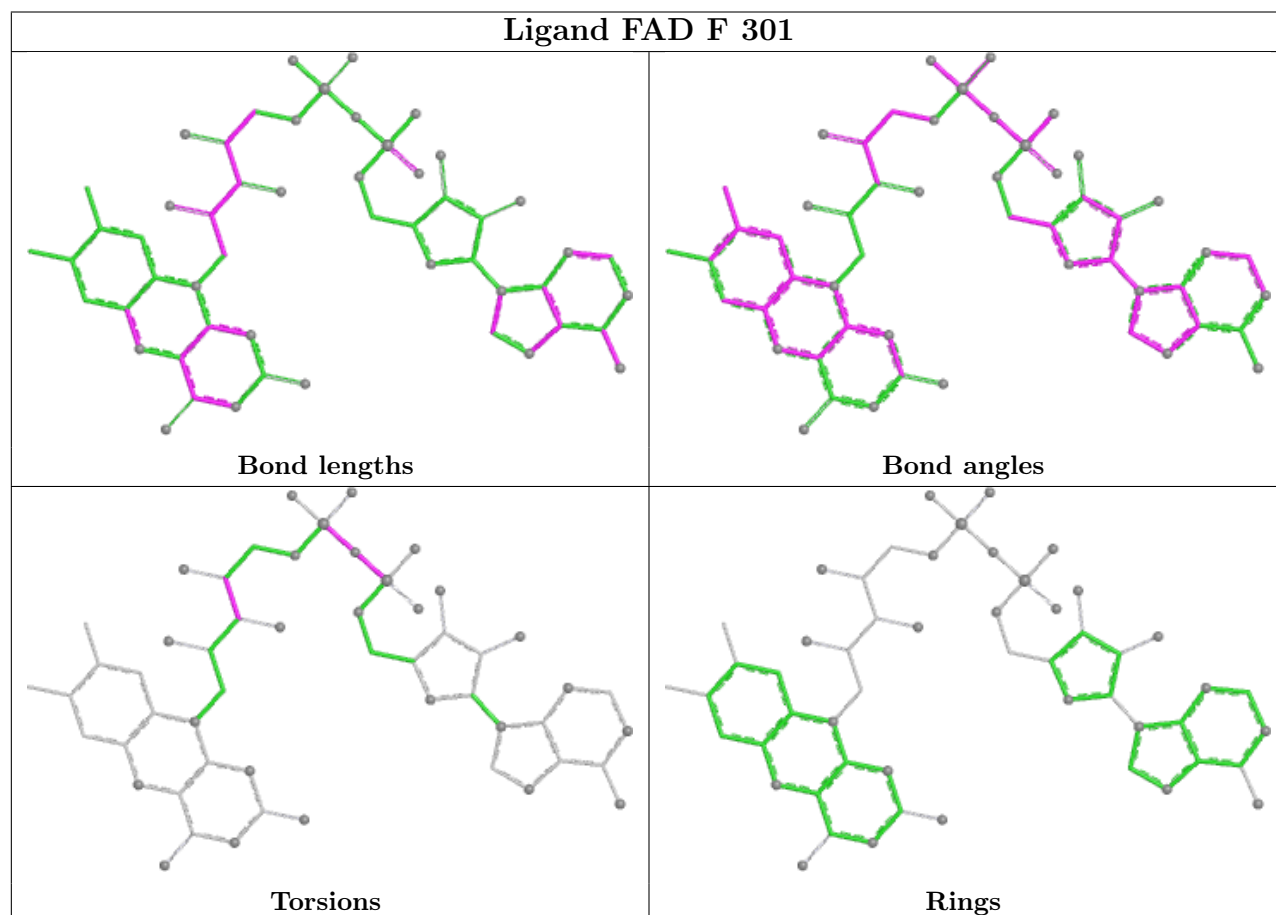
There are no ring outliers.

28 monomers are involved in 46 short contacts:

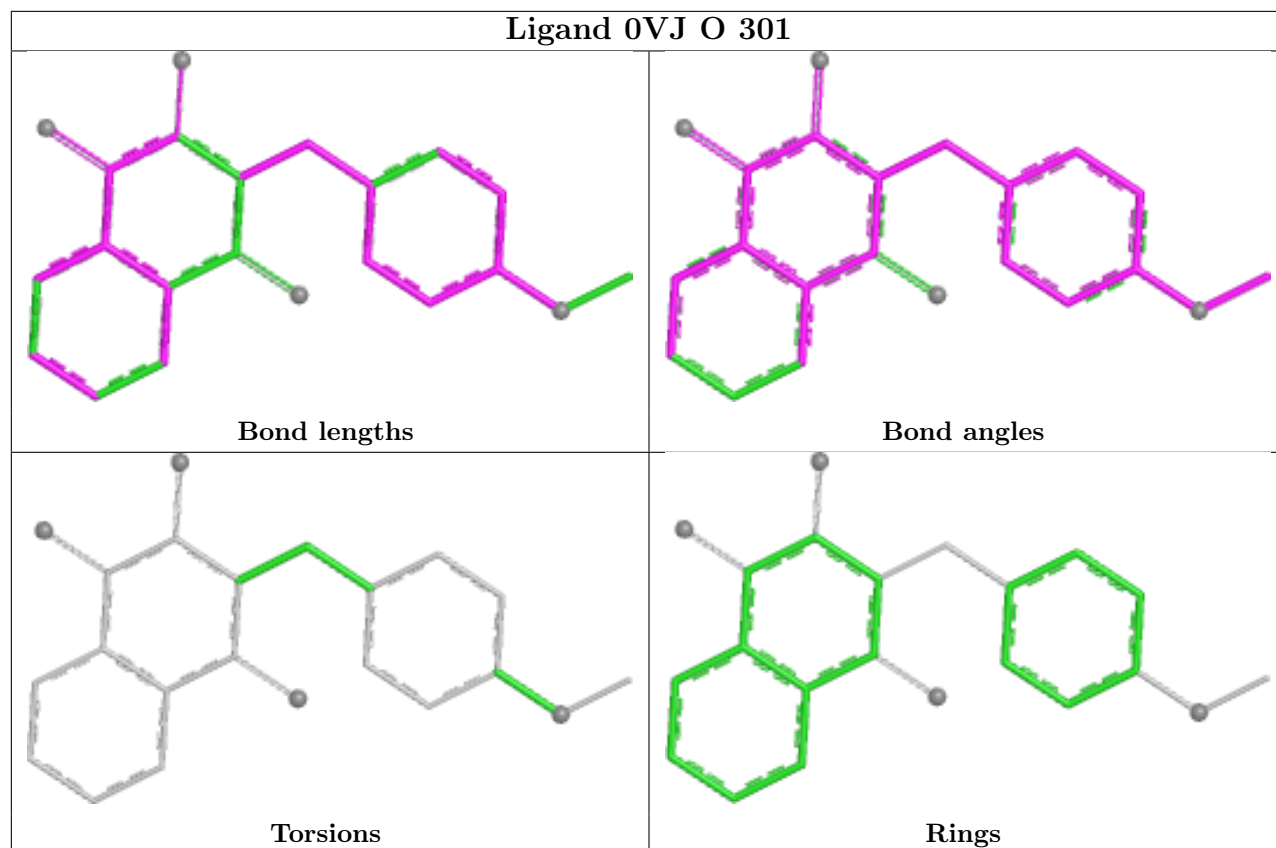
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	FAD	1	0
3	O	301	0VJ	3	0
3	I	304	0VJ	2	0
3	J	302	0VJ	1	0
2	M	301	FAD	1	0
2	C	301	FAD	1	0
2	I	301	FAD	1	0
4	M	302	DMS	4	0
3	P	302	0VJ	1	0
3	D	301	0VJ	1	0
2	J	301	FAD	3	0
4	C	302	DMS	2	0
4	I	303	DMS	2	0
4	K	303	DMS	2	0
3	B	303	0VJ	2	0
2	N	301	FAD	1	0
2	H	302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

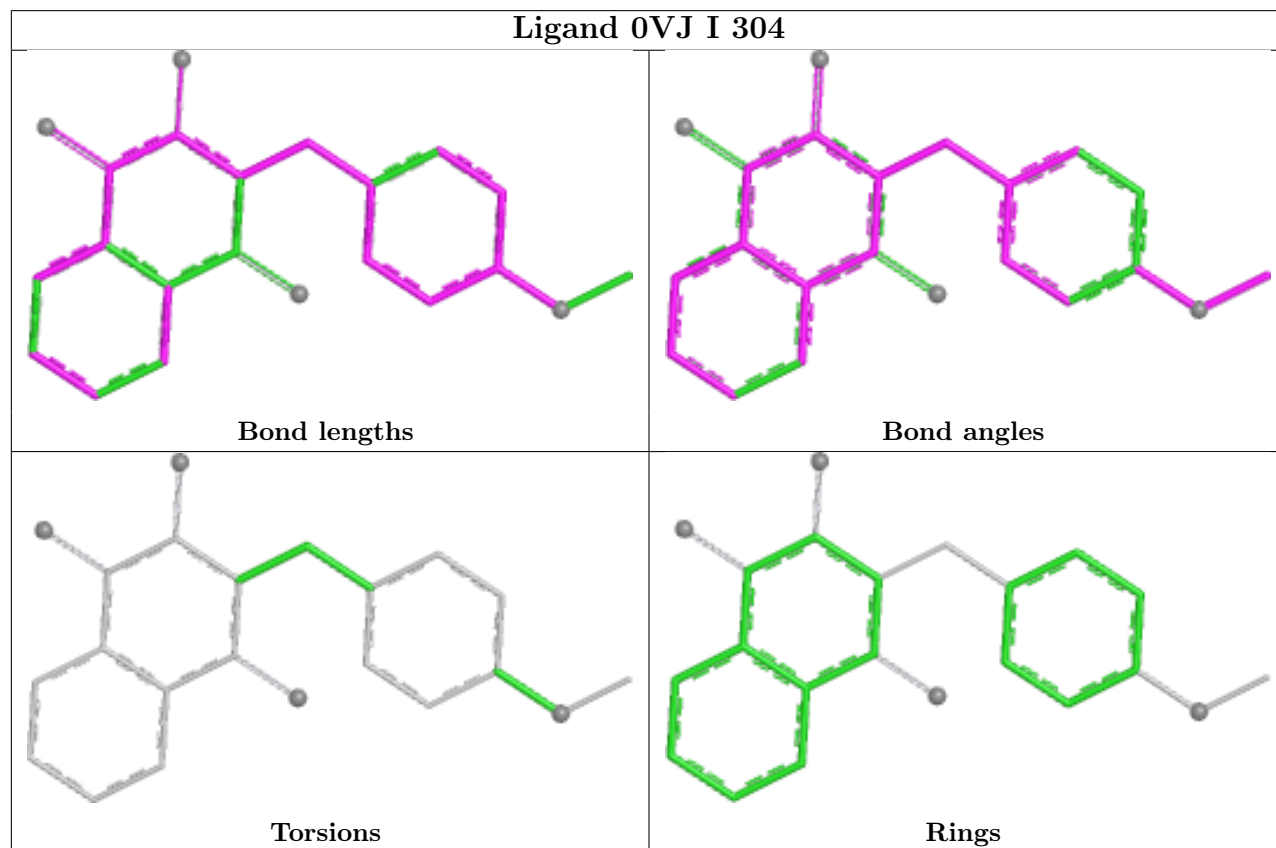
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



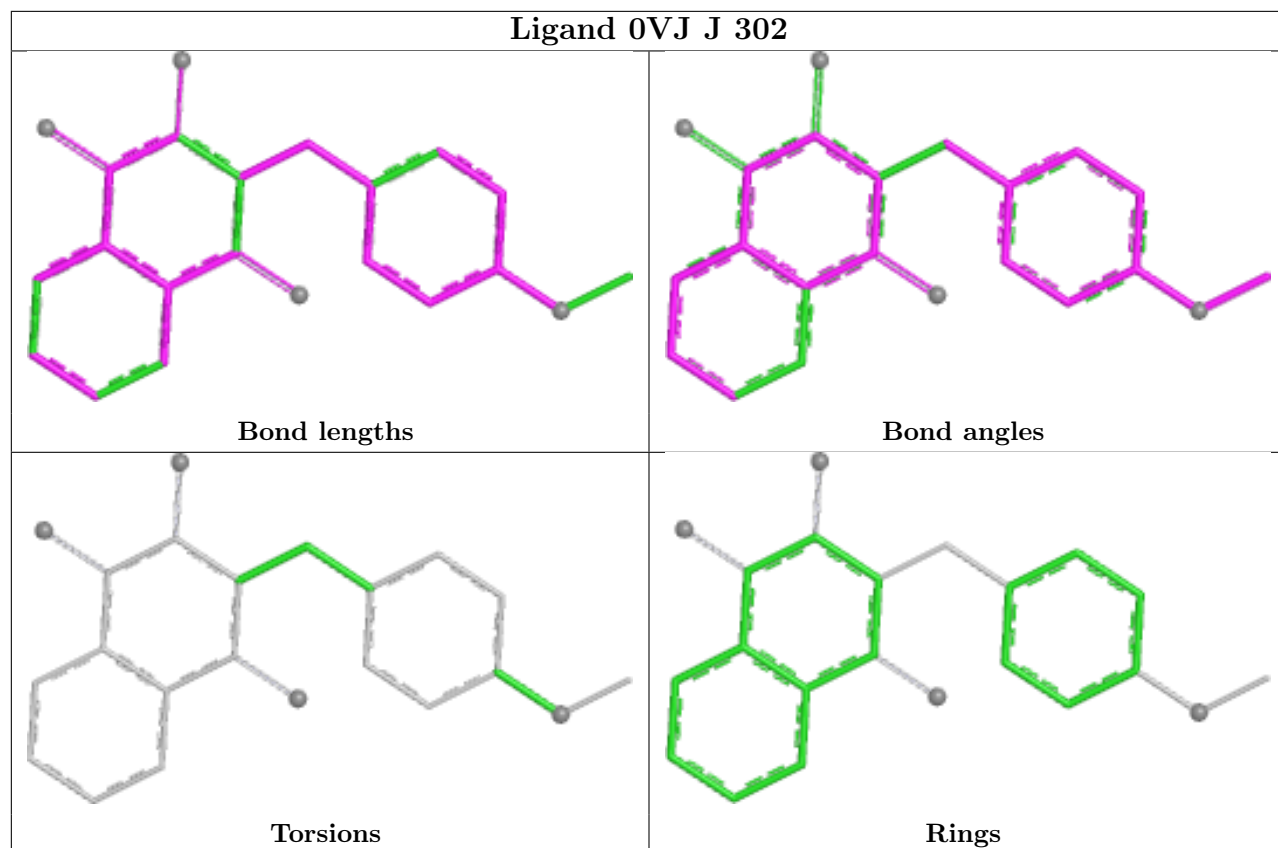
Ligand 0VJ O 301



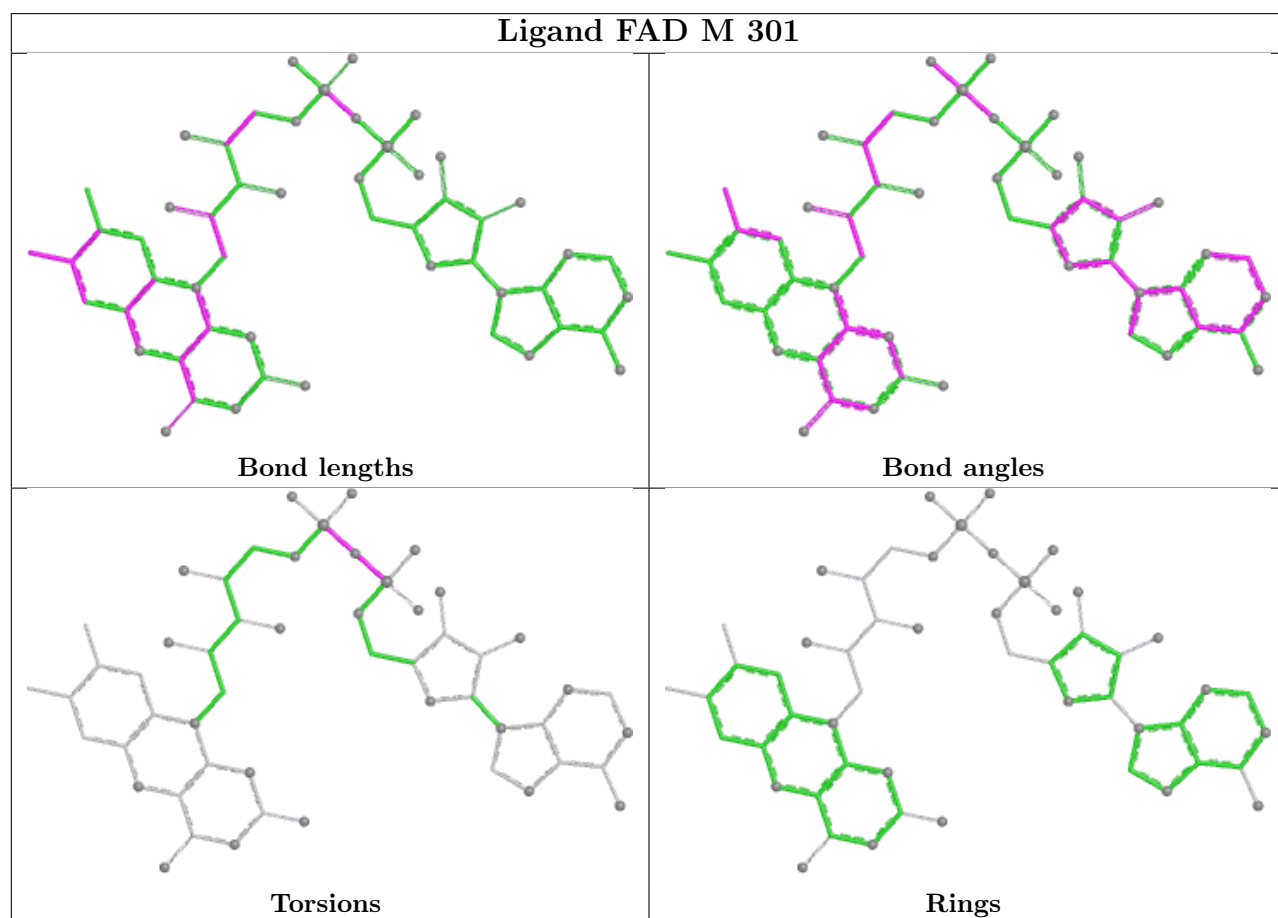
Ligand 0VJ I 304

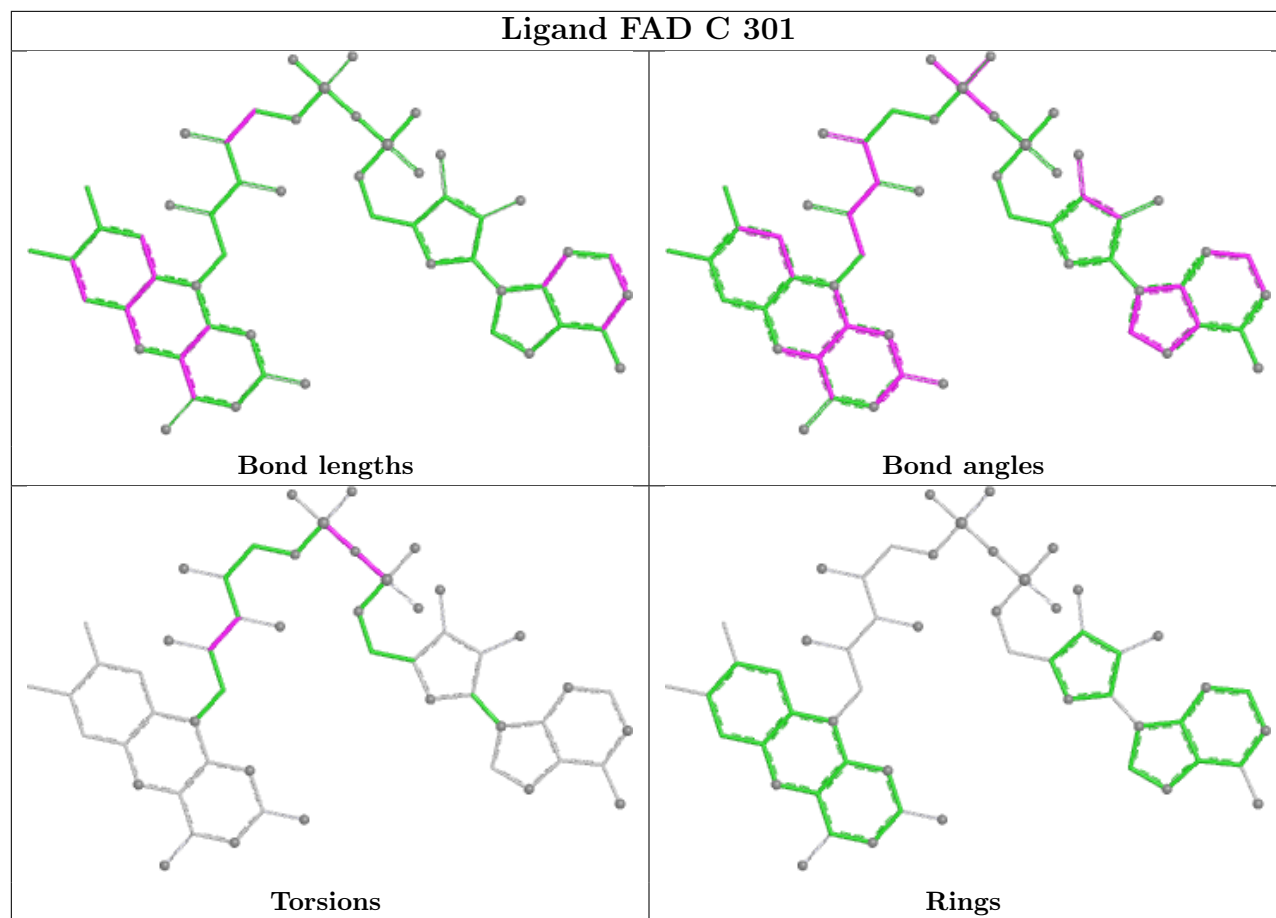


Ligand 0VJ J 302

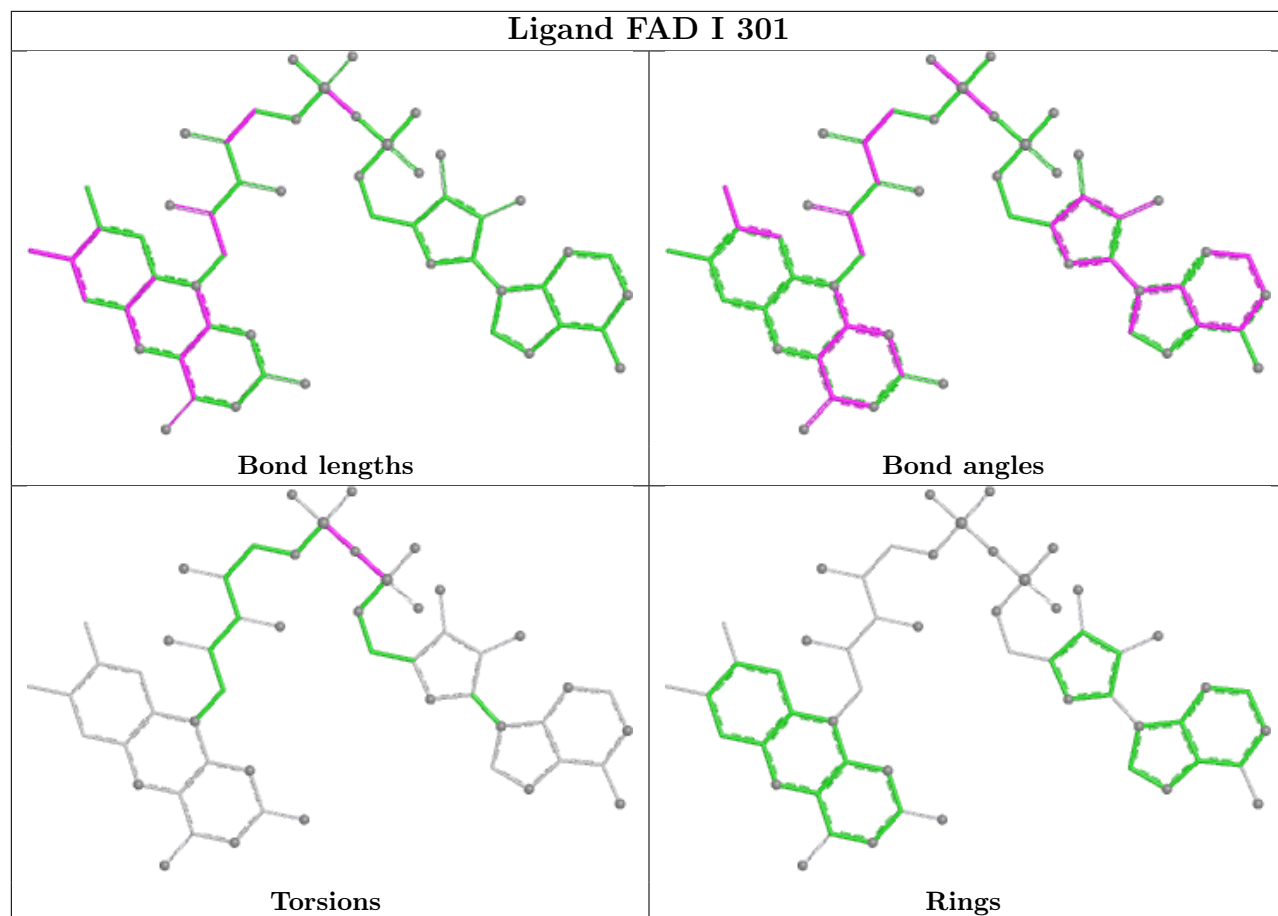


Ligand FAD M 301

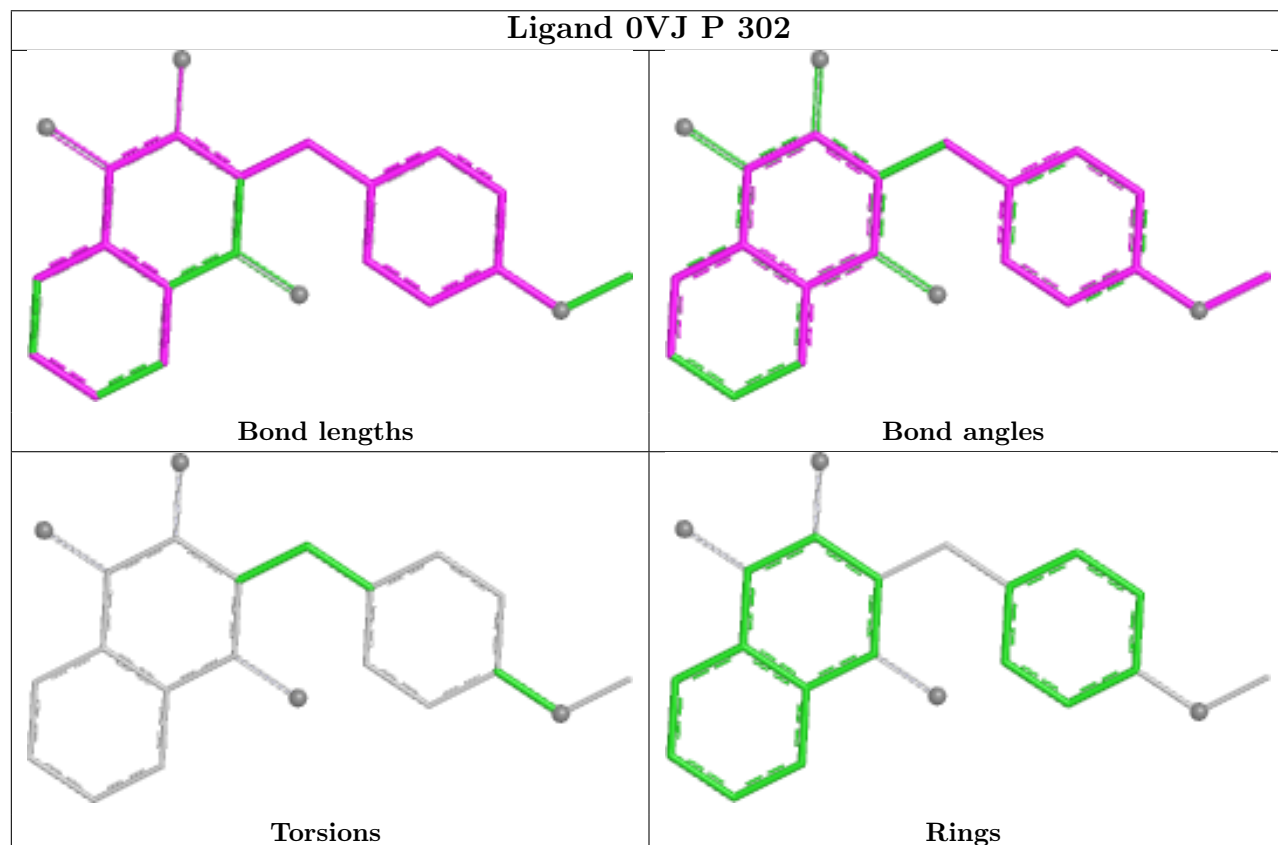




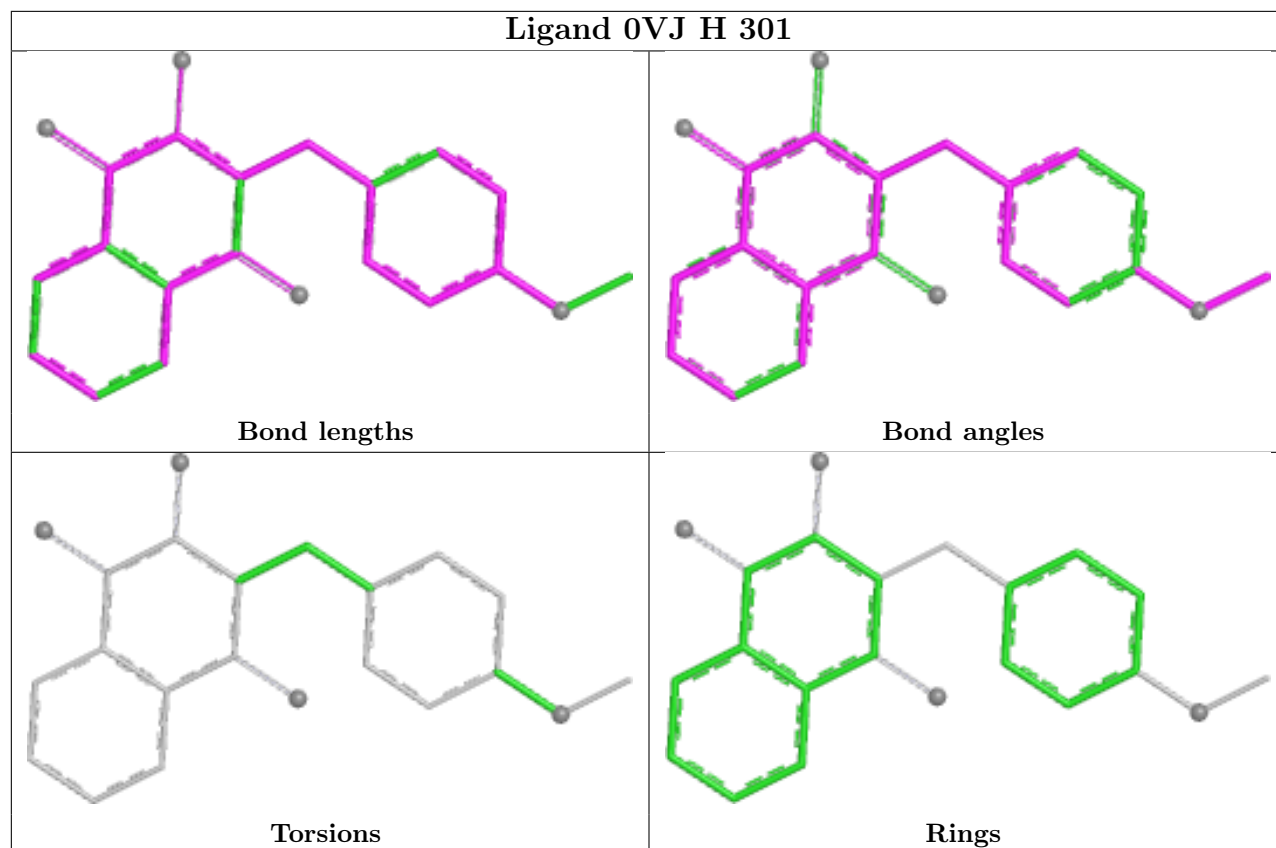
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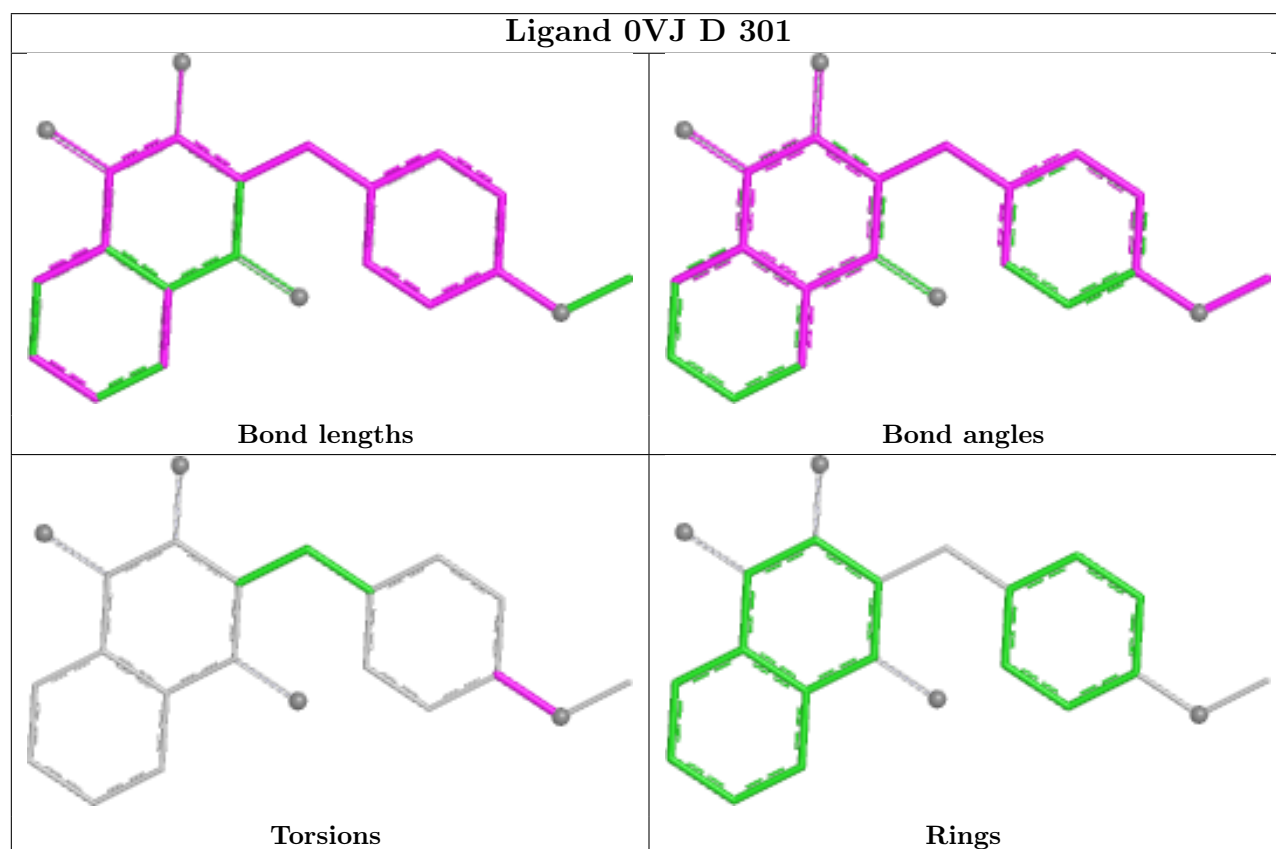
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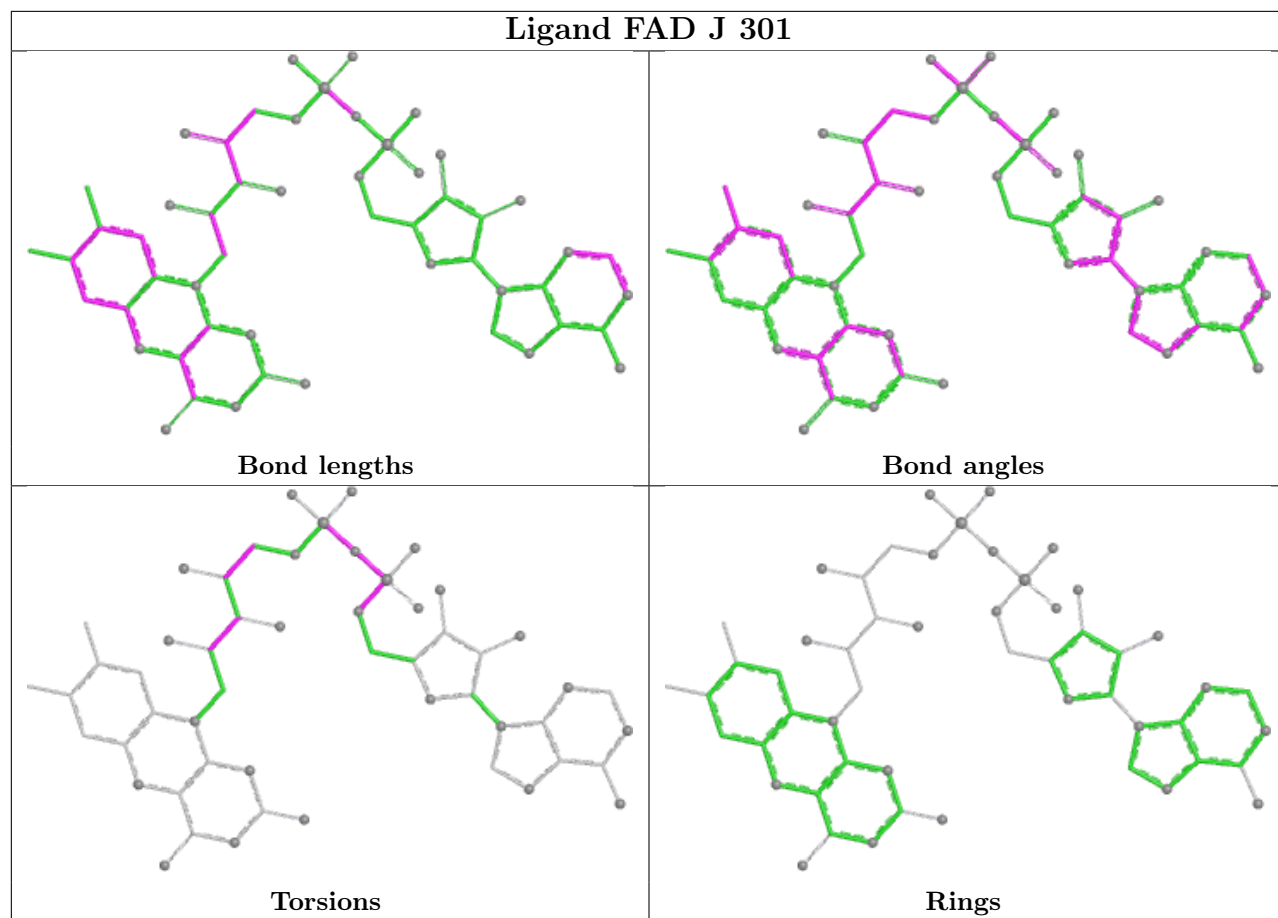
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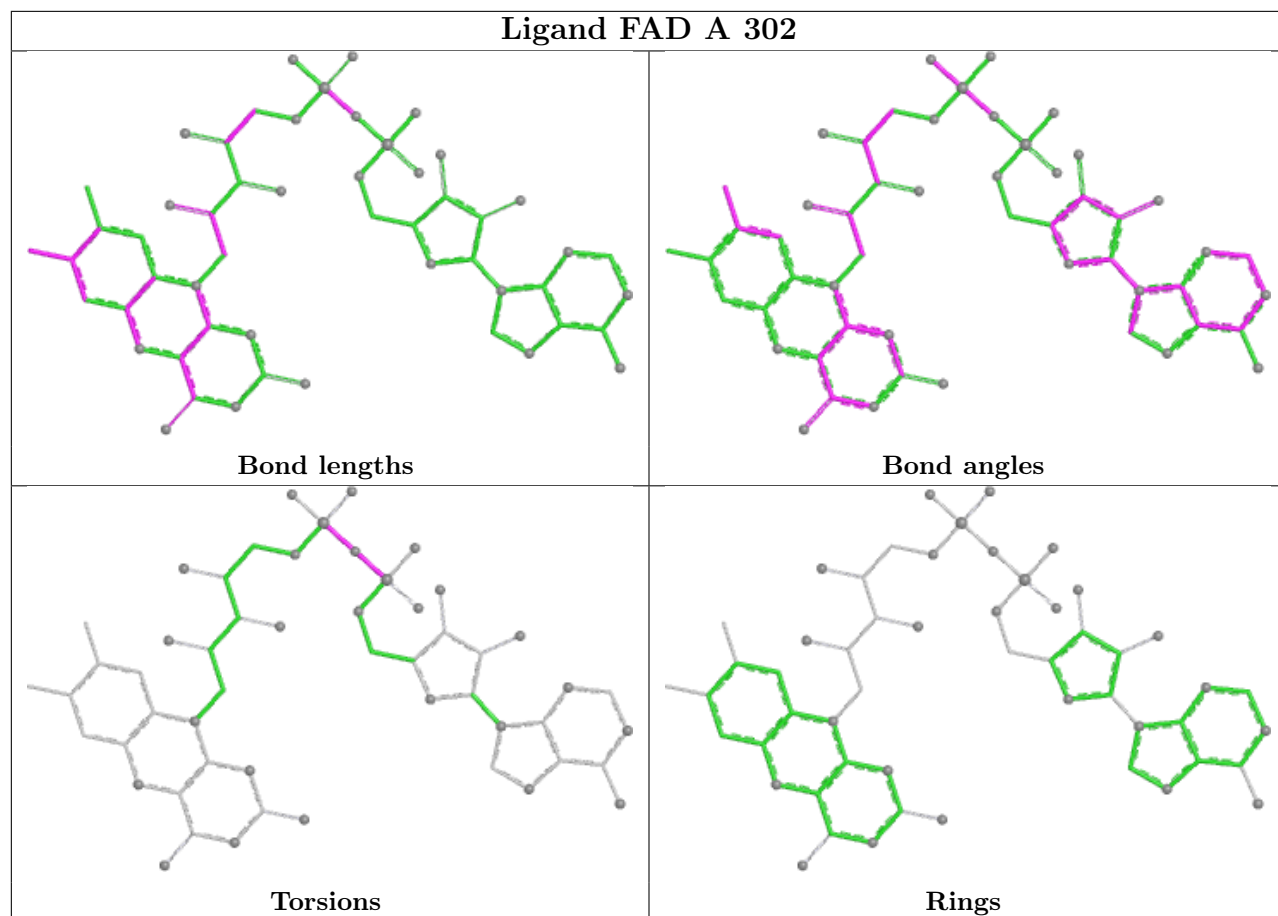
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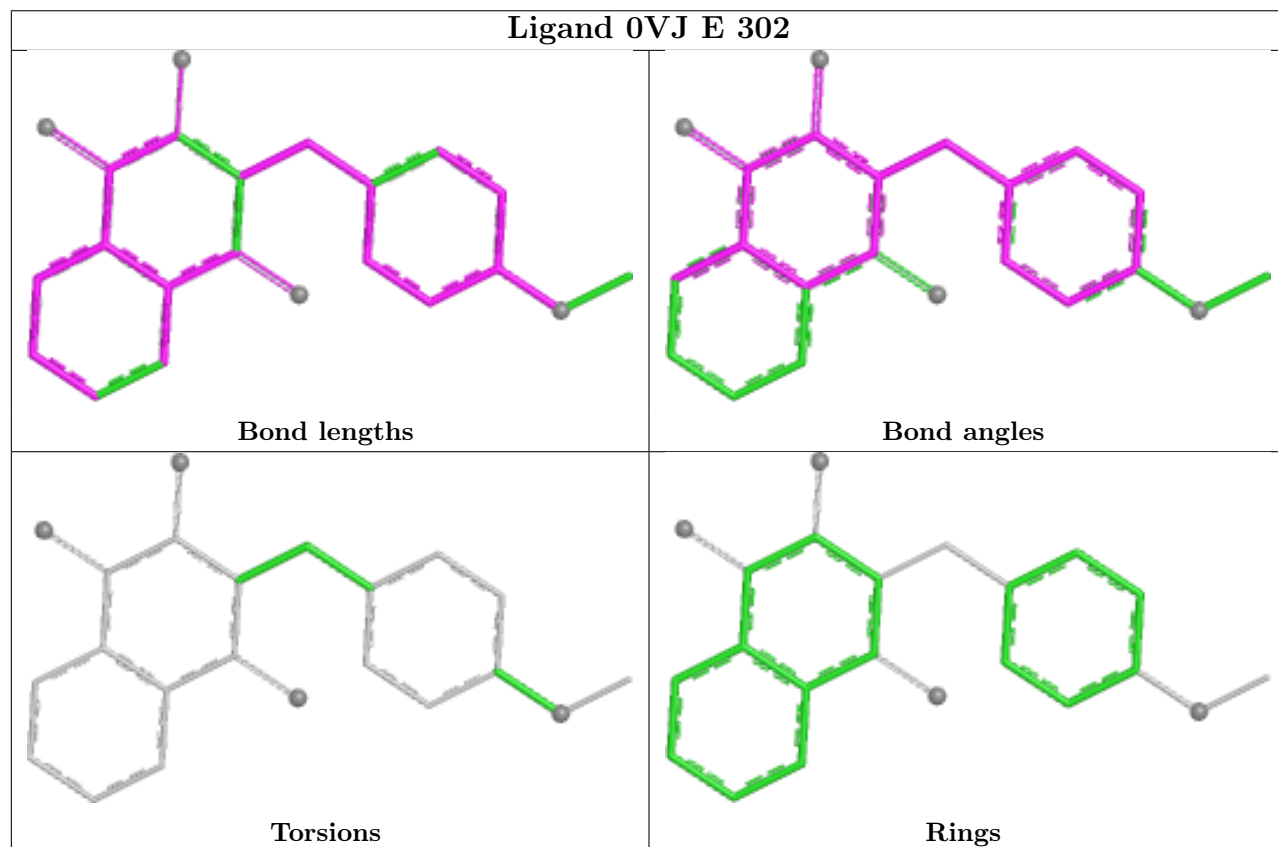
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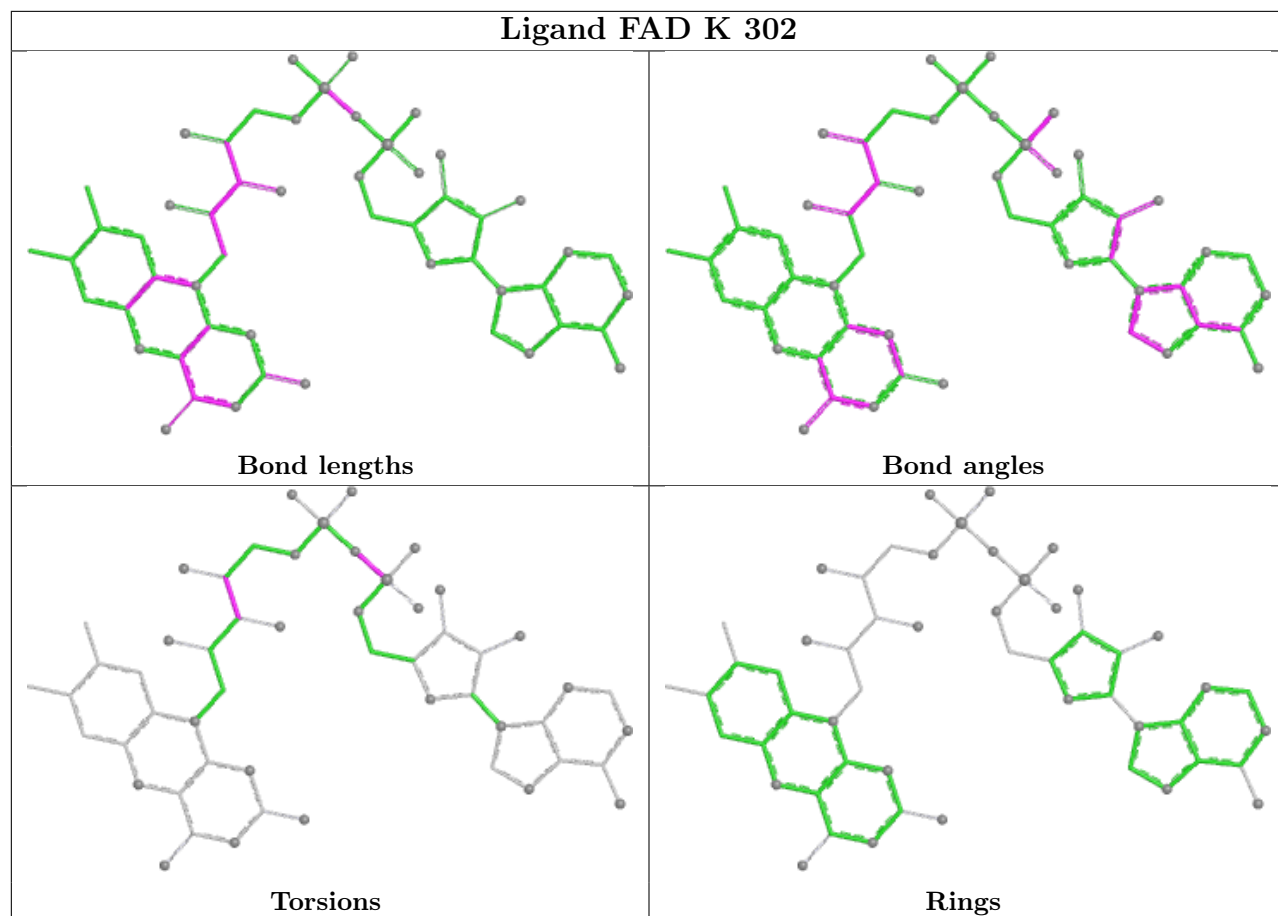
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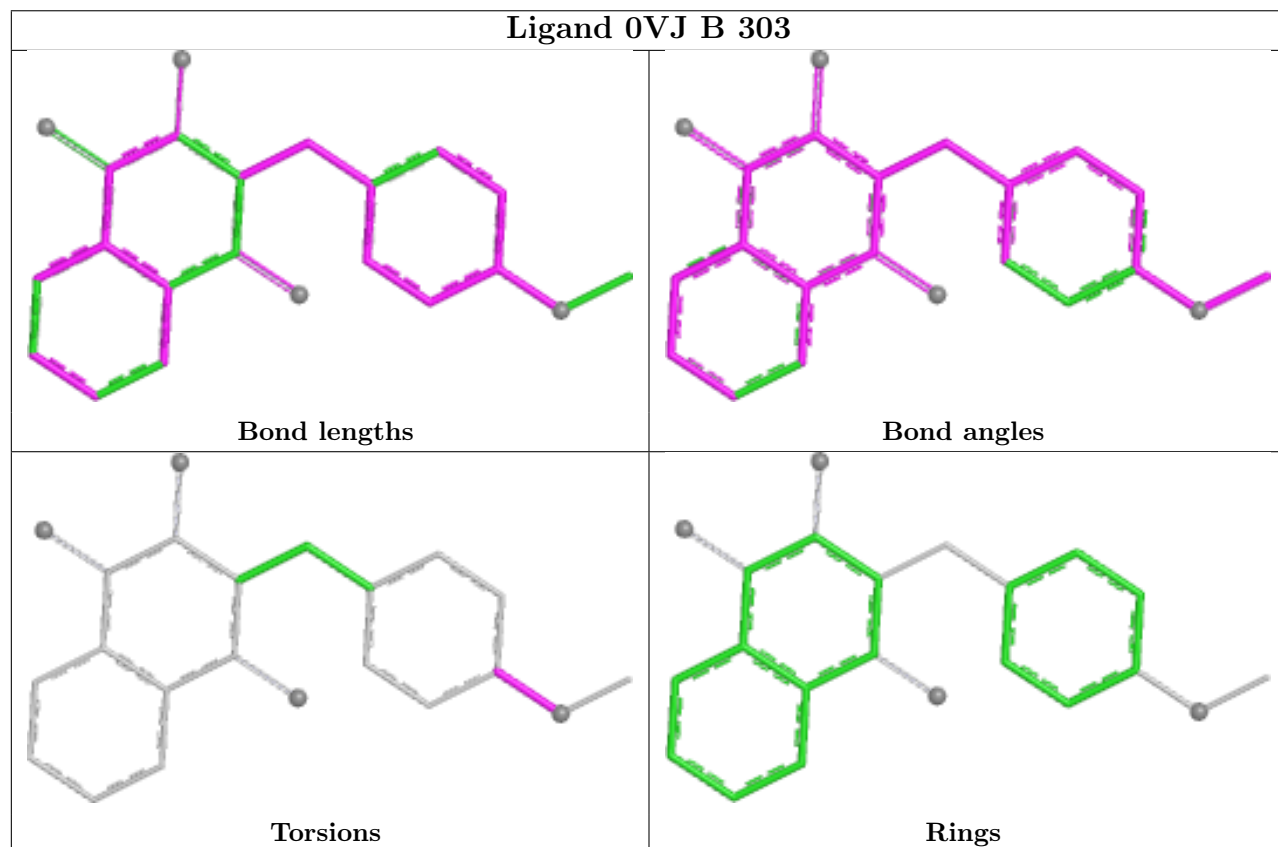
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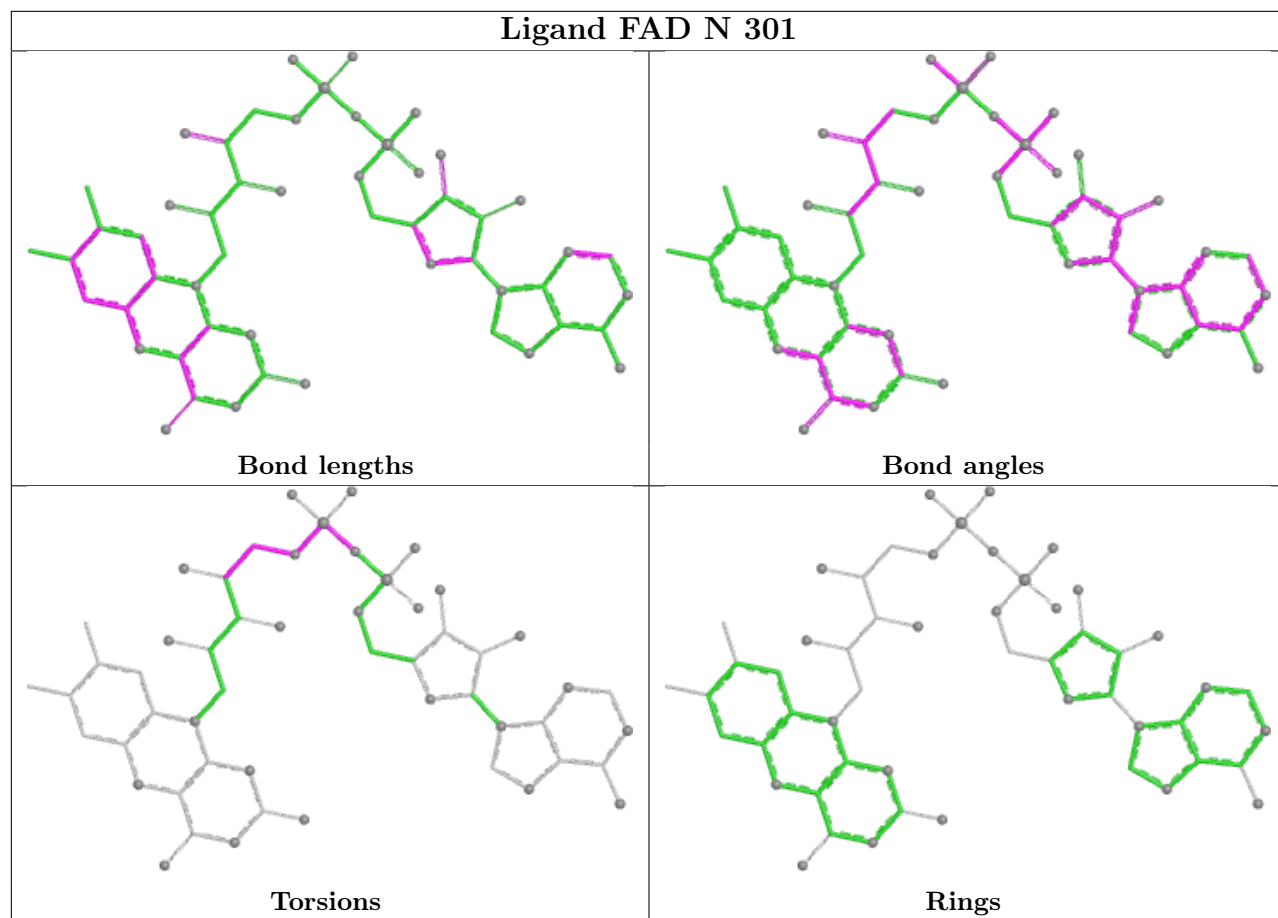


Ligand FAD K 302

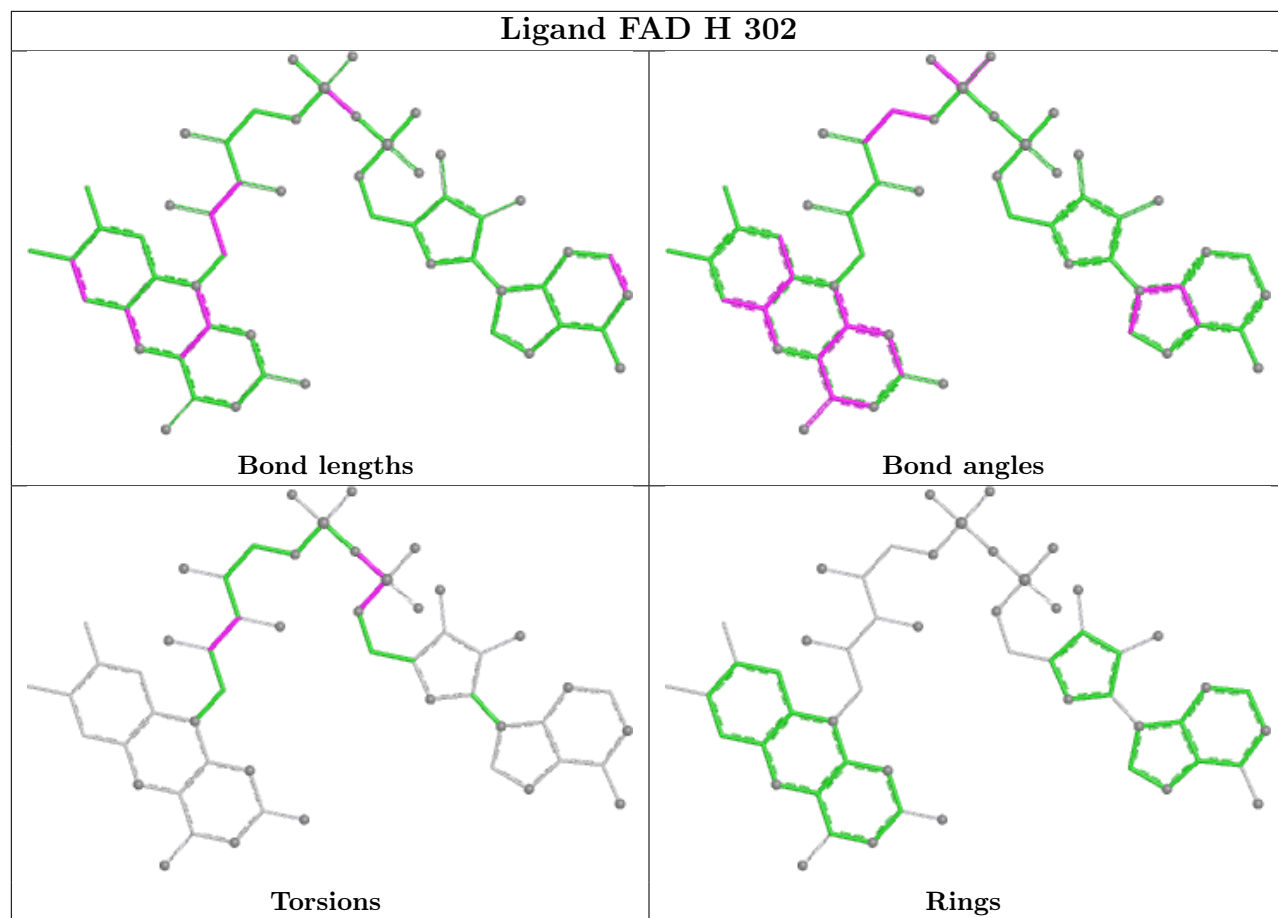


Ligand 0VJ B 303

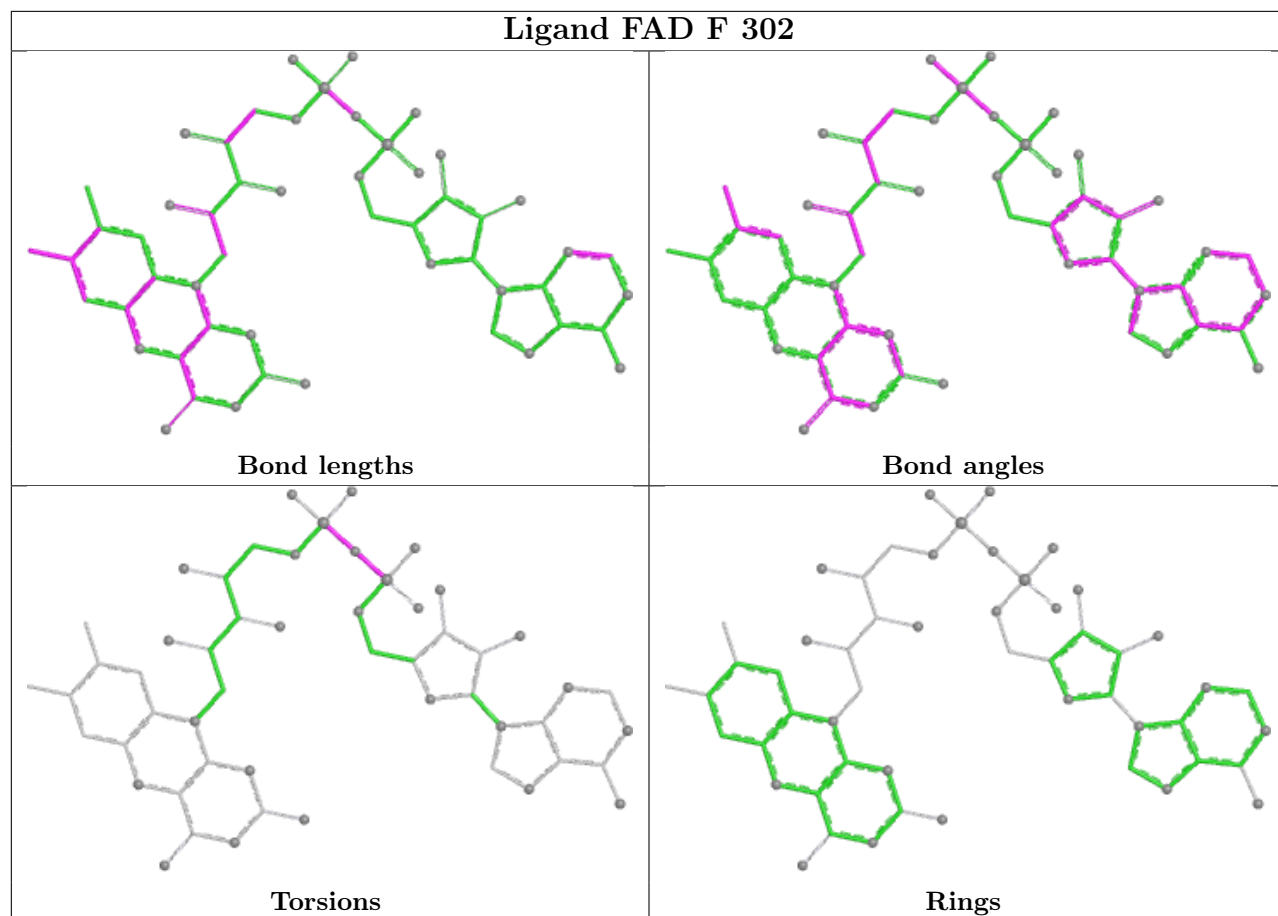




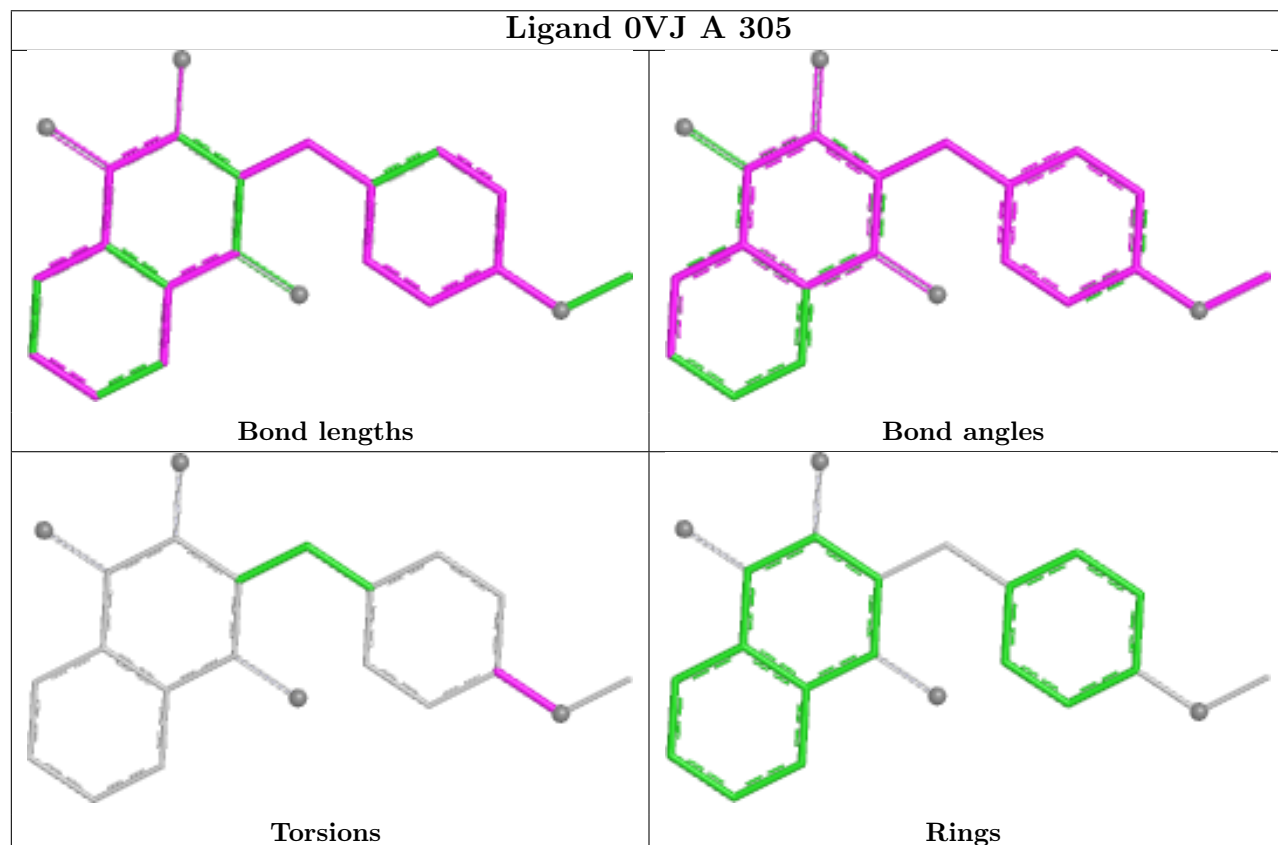
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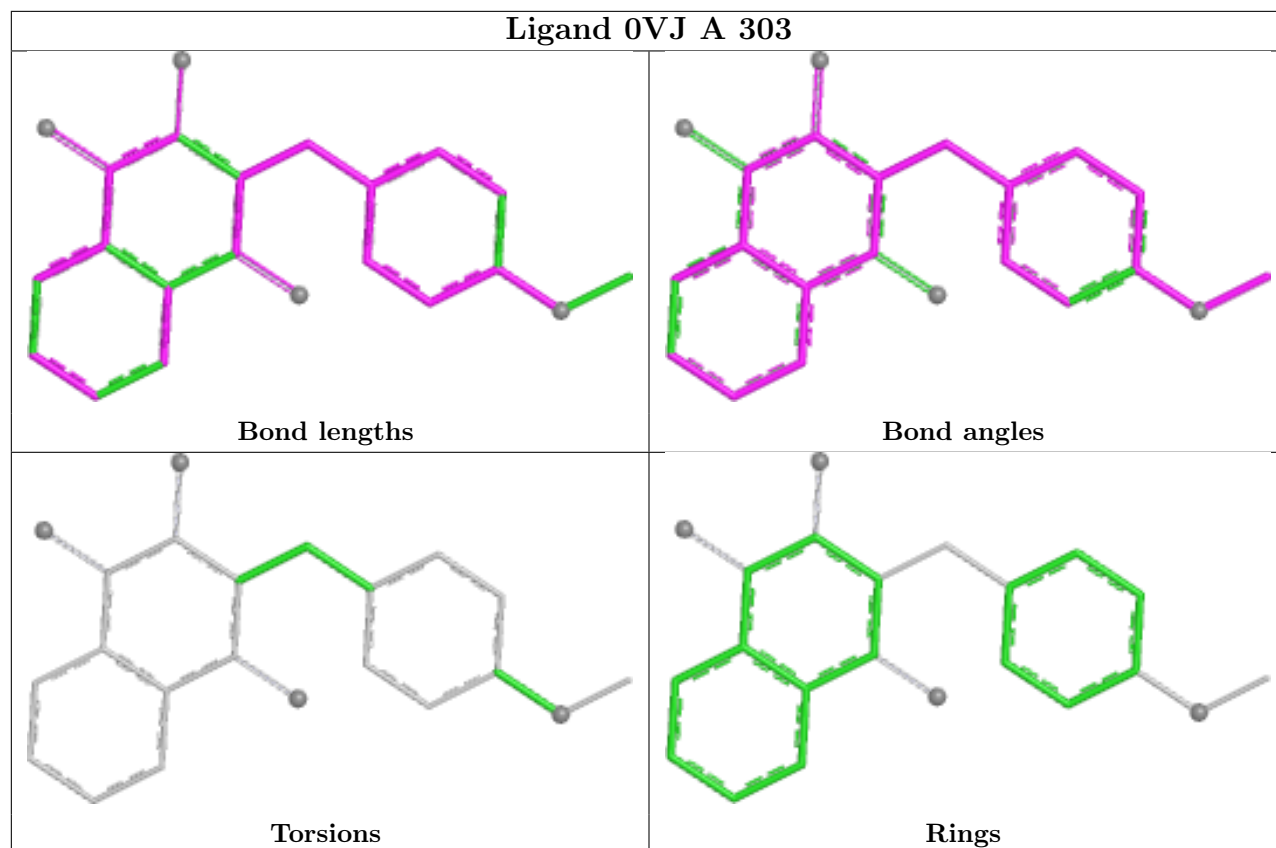
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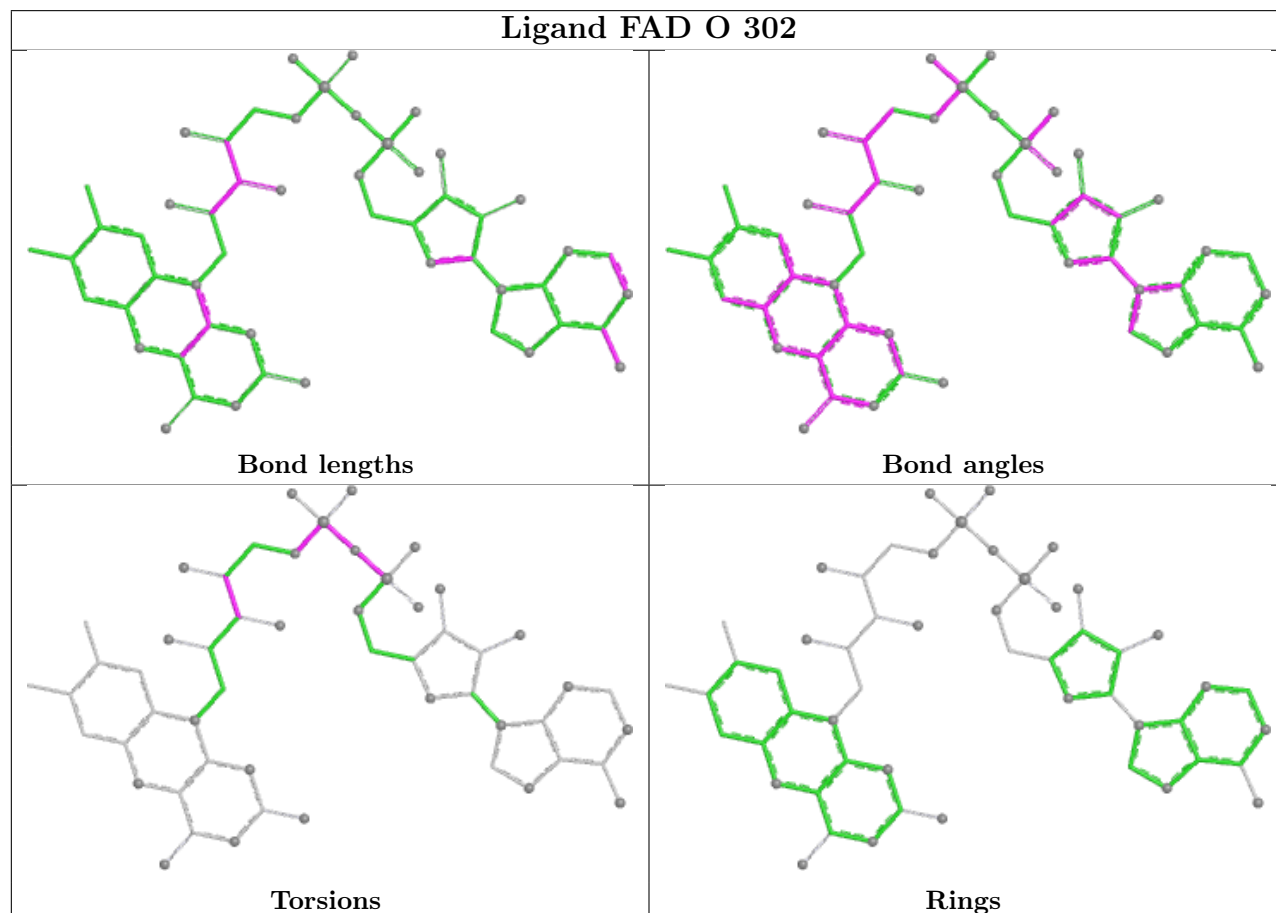
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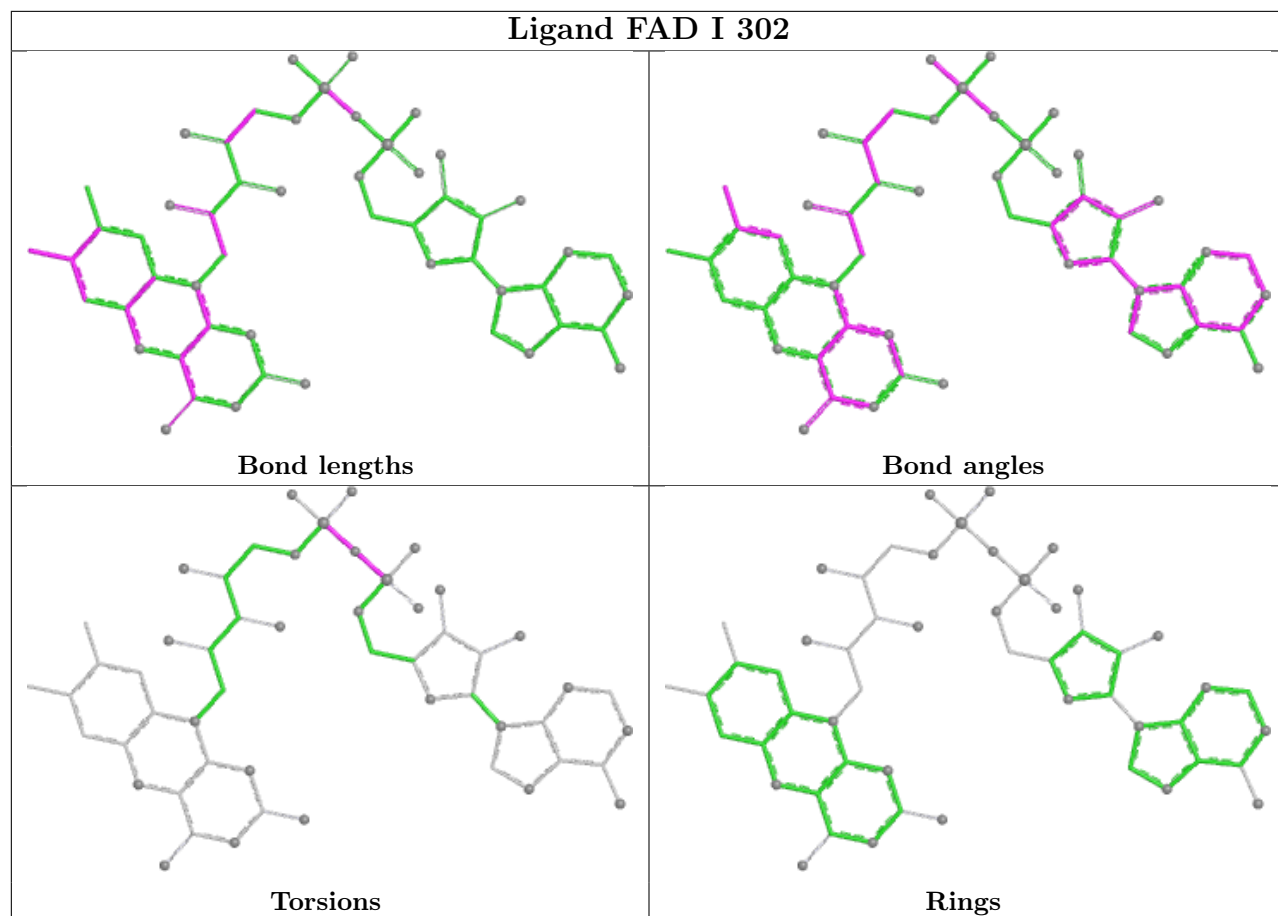
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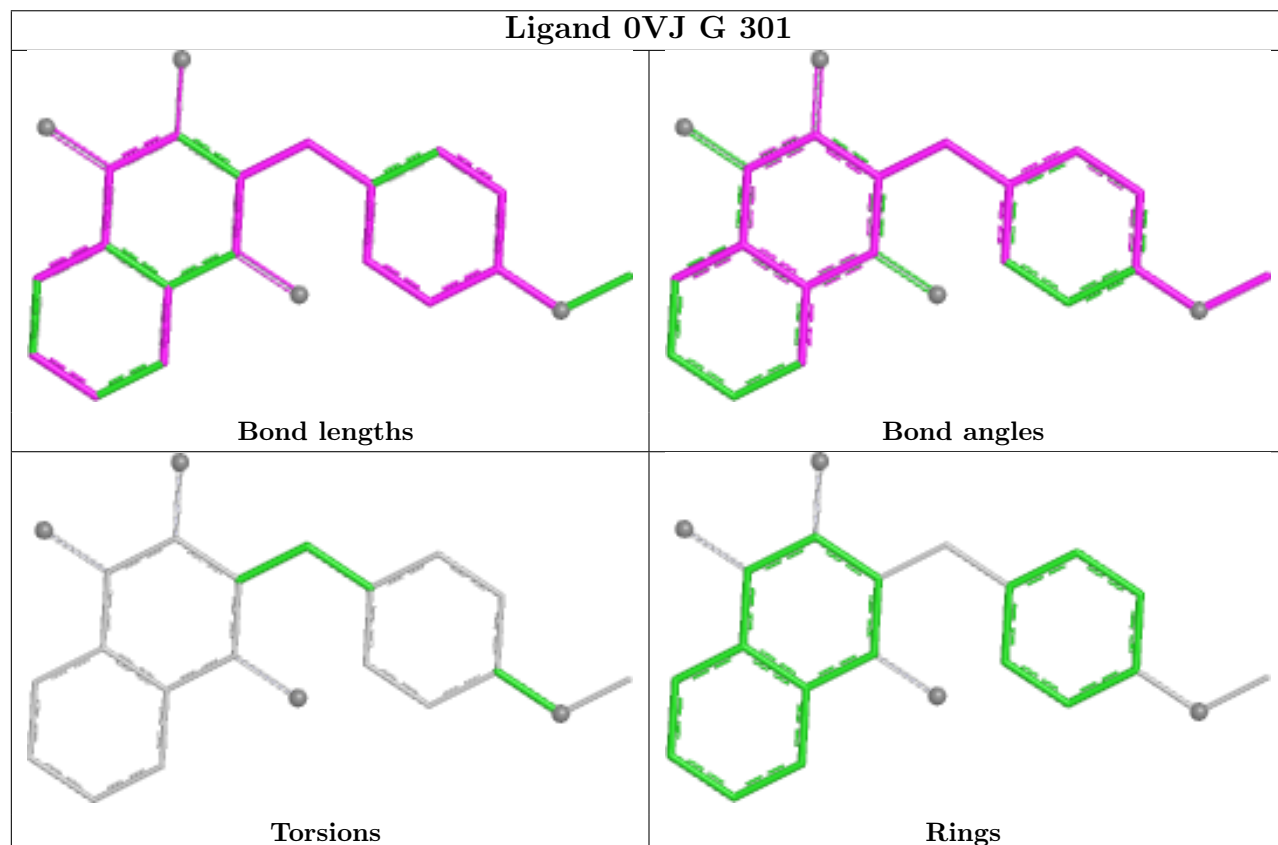
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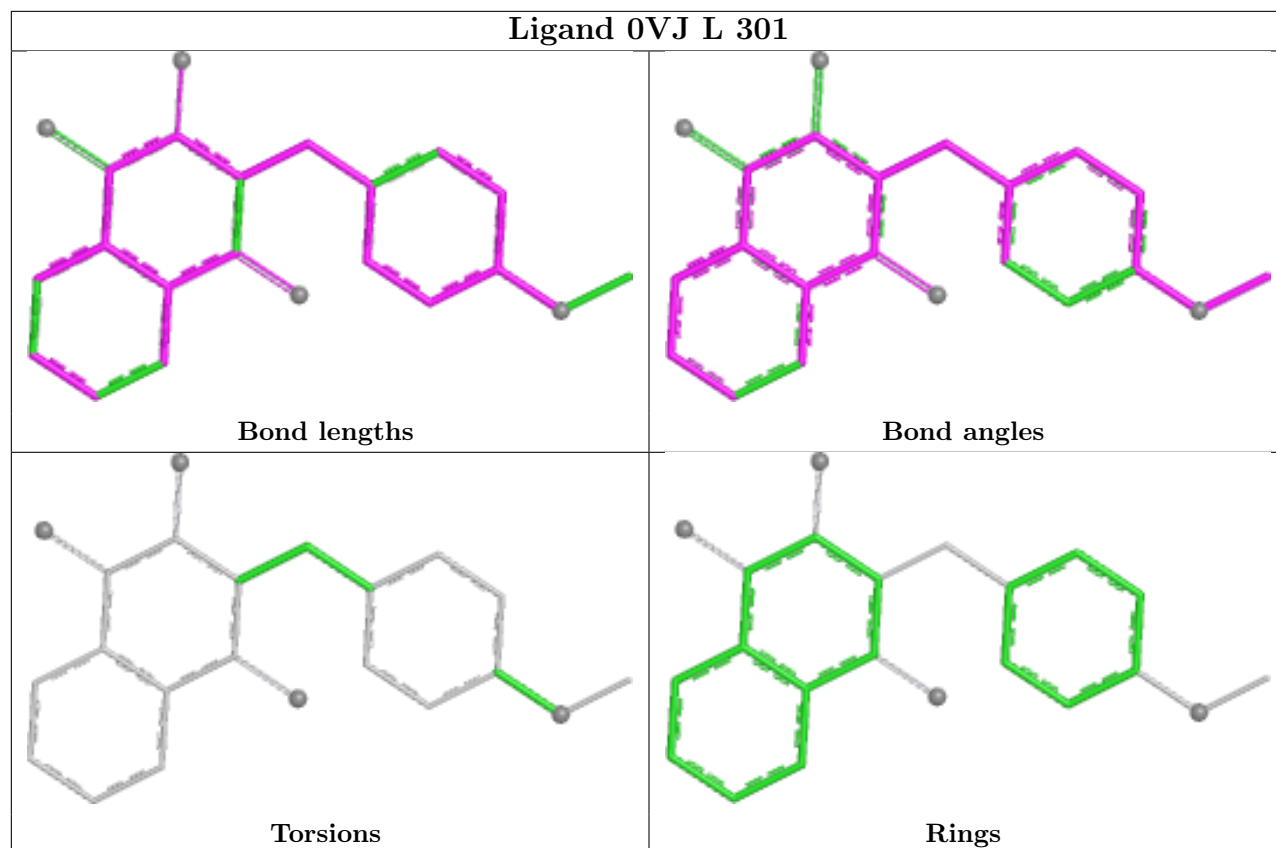
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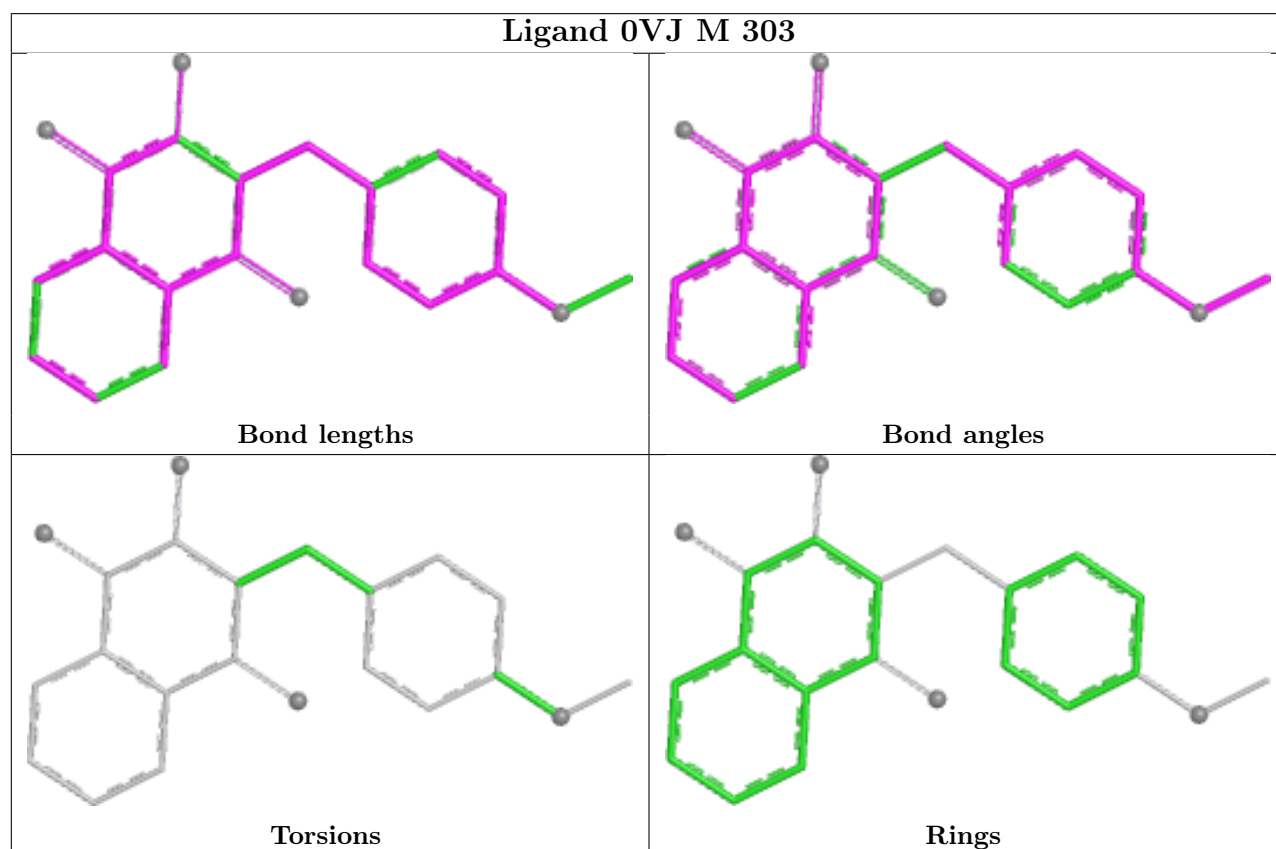
Ligand 0VJ G 301



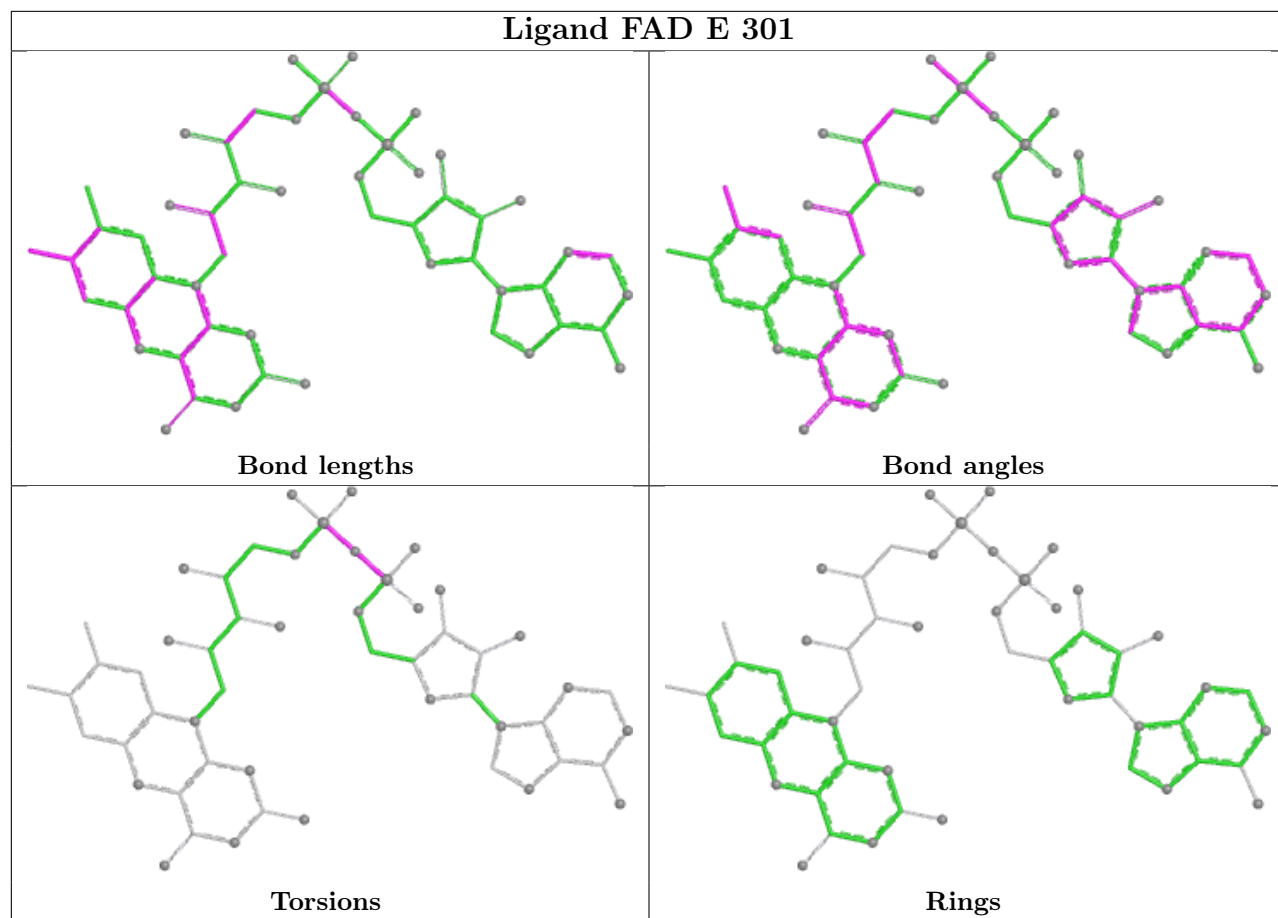
Ligand 0VJ L 301

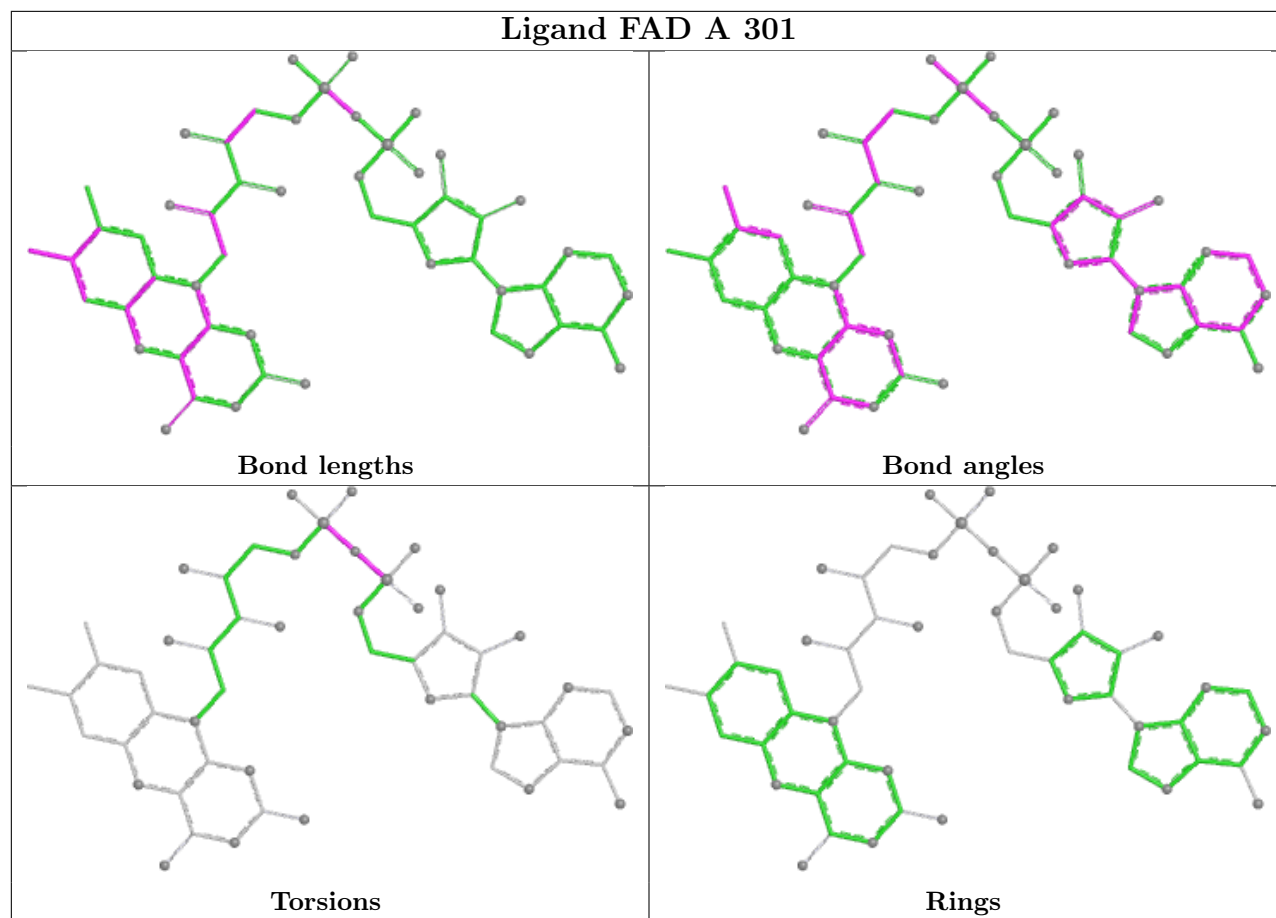


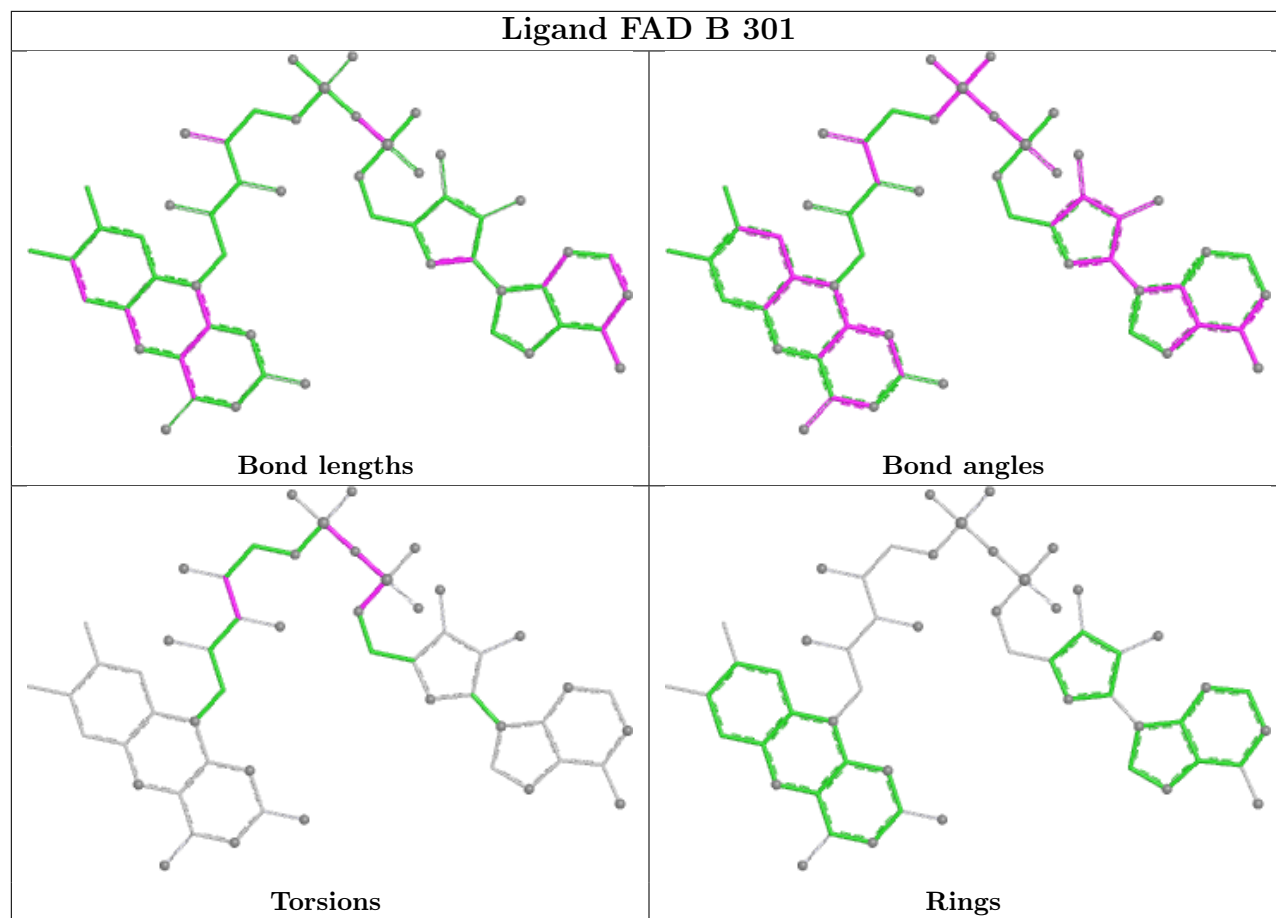
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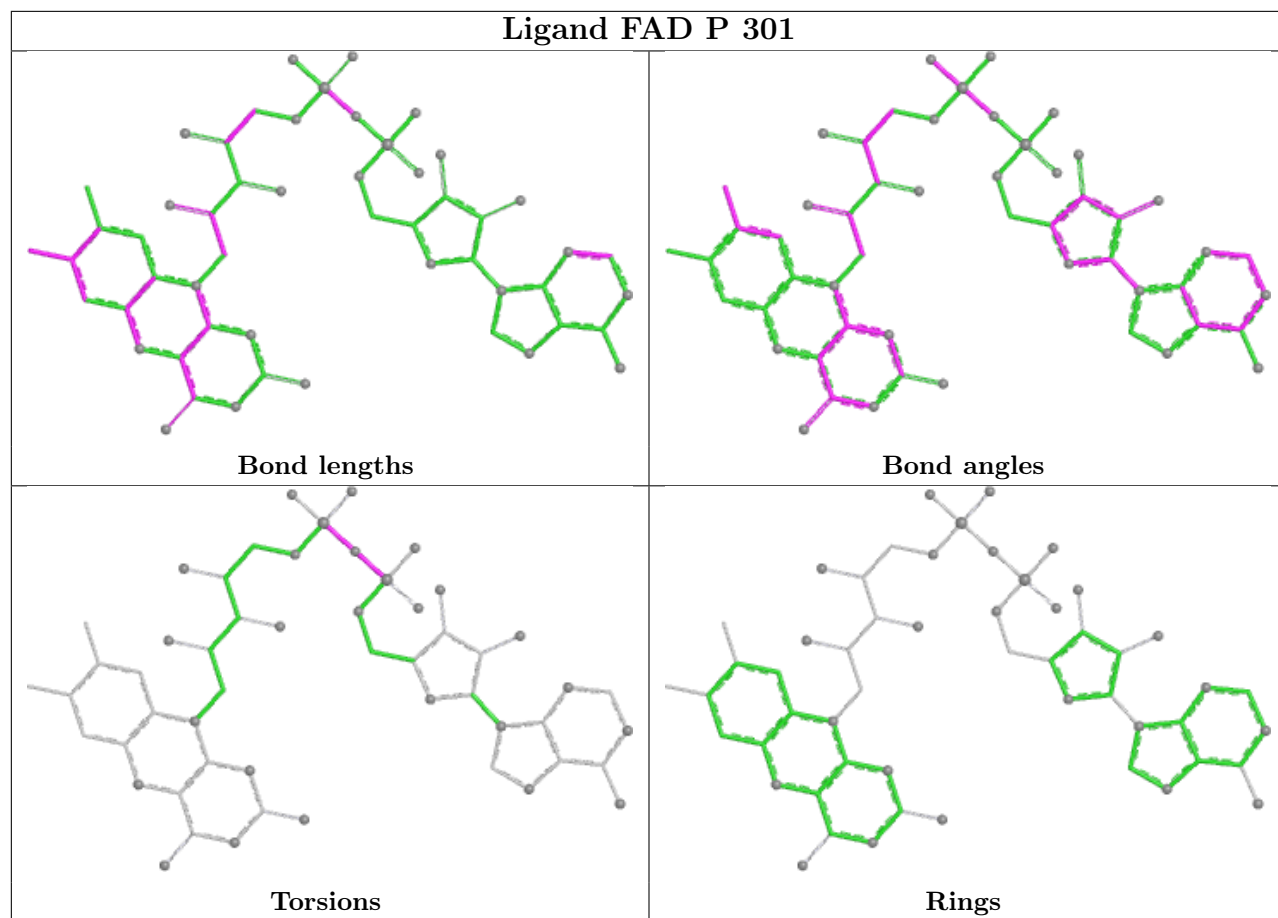
Ligand FAD E 301



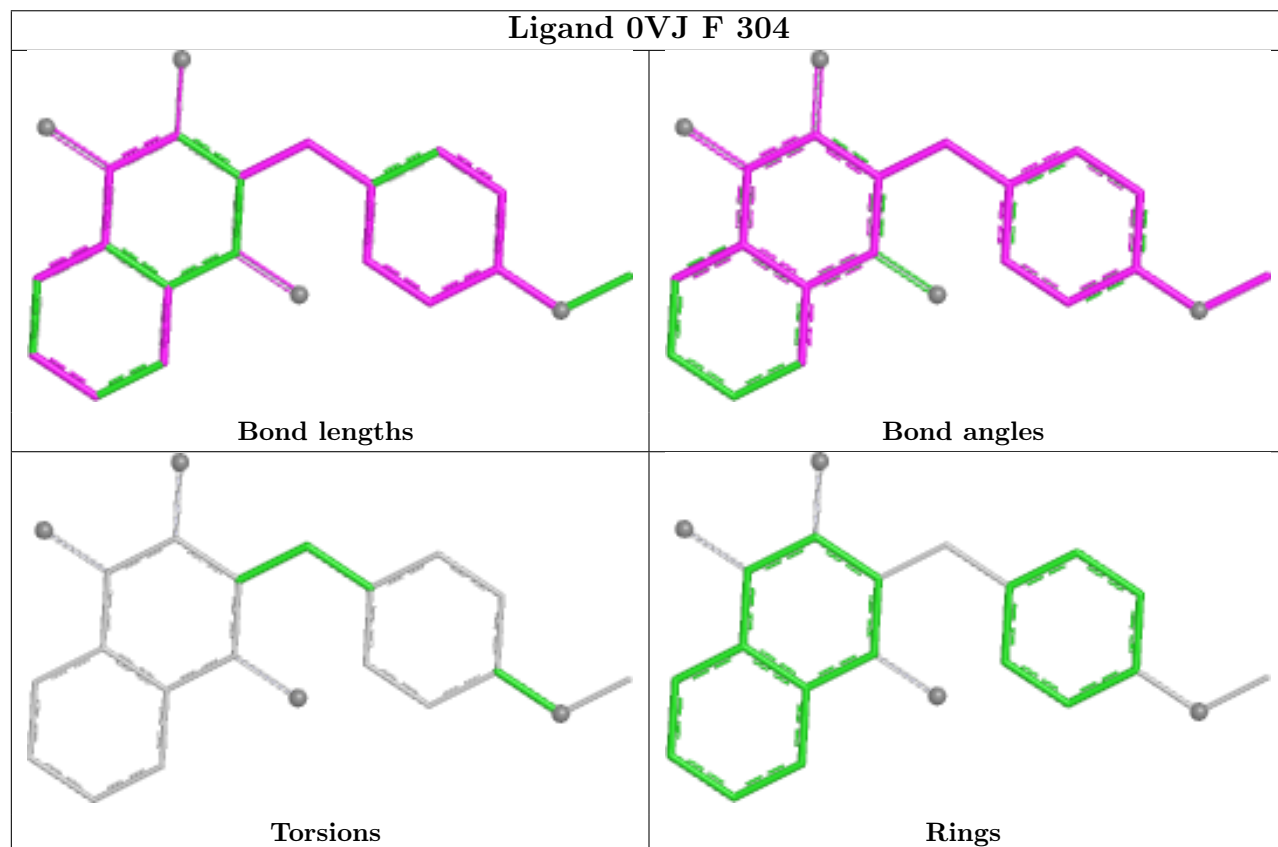




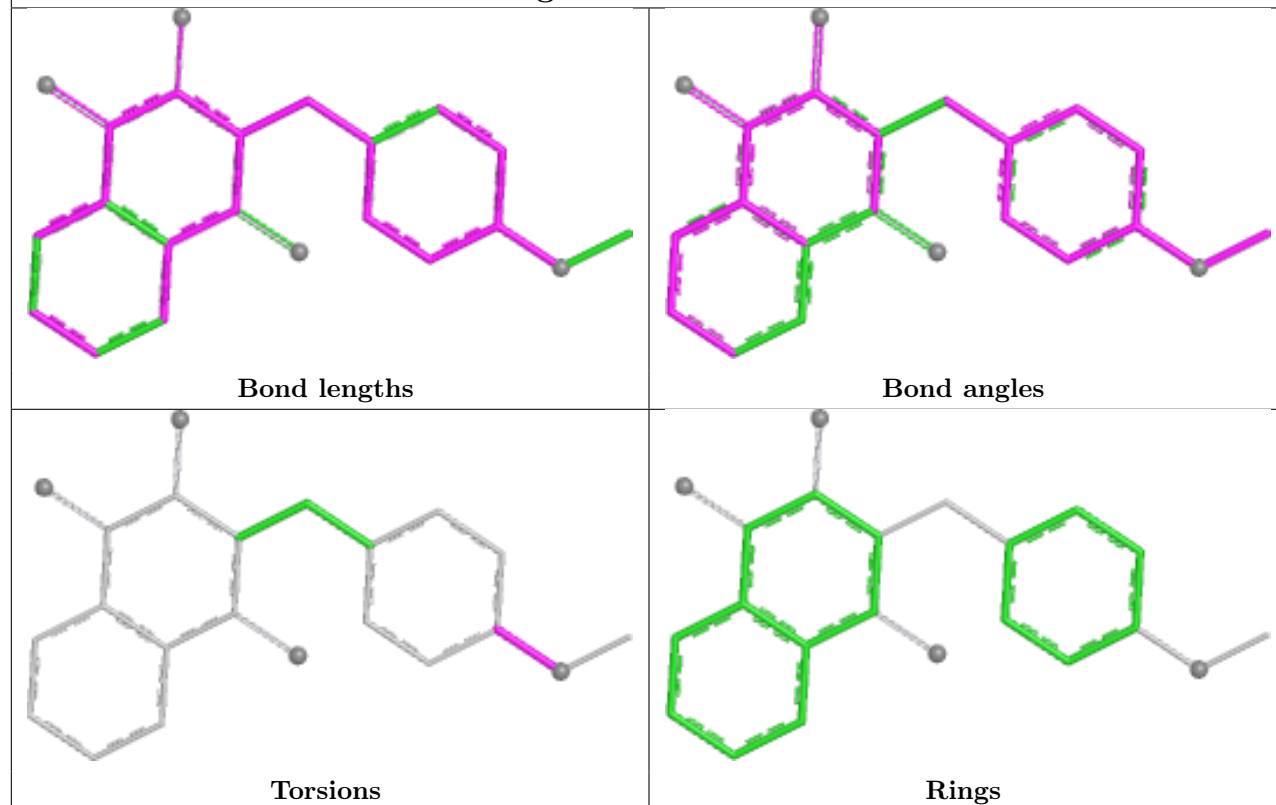
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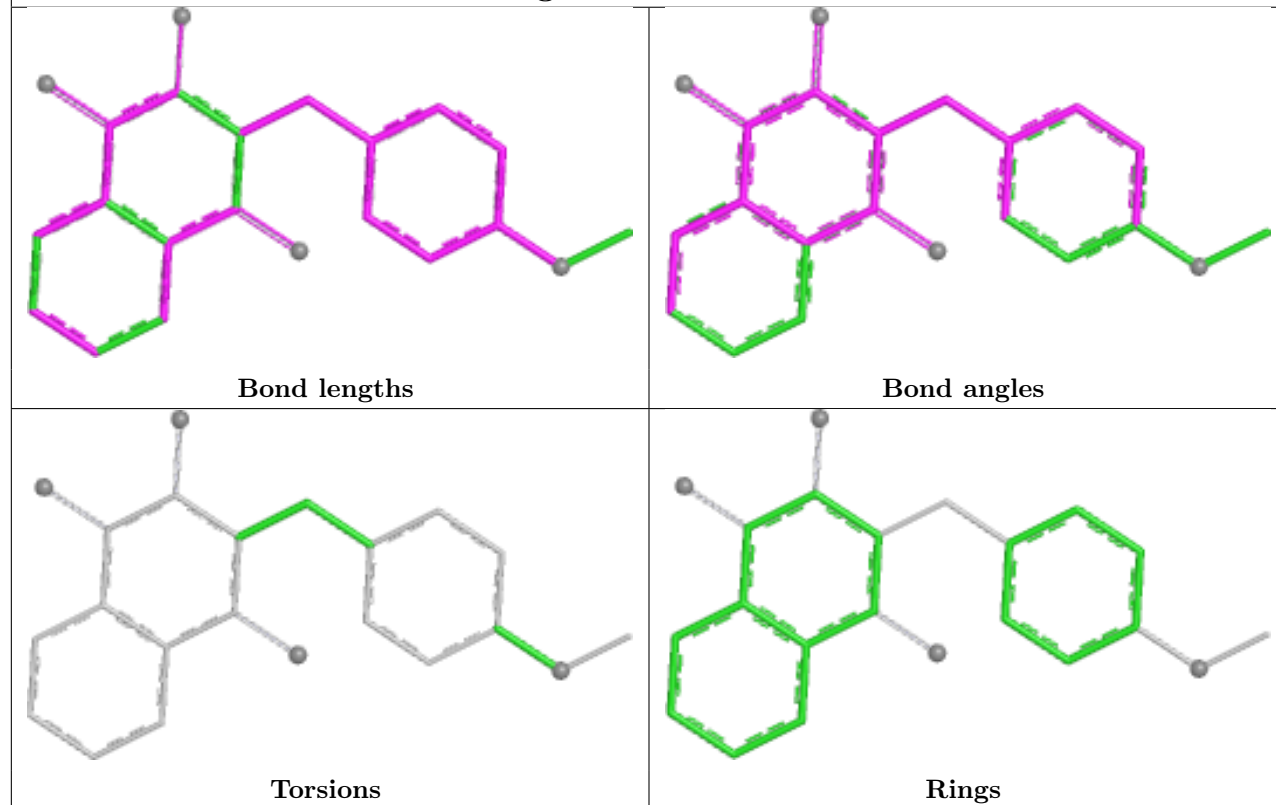
Ligand 0VJ F 304



Ligand 0VJ N 302



Ligand 0VJ K 301



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	191/227 (84%)	-0.86	0 100 100	27, 46, 77, 94	0
1	B	188/227 (82%)	-0.76	0 100 100	28, 50, 89, 119	0
1	C	207/227 (91%)	-0.75	0 100 100	27, 51, 91, 104	0
1	D	203/227 (89%)	-0.92	0 100 100	28, 45, 71, 90	0
1	E	206/227 (90%)	-0.84	0 100 100	26, 49, 86, 107	1 (0%)
1	F	206/227 (90%)	-0.91	0 100 100	24, 44, 74, 111	0
1	G	188/227 (82%)	-0.91	0 100 100	27, 46, 71, 99	0
1	H	179/227 (78%)	-0.82	0 100 100	30, 48, 72, 108	0
1	I	193/227 (85%)	-0.87	0 100 100	23, 49, 74, 91	0
1	J	179/227 (78%)	-0.65	0 100 100	32, 57, 91, 101	0
1	K	201/227 (88%)	-0.78	0 100 100	32, 51, 90, 110	0
1	L	201/227 (88%)	-0.68	0 100 100	31, 54, 99, 130	0
1	M	197/227 (86%)	-0.82	0 100 100	29, 51, 78, 92	0
1	N	177/227 (77%)	-0.57	0 100 100	29, 58, 102, 138	0
1	O	200/227 (88%)	-0.75	0 100 100	34, 53, 93, 119	0
1	P	197/227 (86%)	-0.60	0 100 100	29, 60, 101, 120	0
All	All	3113/3632 (85%)	-0.78	0 100 100	23, 51, 89, 138	1 (0%)

There are no RSRZ outliers to report.

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DMS	P	303	4/4	0.95	0.10	78,87,87,91	0
4	DMS	A	304	4/4	0.96	0.16	63,70,74,74	0
3	0VJ	J	302	22/22	0.97	0.06	51,55,59,60	0
4	DMS	G	302	4/4	0.97	0.10	70,70,71,76	0
4	DMS	H	303	4/4	0.97	0.09	60,62,63,69	0
3	0VJ	N	302	22/22	0.97	0.07	59,65,70,71	0
2	FAD	N	301	53/53	0.98	0.05	44,45,47,48	0
2	FAD	P	301	53/53	0.98	0.05	33,34,35,37	0
3	0VJ	A	303	22/22	0.98	0.05	34,39,43,47	0
3	0VJ	A	305	22/22	0.98	0.05	35,40,44,48	0
3	0VJ	D	301	22/22	0.98	0.05	45,50,56,56	0
3	0VJ	F	304	22/22	0.98	0.06	52,58,61,62	0
3	0VJ	G	301	22/22	0.98	0.05	30,39,47,47	0
3	0VJ	I	304	22/22	0.98	0.06	38,44,48,49	0
2	FAD	E	301	53/53	0.98	0.05	33,34,35,37	0
3	0VJ	K	301	22/22	0.98	0.05	21,26,34,35	0
3	0VJ	L	301	22/22	0.98	0.06	39,42,48,51	0
2	FAD	F	302	53/53	0.98	0.06	33,34,35,37	0
3	0VJ	P	302	22/22	0.98	0.06	44,47,53,57	0
2	FAD	I	301	53/53	0.98	0.06	33,34,35,37	0
4	DMS	B	302	4/4	0.98	0.08	44,46,55,55	0
4	DMS	F	303	4/4	0.98	0.07	60,63,67,74	0
2	FAD	I	302	53/53	0.98	0.06	33,34,35,37	0
2	FAD	J	301	53/53	0.98	0.05	42,44,46,48	0
4	DMS	I	303	4/4	0.98	0.08	81,84,87,89	0
4	DMS	M	302	4/4	0.98	0.07	80,87,87,88	0
2	FAD	M	301	53/53	0.98	0.07	33,34,35,37	0
2	FAD	B	301	53/53	0.99	0.04	40,41,43,44	0
3	0VJ	M	303	22/22	0.99	0.05	33,43,52,53	0
2	FAD	C	301	53/53	0.99	0.04	33,34,36,38	0
3	0VJ	O	301	22/22	0.99	0.04	18,27,33,36	0
3	0VJ	B	303	22/22	0.99	0.04	24,27,36,40	0

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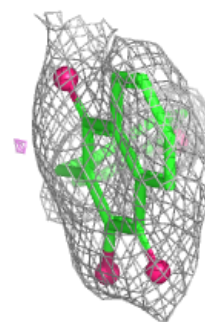
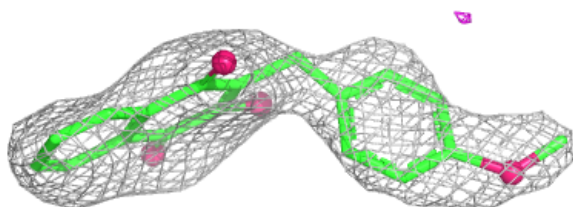
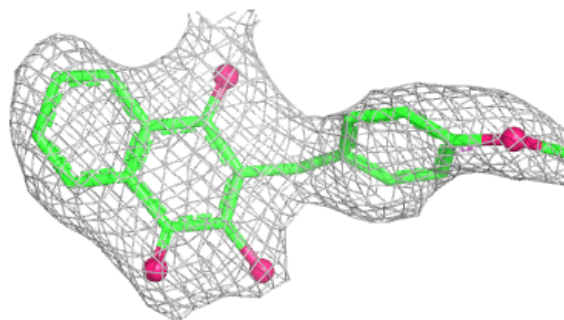
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	A	301	53/53	0.99	0.04	33,34,35,37	0
3	0VJ	E	302	22/22	0.99	0.04	32,39,43,44	0
4	DMS	C	302	4/4	0.99	0.08	63,64,65,65	0
4	DMS	D	302	4/4	0.99	0.06	63,63,67,74	0
4	DMS	E	303	4/4	0.99	0.07	57,64,68,70	0
2	FAD	K	302	53/53	0.99	0.04	37,38,40,40	0
2	FAD	F	301	53/53	0.99	0.04	28,29,30,32	0
3	0VJ	H	301	22/22	0.99	0.04	27,33,39,39	0
2	FAD	A	302	53/53	0.99	0.05	33,34,35,37	0
4	DMS	K	303	4/4	0.99	0.05	54,54,60,61	0
2	FAD	O	302	53/53	0.99	0.05	40,41,43,44	0
4	DMS	O	303	4/4	0.99	0.06	53,56,60,63	0
2	FAD	H	302	53/53	0.99	0.05	45,46,47,49	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.

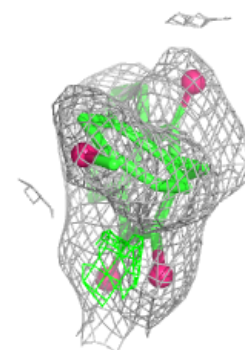
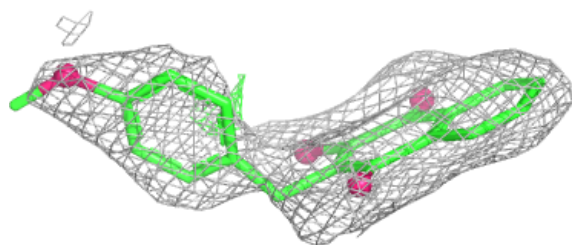
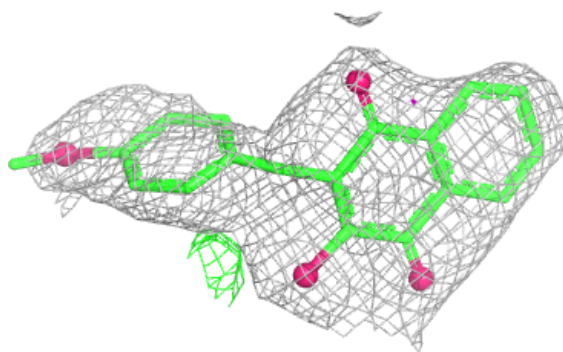
Electron density around 0VJ J 302:

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

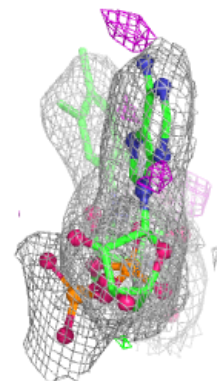
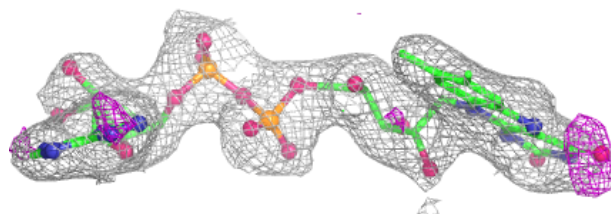
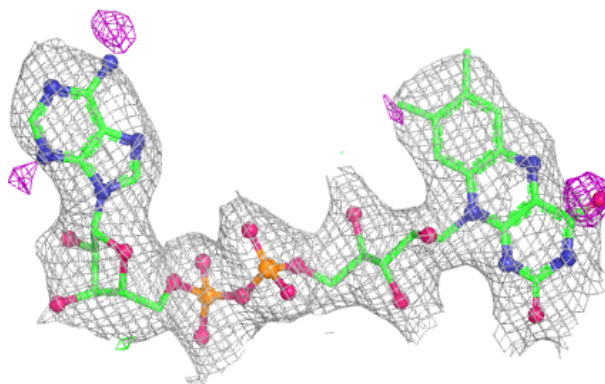


Electron density around 0VJ N 302:

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

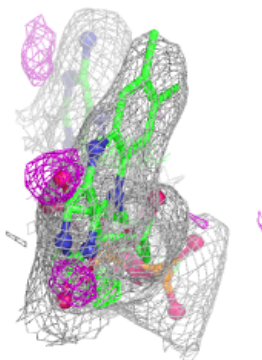
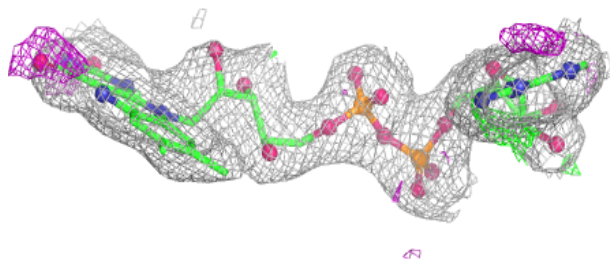
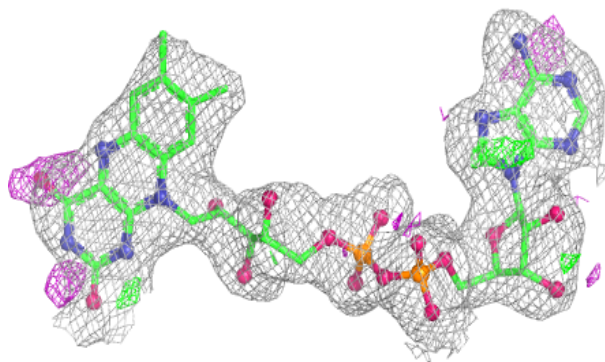
**Electron density around FAD N 301:**

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

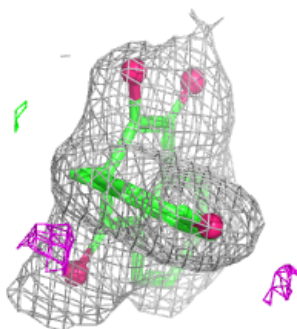
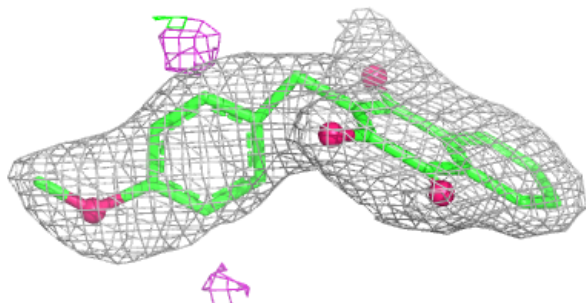
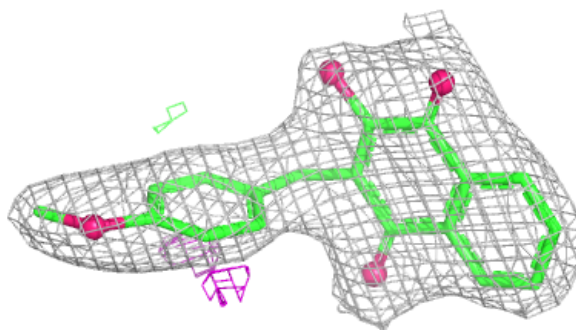


Electron density around FAD P 301:

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

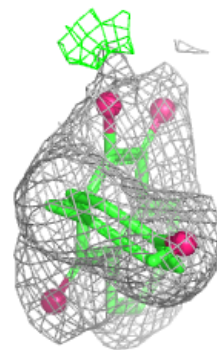
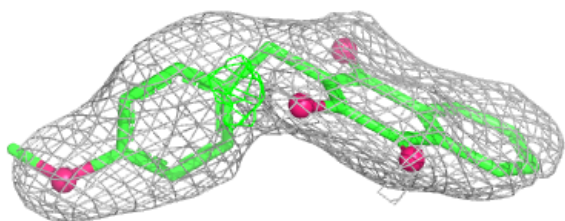
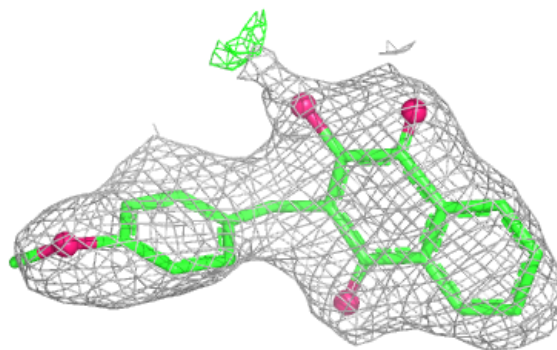
**Electron density around 0VJ A 303:**

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

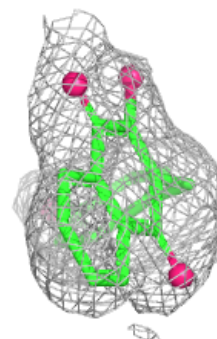
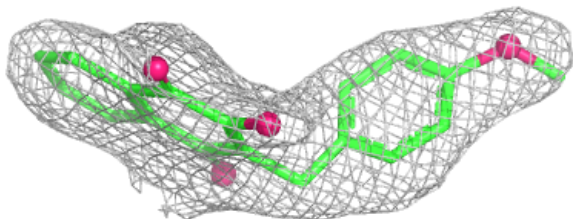
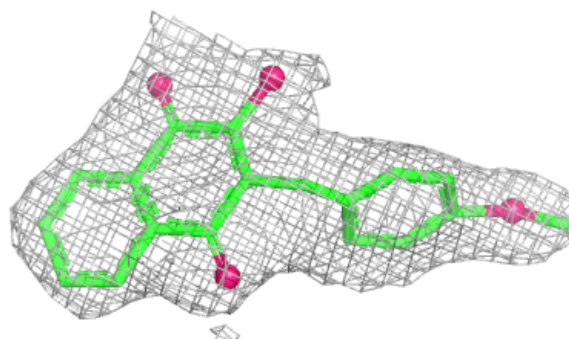


Electron density around 0VJ A 305:

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

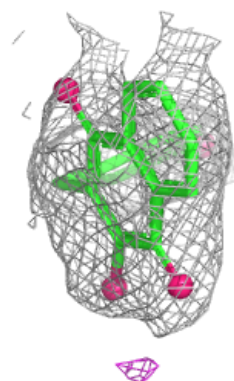
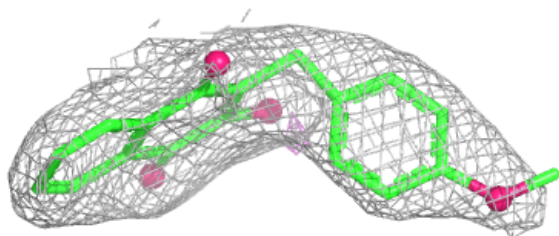
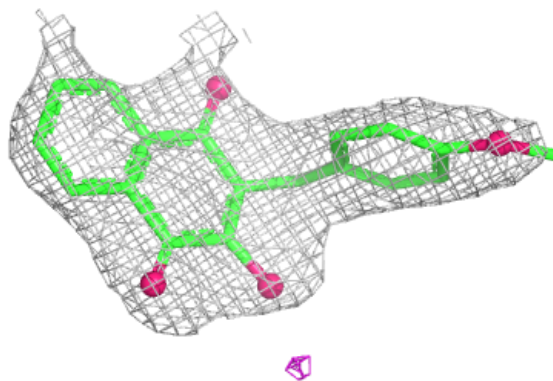
**Electron density around 0VJ D 301:**

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

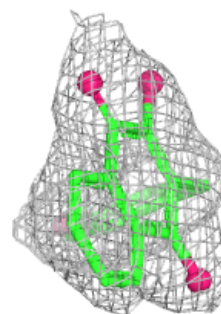
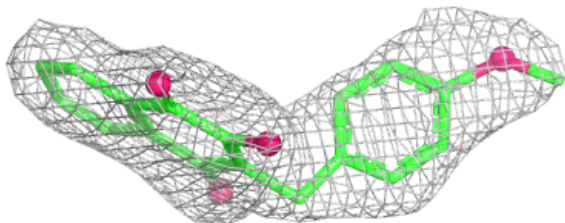
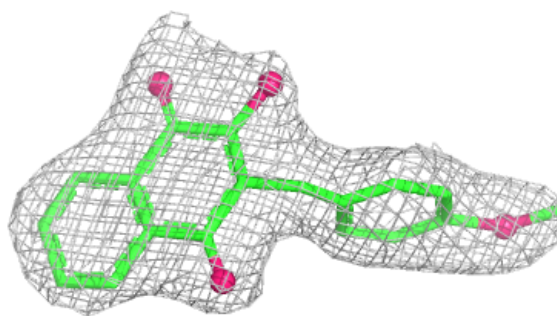


Electron density around 0VJ F 304:

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

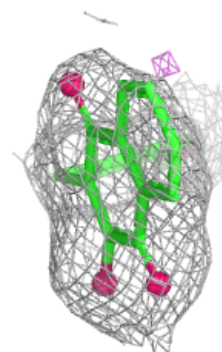
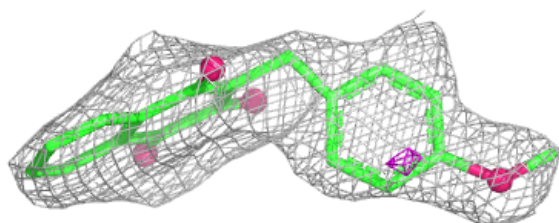
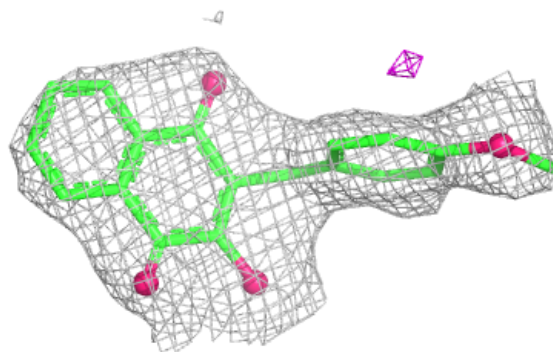
**Electron density around 0VJ G 301:**

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

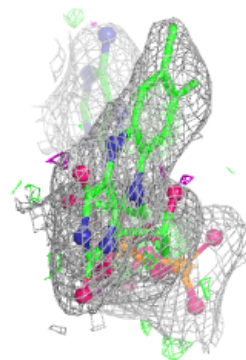
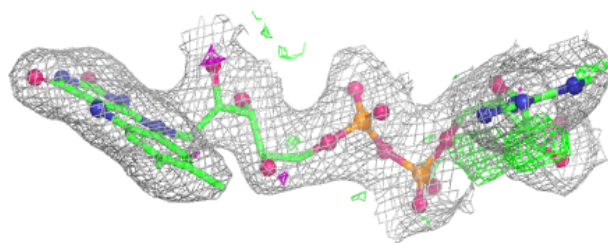
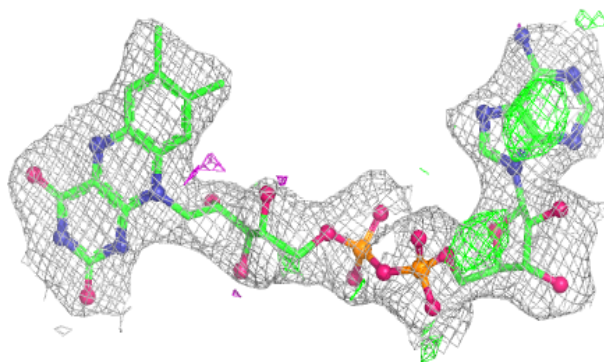


Electron density around 0VJ I 304:

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

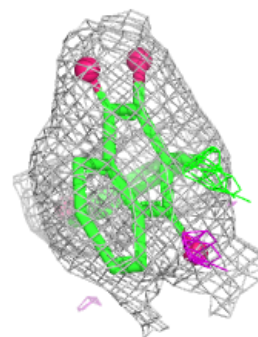
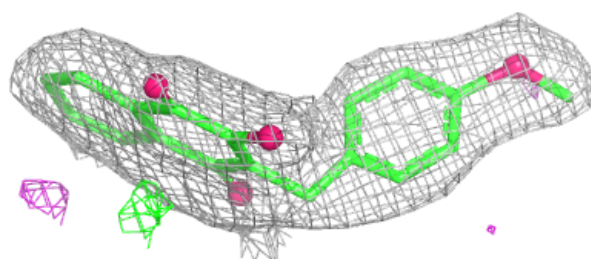
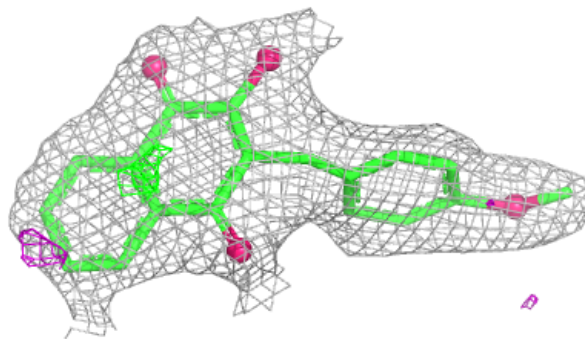
**Electron density around FAD E 301:**

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

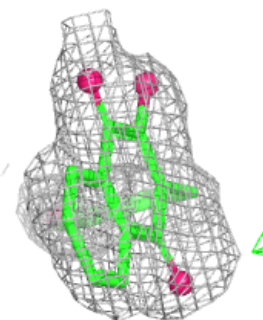
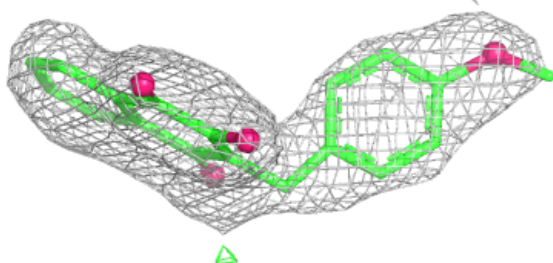
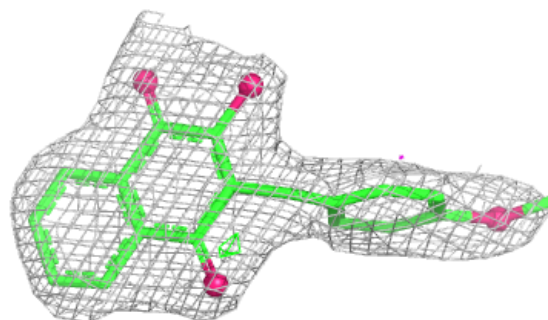


Electron density around 0VJ K 301:

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

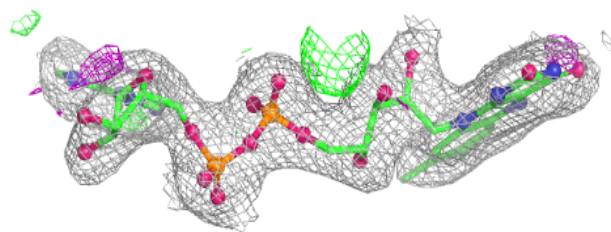
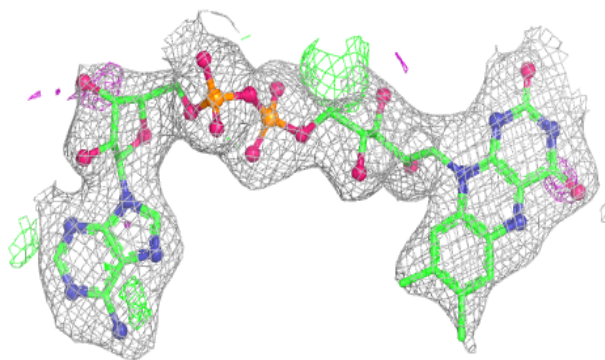
**Electron density around 0VJ L 301:**

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

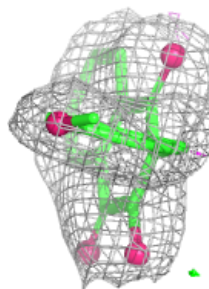
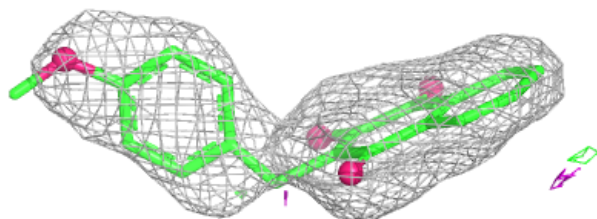
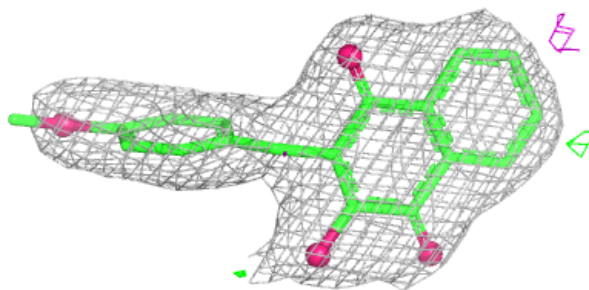


Electron density around FAD F 302:

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

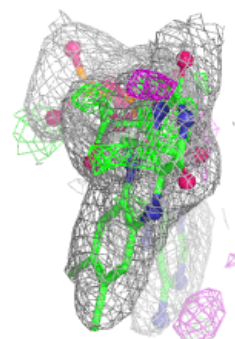
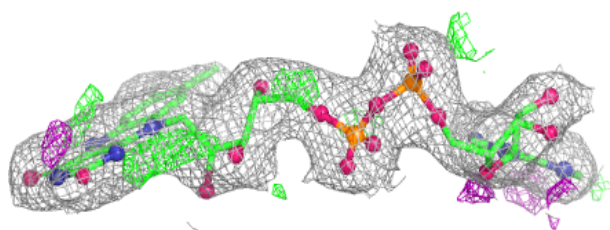
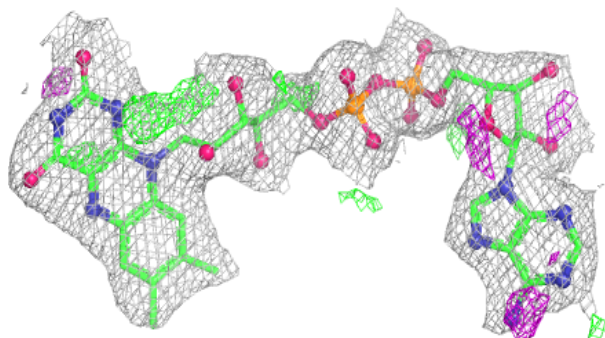
**Electron density around 0VJ P 302:**

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

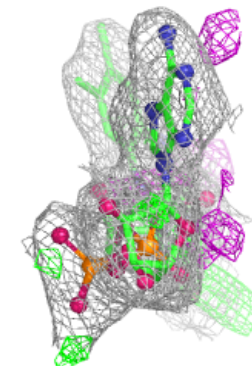
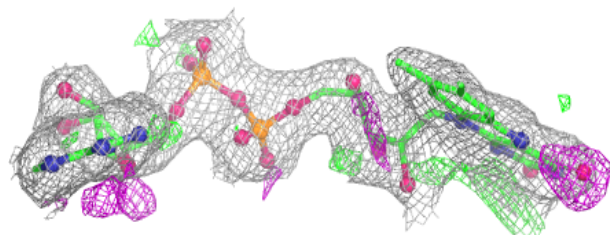
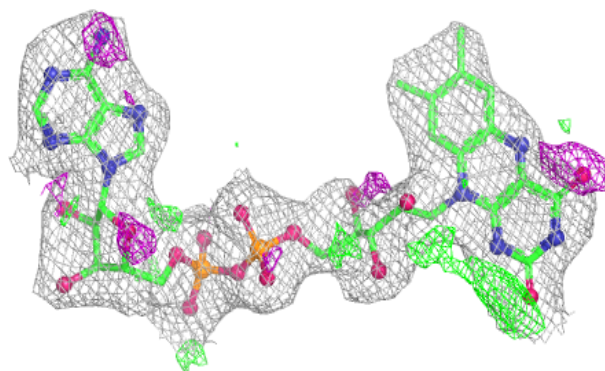


Electron density around FAD I 301:

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

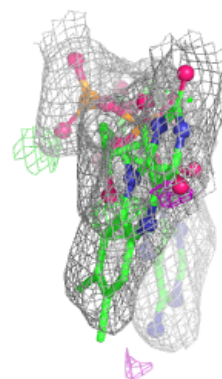
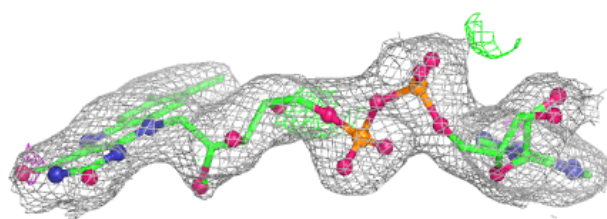
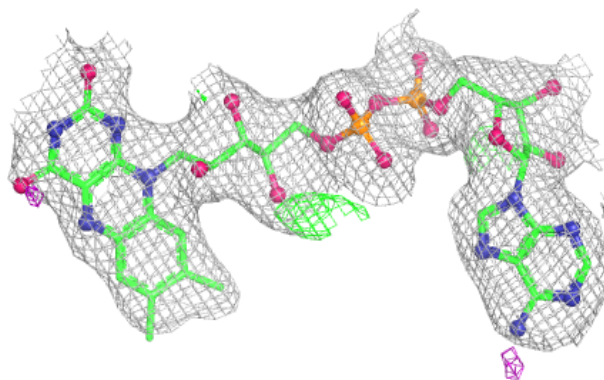
**Electron density around FAD I 302:**

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

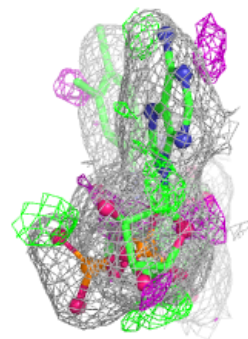
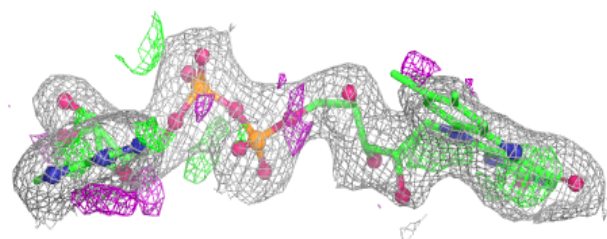
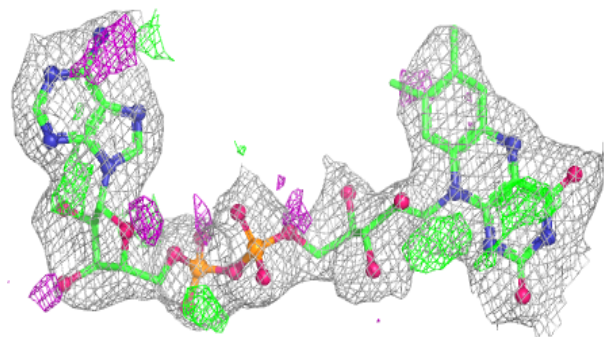


Electron density around FAD J 301:

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

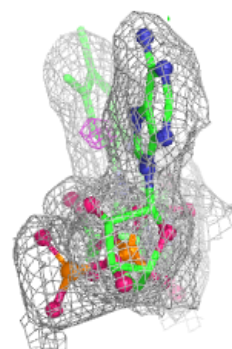
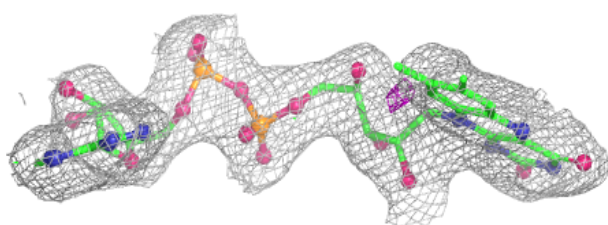
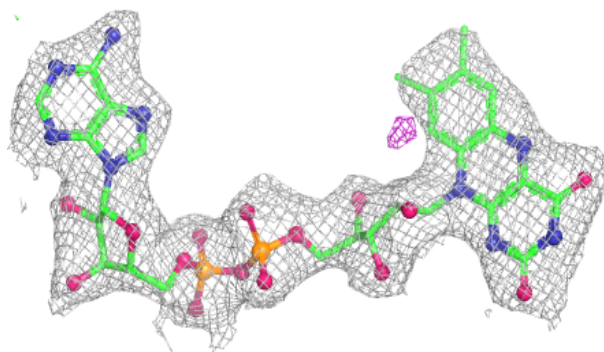
**Electron density around FAD M 301:**

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

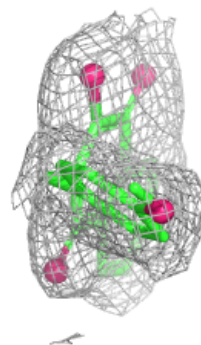
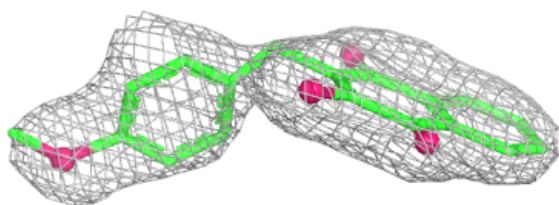
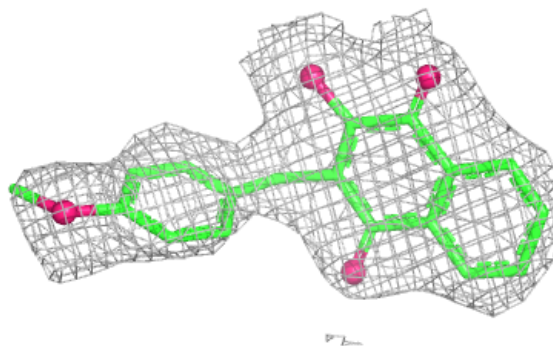


Electron density around FAD B 301:

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

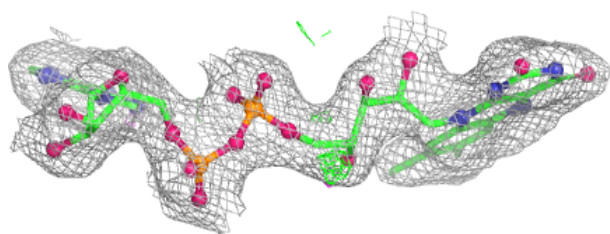
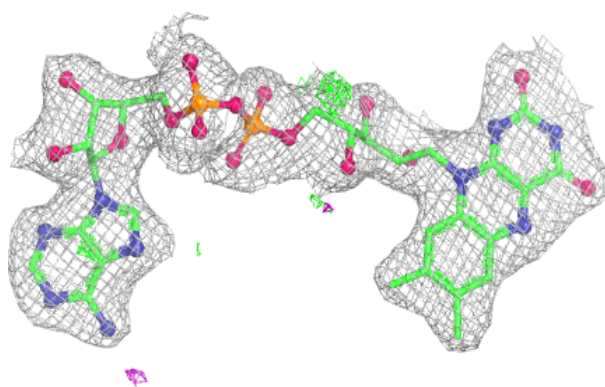
**Electron density around 0VJ M 303:**

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

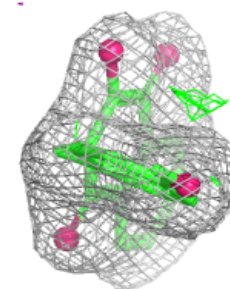
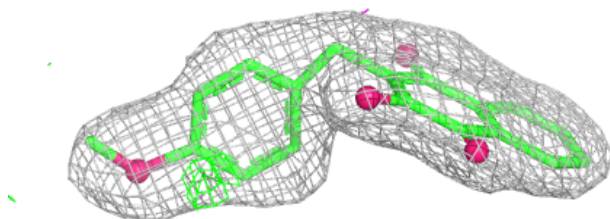
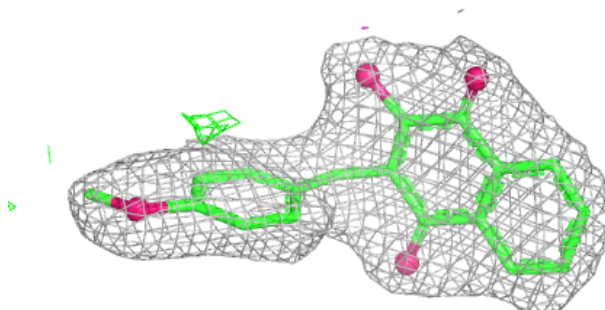


Electron density around FAD C 301:

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

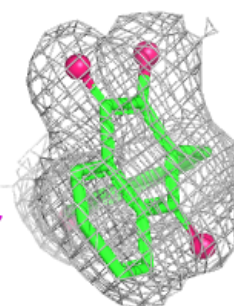
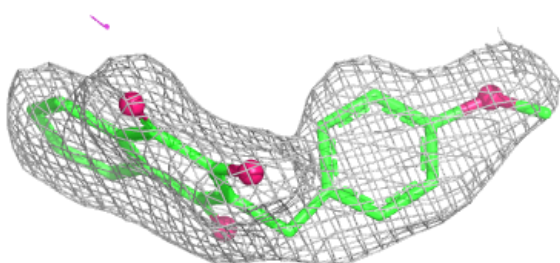
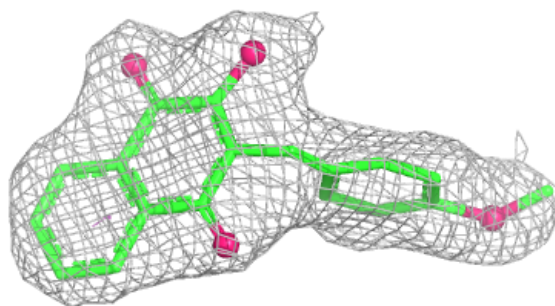
**Electron density around 0VJ O 301:**

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

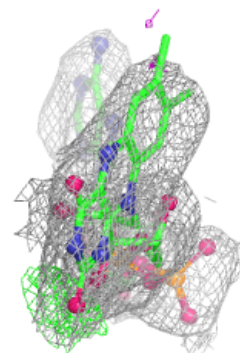
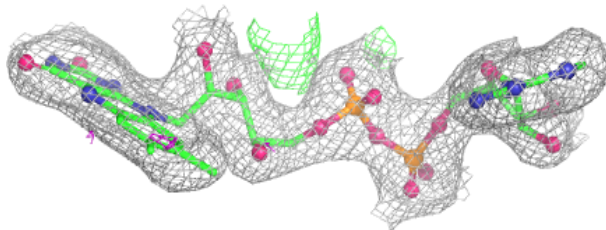
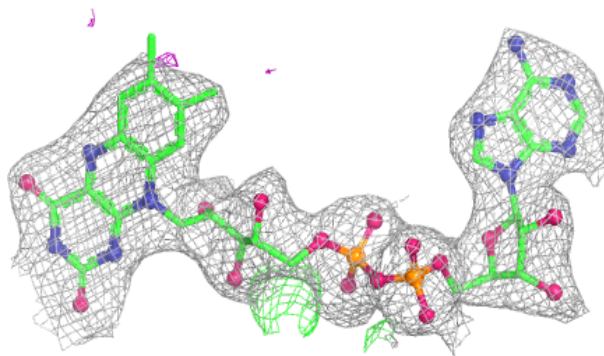


Electron density around 0VJ B 303:

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

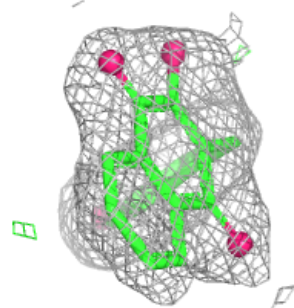
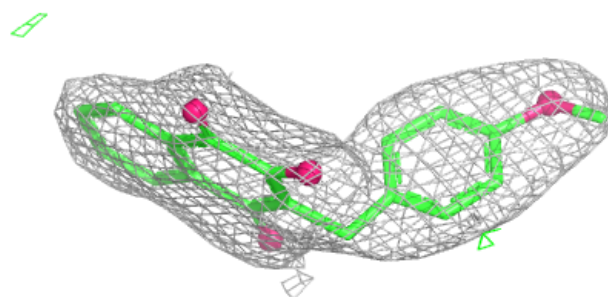
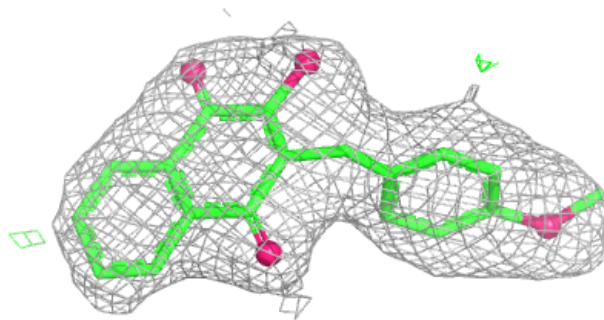
**Electron density around FAD A 301:**

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

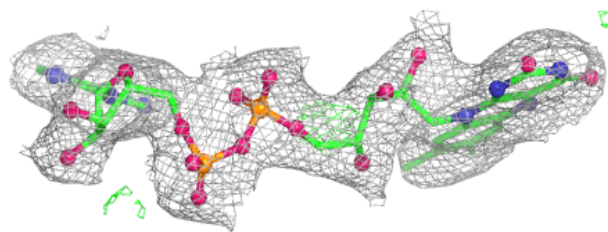
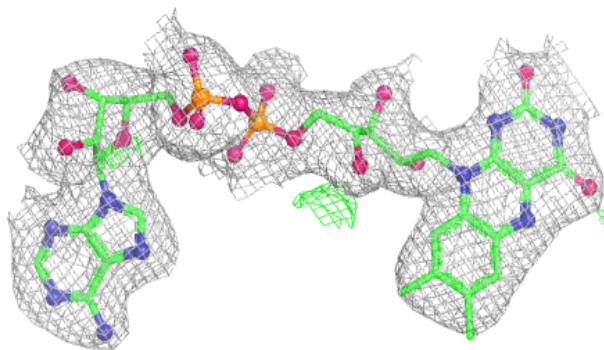


Electron density around 0VJ E 302:

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

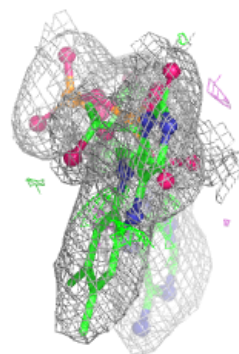
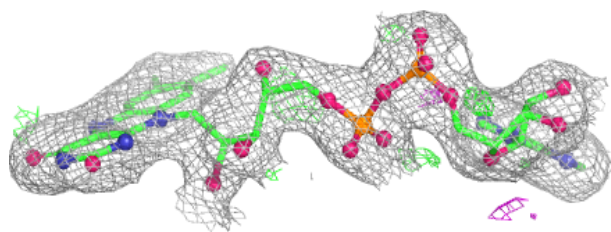
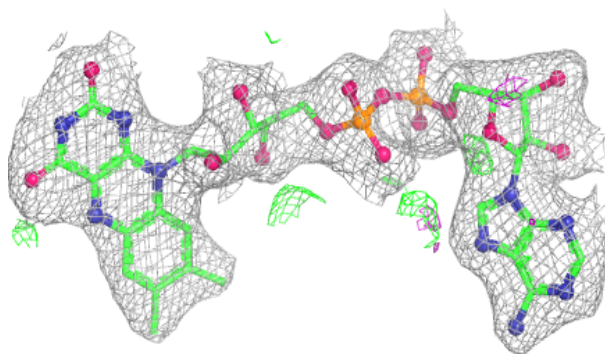
**Electron density around FAD K 302:**

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

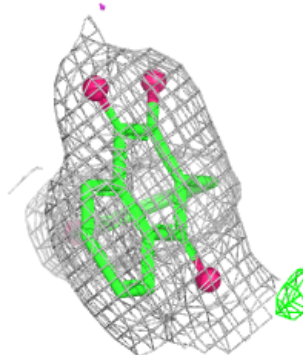
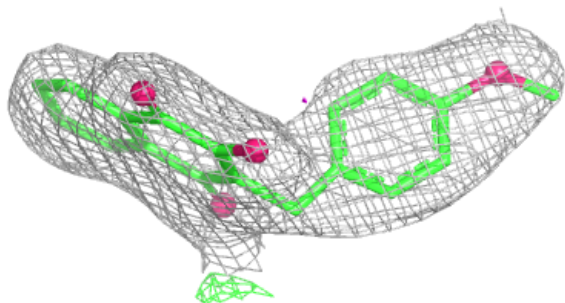
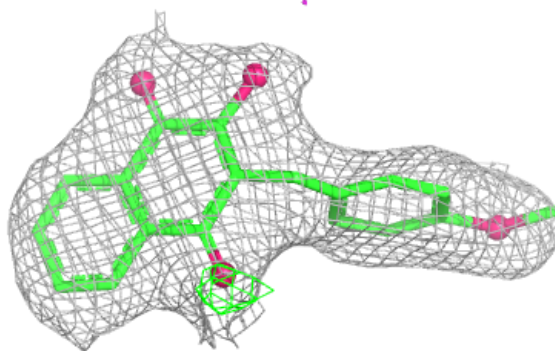


Electron density around FAD F 301:

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

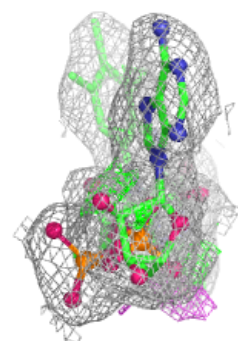
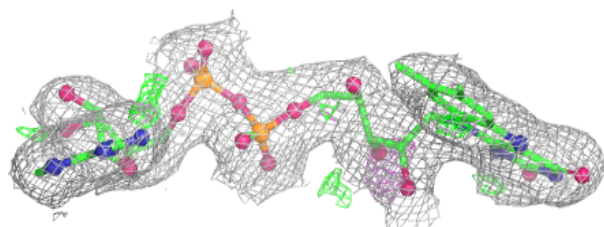
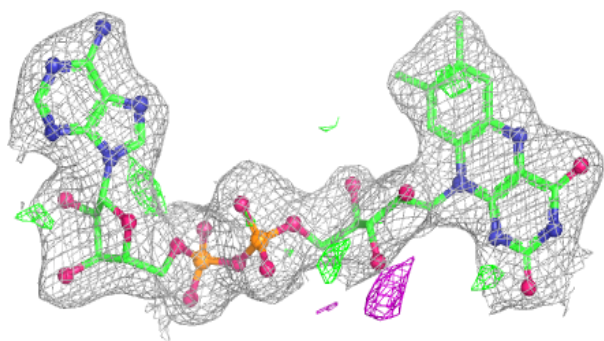
**Electron density around 0VJ H 301:**

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

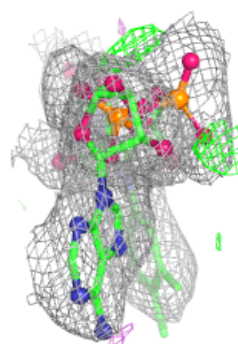
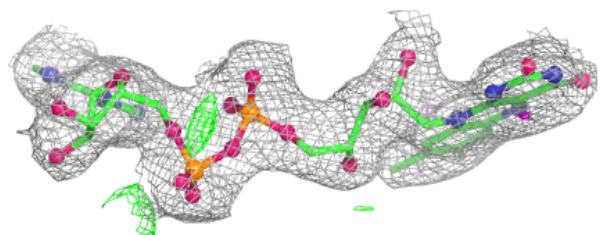
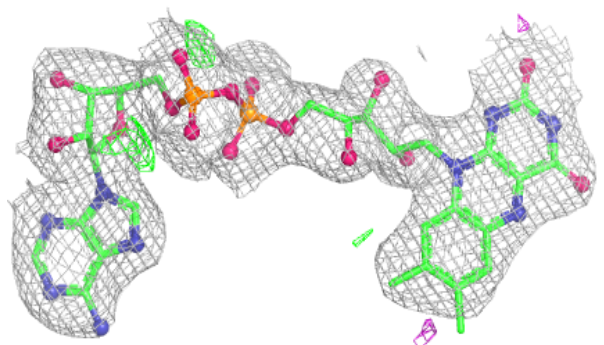


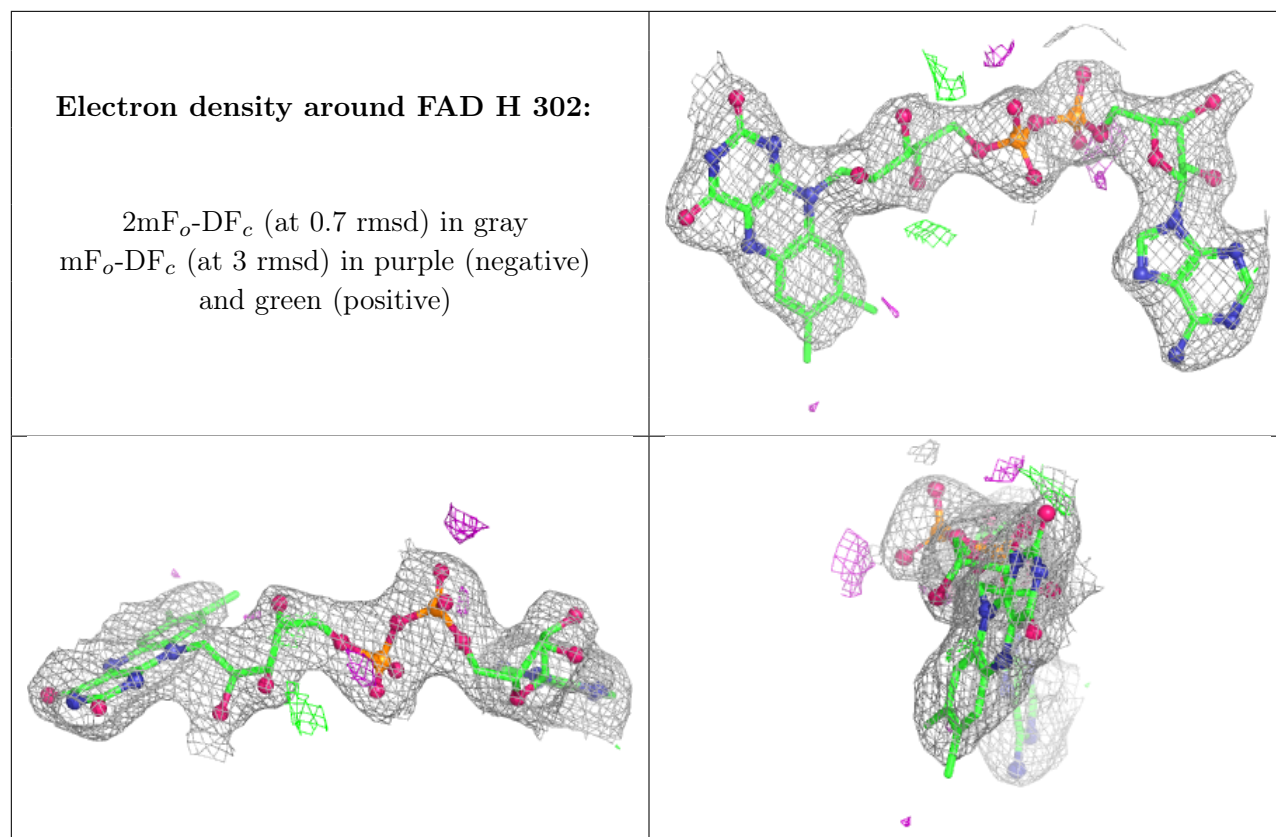
Electron density around FAD A 302:

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

**Electron density around FAD 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.