



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 01:13 am BST

PDB ID : 6QLV  
Title : Crystal structure of W200H UbiX in complex with a geranyl-FMN N5 adduct  
Authors : Marshall, S.A.; Leys, D.  
Deposited on : 2019-02-01  
Resolution : 2.39 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

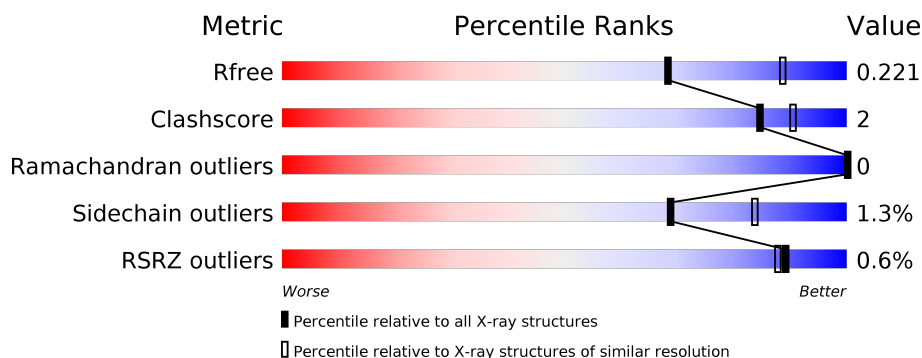
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	230	
1	B	230	
1	C	230	
1	D	230	
1	E	230	
1	F	230	

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Mol	Chain	Length	Quality of chain
1	G	230	<div><div></div><div>80%</div><div></div><div>15%</div></div>
1	H	230	<div><div></div><div>79%</div><div>5%</div><div>16%</div></div>
1	I	230	<div><div>%</div><div></div><div>79%</div><div>6%</div><div>15%</div></div>
1	J	230	<div><div></div><div>79%</div><div>5%</div><div>16%</div></div>
1	K	230	<div><div>%</div><div></div><div>79%</div><div>6%</div><div>15%</div></div>
1	L	230	<div><div></div><div>77%</div><div>7%</div><div>16%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18765 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 Flavin prenyltransferase UbiX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	2	0
			1428	902	247	268	11			
1	B	196	Total	C	N	O	S	0	2	0
			1464	923	253	275	13			
1	C	193	Total	C	N	O	S	0	1	0
			1427	901	247	268	11			
1	D	195	Total	C	N	O	S	0	5	0
			1470	929	255	274	12			
1	E	193	Total	C	N	O	S	0	3	0
			1445	913	252	269	11			
1	F	195	Total	C	N	O	S	0	2	0
			1450	914	252	272	12			
1	G	195	Total	C	N	O	S	0	2	0
			1440	909	249	270	12			
1	H	193	Total	C	N	O	S	0	1	0
			1423	899	246	267	11			
1	I	195	Total	C	N	O	S	0	1	0
			1443	910	249	272	12			
1	J	193	Total	C	N	O	S	0	1	0
			1431	904	248	268	11			
1	K	196	Total	C	N	O	S	0	1	0
			1451	917	251	271	12			
1	L	193	Total	C	N	O	S	0	1	0
			1427	901	247	268	11			

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A072ZCW8
A	-19	HIS	-	expression tag	UNP A0A072ZCW8
A	-18	HIS	-	expression tag	UNP A0A072ZCW8
A	-17	HIS	-	expression tag	UNP A0A072ZCW8
A	-16	HIS	-	expression tag	UNP A0A072ZCW8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP A0A072ZCW8
A	-14	HIS	-	expression tag	UNP A0A072ZCW8
A	-13	SER	-	expression tag	UNP A0A072ZCW8
A	-12	SER	-	expression tag	UNP A0A072ZCW8
A	-11	GLY	-	expression tag	UNP A0A072ZCW8
A	-10	VAL	-	expression tag	UNP A0A072ZCW8
A	-9	ASP	-	expression tag	UNP A0A072ZCW8
A	-8	LEU	-	expression tag	UNP A0A072ZCW8
A	-7	GLY	-	expression tag	UNP A0A072ZCW8
A	-6	THR	-	expression tag	UNP A0A072ZCW8
A	-5	GLU	-	expression tag	UNP A0A072ZCW8
A	-4	ASN	-	expression tag	UNP A0A072ZCW8
A	-3	LEU	-	expression tag	UNP A0A072ZCW8
A	-2	TYR	-	expression tag	UNP A0A072ZCW8
A	-1	GLN	-	expression tag	UNP A0A072ZCW8
A	0	SER	-	expression tag	UNP A0A072ZCW8
A	200	HIS	TRP	engineered mutation	UNP A0A072ZCW8
B	-20	MET	-	initiating methionine	UNP A0A072ZCW8
B	-19	HIS	-	expression tag	UNP A0A072ZCW8
B	-18	HIS	-	expression tag	UNP A0A072ZCW8
B	-17	HIS	-	expression tag	UNP A0A072ZCW8
B	-16	HIS	-	expression tag	UNP A0A072ZCW8
B	-15	HIS	-	expression tag	UNP A0A072ZCW8
B	-14	HIS	-	expression tag	UNP A0A072ZCW8
B	-13	SER	-	expression tag	UNP A0A072ZCW8
B	-12	SER	-	expression tag	UNP A0A072ZCW8
B	-11	GLY	-	expression tag	UNP A0A072ZCW8
B	-10	VAL	-	expression tag	UNP A0A072ZCW8
B	-9	ASP	-	expression tag	UNP A0A072ZCW8
B	-8	LEU	-	expression tag	UNP A0A072ZCW8
B	-7	GLY	-	expression tag	UNP A0A072ZCW8
B	-6	THR	-	expression tag	UNP A0A072ZCW8
B	-5	GLU	-	expression tag	UNP A0A072ZCW8
B	-4	ASN	-	expression tag	UNP A0A072ZCW8
B	-3	LEU	-	expression tag	UNP A0A072ZCW8
B	-2	TYR	-	expression tag	UNP A0A072ZCW8
B	-1	GLN	-	expression tag	UNP A0A072ZCW8
B	0	SER	-	expression tag	UNP A0A072ZCW8
B	200	HIS	TRP	engineered mutation	UNP A0A072ZCW8
C	-20	MET	-	initiating methionine	UNP A0A072ZCW8
C	-19	HIS	-	expression tag	UNP A0A072ZCW8
C	-18	HIS	-	expression tag	UNP A0A072ZCW8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	HIS	-	expression tag	UNP A0A072ZCW8
C	-16	HIS	-	expression tag	UNP A0A072ZCW8
C	-15	HIS	-	expression tag	UNP A0A072ZCW8
C	-14	HIS	-	expression tag	UNP A0A072ZCW8
C	-13	SER	-	expression tag	UNP A0A072ZCW8
C	-12	SER	-	expression tag	UNP A0A072ZCW8
C	-11	GLY	-	expression tag	UNP A0A072ZCW8
C	-10	VAL	-	expression tag	UNP A0A072ZCW8
C	-9	ASP	-	expression tag	UNP A0A072ZCW8
C	-8	LEU	-	expression tag	UNP A0A072ZCW8
C	-7	GLY	-	expression tag	UNP A0A072ZCW8
C	-6	THR	-	expression tag	UNP A0A072ZCW8
C	-5	GLU	-	expression tag	UNP A0A072ZCW8
C	-4	ASN	-	expression tag	UNP A0A072ZCW8
C	-3	LEU	-	expression tag	UNP A0A072ZCW8
C	-2	TYR	-	expression tag	UNP A0A072ZCW8
C	-1	GLN	-	expression tag	UNP A0A072ZCW8
C	0	SER	-	expression tag	UNP A0A072ZCW8
C	200	HIS	TRP	engineered mutation	UNP A0A072ZCW8
D	-20	MET	-	initiating methionine	UNP A0A072ZCW8
D	-19	HIS	-	expression tag	UNP A0A072ZCW8
D	-18	HIS	-	expression tag	UNP A0A072ZCW8
D	-17	HIS	-	expression tag	UNP A0A072ZCW8
D	-16	HIS	-	expression tag	UNP A0A072ZCW8
D	-15	HIS	-	expression tag	UNP A0A072ZCW8
D	-14	HIS	-	expression tag	UNP A0A072ZCW8
D	-13	SER	-	expression tag	UNP A0A072ZCW8
D	-12	SER	-	expression tag	UNP A0A072ZCW8
D	-11	GLY	-	expression tag	UNP A0A072ZCW8
D	-10	VAL	-	expression tag	UNP A0A072ZCW8
D	-9	ASP	-	expression tag	UNP A0A072ZCW8
D	-8	LEU	-	expression tag	UNP A0A072ZCW8
D	-7	GLY	-	expression tag	UNP A0A072ZCW8
D	-6	THR	-	expression tag	UNP A0A072ZCW8
D	-5	GLU	-	expression tag	UNP A0A072ZCW8
D	-4	ASN	-	expression tag	UNP A0A072ZCW8
D	-3	LEU	-	expression tag	UNP A0A072ZCW8
D	-2	TYR	-	expression tag	UNP A0A072ZCW8
D	-1	GLN	-	expression tag	UNP A0A072ZCW8
D	0	SER	-	expression tag	UNP A0A072ZCW8
D	200	HIS	TRP	engineered mutation	UNP A0A072ZCW8
E	-20	MET	-	initiating methionine	UNP A0A072ZCW8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	HIS	-	expression tag	UNP A0A072ZCW8
E	-18	HIS	-	expression tag	UNP A0A072ZCW8
E	-17	HIS	-	expression tag	UNP A0A072ZCW8
E	-16	HIS	-	expression tag	UNP A0A072ZCW8
E	-15	HIS	-	expression tag	UNP A0A072ZCW8
E	-14	HIS	-	expression tag	UNP A0A072ZCW8
E	-13	SER	-	expression tag	UNP A0A072ZCW8
E	-12	SER	-	expression tag	UNP A0A072ZCW8
E	-11	GLY	-	expression tag	UNP A0A072ZCW8
E	-10	VAL	-	expression tag	UNP A0A072ZCW8
E	-9	ASP	-	expression tag	UNP A0A072ZCW8
E	-8	LEU	-	expression tag	UNP A0A072ZCW8
E	-7	GLY	-	expression tag	UNP A0A072ZCW8
E	-6	THR	-	expression tag	UNP A0A072ZCW8
E	-5	GLU	-	expression tag	UNP A0A072ZCW8
E	-4	ASN	-	expression tag	UNP A0A072ZCW8
E	-3	LEU	-	expression tag	UNP A0A072ZCW8
E	-2	TYR	-	expression tag	UNP A0A072ZCW8
E	-1	GLN	-	expression tag	UNP A0A072ZCW8
E	0	SER	-	expression tag	UNP A0A072ZCW8
E	200	HIS	TRP	engineered mutation	UNP A0A072ZCW8
F	-20	MET	-	initiating methionine	UNP A0A072ZCW8
F	-19	HIS	-	expression tag	UNP A0A072ZCW8
F	-18	HIS	-	expression tag	UNP A0A072ZCW8
F	-17	HIS	-	expression tag	UNP A0A072ZCW8
F	-16	HIS	-	expression tag	UNP A0A072ZCW8
F	-15	HIS	-	expression tag	UNP A0A072ZCW8
F	-14	HIS	-	expression tag	UNP A0A072ZCW8
F	-13	SER	-	expression tag	UNP A0A072ZCW8
F	-12	SER	-	expression tag	UNP A0A072ZCW8
F	-11	GLY	-	expression tag	UNP A0A072ZCW8
F	-10	VAL	-	expression tag	UNP A0A072ZCW8
F	-9	ASP	-	expression tag	UNP A0A072ZCW8
F	-8	LEU	-	expression tag	UNP A0A072ZCW8
F	-7	GLY	-	expression tag	UNP A0A072ZCW8
F	-6	THR	-	expression tag	UNP A0A072ZCW8
F	-5	GLU	-	expression tag	UNP A0A072ZCW8
F	-4	ASN	-	expression tag	UNP A0A072ZCW8
F	-3	LEU	-	expression tag	UNP A0A072ZCW8
F	-2	TYR	-	expression tag	UNP A0A072ZCW8
F	-1	GLN	-	expression tag	UNP A0A072ZCW8
F	0	SER	-	expression tag	UNP A0A072ZCW8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	200	HIS	TRP	engineered mutation	UNP A0A072ZCW8
G	-20	MET	-	initiating methionine	UNP A0A072ZCW8
G	-19	HIS	-	expression tag	UNP A0A072ZCW8
G	-18	HIS	-	expression tag	UNP A0A072ZCW8
G	-17	HIS	-	expression tag	UNP A0A072ZCW8
G	-16	HIS	-	expression tag	UNP A0A072ZCW8
G	-15	HIS	-	expression tag	UNP A0A072ZCW8
G	-14	HIS	-	expression tag	UNP A0A072ZCW8
G	-13	SER	-	expression tag	UNP A0A072ZCW8
G	-12	SER	-	expression tag	UNP A0A072ZCW8
G	-11	GLY	-	expression tag	UNP A0A072ZCW8
G	-10	VAL	-	expression tag	UNP A0A072ZCW8
G	-9	ASP	-	expression tag	UNP A0A072ZCW8
G	-8	LEU	-	expression tag	UNP A0A072ZCW8
G	-7	GLY	-	expression tag	UNP A0A072ZCW8
G	-6	THR	-	expression tag	UNP A0A072ZCW8
G	-5	GLU	-	expression tag	UNP A0A072ZCW8
G	-4	ASN	-	expression tag	UNP A0A072ZCW8
G	-3	LEU	-	expression tag	UNP A0A072ZCW8
G	-2	TYR	-	expression tag	UNP A0A072ZCW8
G	-1	GLN	-	expression tag	UNP A0A072ZCW8
G	0	SER	-	expression tag	UNP A0A072ZCW8
G	200	HIS	TRP	engineered mutation	UNP A0A072ZCW8
H	-20	MET	-	initiating methionine	UNP A0A072ZCW8
H	-19	HIS	-	expression tag	UNP A0A072ZCW8
H	-18	HIS	-	expression tag	UNP A0A072ZCW8
H	-17	HIS	-	expression tag	UNP A0A072ZCW8
H	-16	HIS	-	expression tag	UNP A0A072ZCW8
H	-15	HIS	-	expression tag	UNP A0A072ZCW8
H	-14	HIS	-	expression tag	UNP A0A072ZCW8
H	-13	SER	-	expression tag	UNP A0A072ZCW8
H	-12	SER	-	expression tag	UNP A0A072ZCW8
H	-11	GLY	-	expression tag	UNP A0A072ZCW8
H	-10	VAL	-	expression tag	UNP A0A072ZCW8
H	-9	ASP	-	expression tag	UNP A0A072ZCW8
H	-8	LEU	-	expression tag	UNP A0A072ZCW8
H	-7	GLY	-	expression tag	UNP A0A072ZCW8
H	-6	THR	-	expression tag	UNP A0A072ZCW8
H	-5	GLU	-	expression tag	UNP A0A072ZCW8
H	-4	ASN	-	expression tag	UNP A0A072ZCW8
H	-3	LEU	-	expression tag	UNP A0A072ZCW8
H	-2	TYR	-	expression tag	UNP A0A072ZCW8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	GLN	-	expression tag	UNP A0A072ZCW8
H	0	SER	-	expression tag	UNP A0A072ZCW8
H	200	HIS	TRP	engineered mutation	UNP A0A072ZCW8
I	-20	MET	-	initiating methionine	UNP A0A072ZCW8
I	-19	HIS	-	expression tag	UNP A0A072ZCW8
I	-18	HIS	-	expression tag	UNP A0A072ZCW8
I	-17	HIS	-	expression tag	UNP A0A072ZCW8
I	-16	HIS	-	expression tag	UNP A0A072ZCW8
I	-15	HIS	-	expression tag	UNP A0A072ZCW8
I	-14	HIS	-	expression tag	UNP A0A072ZCW8
I	-13	SER	-	expression tag	UNP A0A072ZCW8
I	-12	SER	-	expression tag	UNP A0A072ZCW8
I	-11	GLY	-	expression tag	UNP A0A072ZCW8
I	-10	VAL	-	expression tag	UNP A0A072ZCW8
I	-9	ASP	-	expression tag	UNP A0A072ZCW8
I	-8	LEU	-	expression tag	UNP A0A072ZCW8
I	-7	GLY	-	expression tag	UNP A0A072ZCW8
I	-6	THR	-	expression tag	UNP A0A072ZCW8
I	-5	GLU	-	expression tag	UNP A0A072ZCW8
I	-4	ASN	-	expression tag	UNP A0A072ZCW8
I	-3	LEU	-	expression tag	UNP A0A072ZCW8
I	-2	TYR	-	expression tag	UNP A0A072ZCW8
I	-1	GLN	-	expression tag	UNP A0A072ZCW8
I	0	SER	-	expression tag	UNP A0A072ZCW8
I	200	HIS	TRP	engineered mutation	UNP A0A072ZCW8
J	-20	MET	-	initiating methionine	UNP A0A072ZCW8
J	-19	HIS	-	expression tag	UNP A0A072ZCW8
J	-18	HIS	-	expression tag	UNP A0A072ZCW8
J	-17	HIS	-	expression tag	UNP A0A072ZCW8
J	-16	HIS	-	expression tag	UNP A0A072ZCW8
J	-15	HIS	-	expression tag	UNP A0A072ZCW8
J	-14	HIS	-	expression tag	UNP A0A072ZCW8
J	-13	SER	-	expression tag	UNP A0A072ZCW8
J	-12	SER	-	expression tag	UNP A0A072ZCW8
J	-11	GLY	-	expression tag	UNP A0A072ZCW8
J	-10	VAL	-	expression tag	UNP A0A072ZCW8
J	-9	ASP	-	expression tag	UNP A0A072ZCW8
J	-8	LEU	-	expression tag	UNP A0A072ZCW8
J	-7	GLY	-	expression tag	UNP A0A072ZCW8
J	-6	THR	-	expression tag	UNP A0A072ZCW8
J	-5	GLU	-	expression tag	UNP A0A072ZCW8
J	-4	ASN	-	expression tag	UNP A0A072ZCW8

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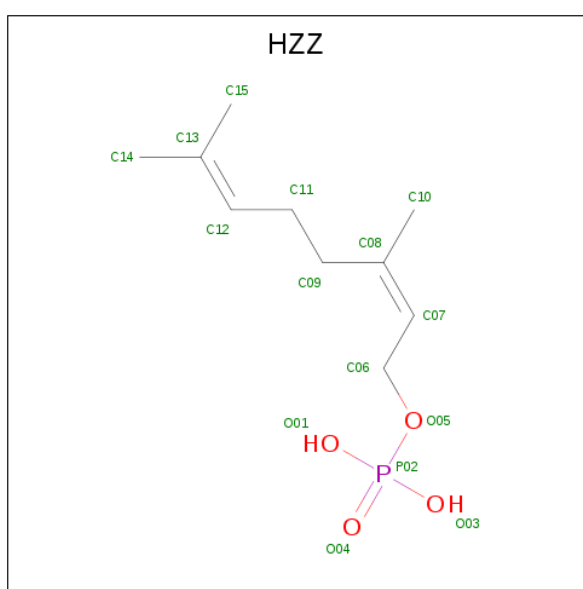
Chain	Residue	Modelled	Actual	Comment	Reference
J	-3	LEU	-	expression tag	UNP A0A072ZCW8
J	-2	TYR	-	expression tag	UNP A0A072ZCW8
J	-1	GLN	-	expression tag	UNP A0A072ZCW8
J	0	SER	-	expression tag	UNP A0A072ZCW8
J	200	HIS	TRP	engineered mutation	UNP A0A072ZCW8
K	-20	MET	-	initiating methionine	UNP A0A072ZCW8
K	-19	HIS	-	expression tag	UNP A0A072ZCW8
K	-18	HIS	-	expression tag	UNP A0A072ZCW8
K	-17	HIS	-	expression tag	UNP A0A072ZCW8
K	-16	HIS	-	expression tag	UNP A0A072ZCW8
K	-15	HIS	-	expression tag	UNP A0A072ZCW8
K	-14	HIS	-	expression tag	UNP A0A072ZCW8
K	-13	SER	-	expression tag	UNP A0A072ZCW8
K	-12	SER	-	expression tag	UNP A0A072ZCW8
K	-11	GLY	-	expression tag	UNP A0A072ZCW8
K	-10	VAL	-	expression tag	UNP A0A072ZCW8
K	-9	ASP	-	expression tag	UNP A0A072ZCW8
K	-8	LEU	-	expression tag	UNP A0A072ZCW8
K	-7	GLY	-	expression tag	UNP A0A072ZCW8
K	-6	THR	-	expression tag	UNP A0A072ZCW8
K	-5	GLU	-	expression tag	UNP A0A072ZCW8
K	-4	ASN	-	expression tag	UNP A0A072ZCW8
K	-3	LEU	-	expression tag	UNP A0A072ZCW8
K	-2	TYR	-	expression tag	UNP A0A072ZCW8
K	-1	GLN	-	expression tag	UNP A0A072ZCW8
K	0	SER	-	expression tag	UNP A0A072ZCW8
K	200	HIS	TRP	engineered mutation	UNP A0A072ZCW8
L	-20	MET	-	initiating methionine	UNP A0A072ZCW8
L	-19	HIS	-	expression tag	UNP A0A072ZCW8
L	-18	HIS	-	expression tag	UNP A0A072ZCW8
L	-17	HIS	-	expression tag	UNP A0A072ZCW8
L	-16	HIS	-	expression tag	UNP A0A072ZCW8
L	-15	HIS	-	expression tag	UNP A0A072ZCW8
L	-14	HIS	-	expression tag	UNP A0A072ZCW8
L	-13	SER	-	expression tag	UNP A0A072ZCW8
L	-12	SER	-	expression tag	UNP A0A072ZCW8
L	-11	GLY	-	expression tag	UNP A0A072ZCW8
L	-10	VAL	-	expression tag	UNP A0A072ZCW8
L	-9	ASP	-	expression tag	UNP A0A072ZCW8
L	-8	LEU	-	expression tag	UNP A0A072ZCW8
L	-7	GLY	-	expression tag	UNP A0A072ZCW8
L	-6	THR	-	expression tag	UNP A0A072ZCW8

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-5	GLU	-	expression tag	UNP A0A072ZCW8
L	-4	ASN	-	expression tag	UNP A0A072ZCW8
L	-3	LEU	-	expression tag	UNP A0A072ZCW8
L	-2	TYR	-	expression tag	UNP A0A072ZCW8
L	-1	GLN	-	expression tag	UNP A0A072ZCW8
L	0	SER	-	expression tag	UNP A0A072ZCW8
L	200	HIS	TRP	engineered mutation	UNP A0A072ZCW8

- Molecule 2 is [(2 {Z})-3,7-dimethylocta-2,6-dienyl] dihydrogen phosphate (three-letter code: HZZ) (formula: C<sub>10</sub>H<sub>19</sub>O<sub>4</sub>P).



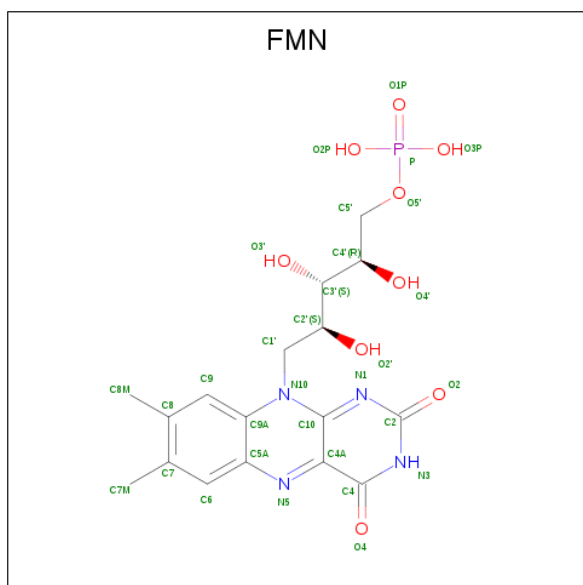
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			15	10	4	1		
2	B	1	Total	C	O	P	0	0
			15	10	4	1		
2	C	1	Total	C	O	P	0	0
			15	10	4	1		
2	G	1	Total	C	O	P	0	0
			15	10	4	1		
2	H	1	Total	C	O	P	0	0
			15	10	4	1		
2	I	1	Total	C	O	P	0	0
			15	10	4	1		
2	J	1	Total	C	O	P	0	0
			15	10	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	K	1	Total	C	O	P	0	0
			15	10	4	1		
2	L	1	Total	C	O	P	0	0
			15	10	4	1		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	B	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	D	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	E	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	F	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	H	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	J	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	K	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	L	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

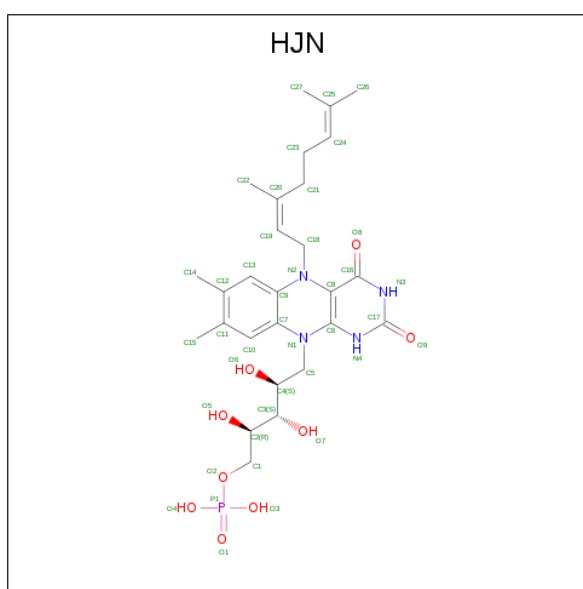
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Na	0	0
			1	1		
5	J	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total	Na	0	0
			1	1		
5	C	1	Total	Na	0	0
			1	1		
5	F	1	Total	Na	0	0
			1	1		

- Molecule 6 is [(2 {R},3 {S},4 {S})-5-[5-[(2 {Z})-3,7-dimethylocta-2,6-dienyl]-7,8-dimethyl-2,4-bis(oxidanylidene)-1 {H}-benzo[g]pteridin-10-yl]-2,3,4-tris(oxidanyl)pentyl] dihydrogen phosphate (three-letter code: HJN) (formula: C<sub>27</sub>H<sub>39</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			41	27	4	9	1		
6	G	1	Total	C	N	O	P	0	0
			41	27	4	9	1		
6	I	1	Total	C	N	O	P	0	0
			41	27	4	9	1		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	O	P	0	0
			5	4	1		
7	E	1	Total	O	P	0	0
			5	4	1		
7	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	68	Total	O	0	0
			68	68		
8	B	79	Total	O	0	0
			79	79		
8	C	74	Total	O	0	0
			74	74		
8	D	97	Total	O	0	0
			97	97		
8	E	74	Total	O	0	0
			74	74		
8	F	66	Total	O	0	0
			66	66		
8	G	77	Total	O	0	0
			77	77		
8	H	73	Total	O	0	0
			73	73		
8	I	59	Total	O	0	0
			59	59		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	71	Total 71	O 71	0	0
8	K	71	Total 71	O 71	0	0
8	L	70	Total 70	O 70	0	0

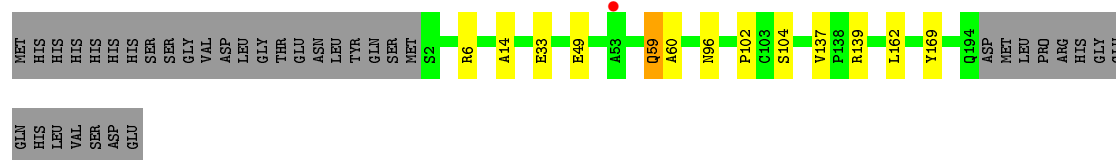


### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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.

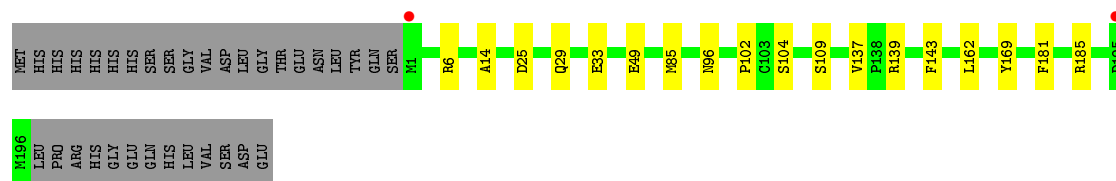
#### • Molecule 1: Flavin prenyltransferase UbiX

Chain A: 




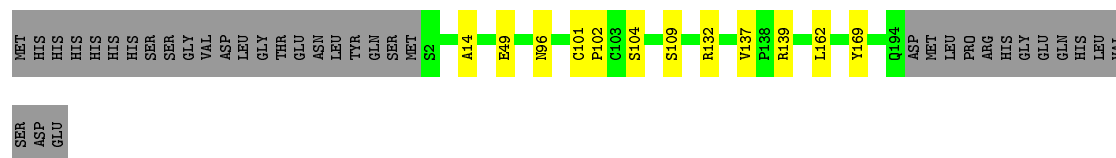
#### • Molecule 1: Flavin prenyltransferase UbiX

Chain B: 



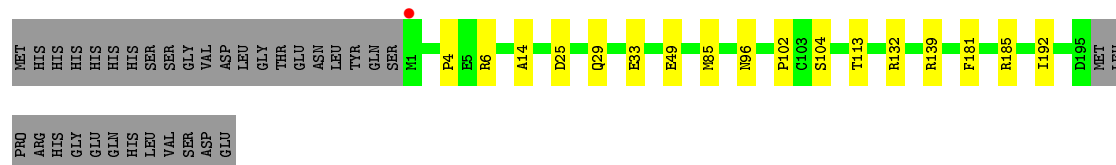
#### • Molecule 1: Flavin prenyltransferase UbiX

Chain C: 




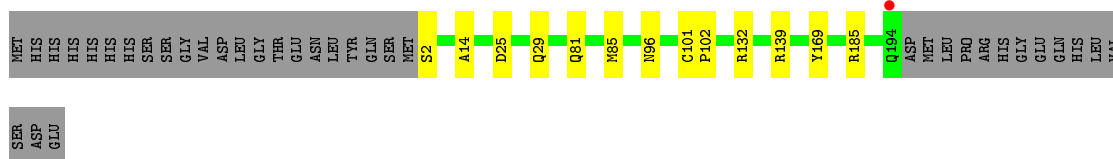
#### • Molecule 1: Flavin prenyltransferase UbiX

Chain D: 




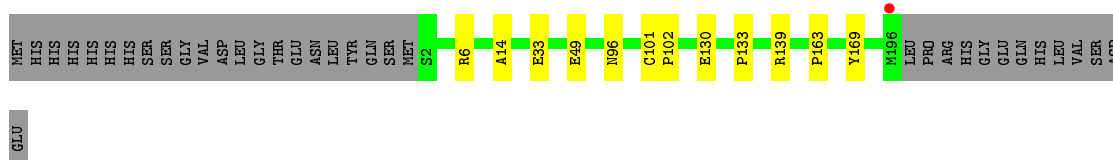
- Molecule 1: Flavin prenyltransferase UbiX

Chain E:  78% 6% 16%




- Molecule 1: Flavin prenyltransferase UbiX

Chain F:  80% 5% 15%




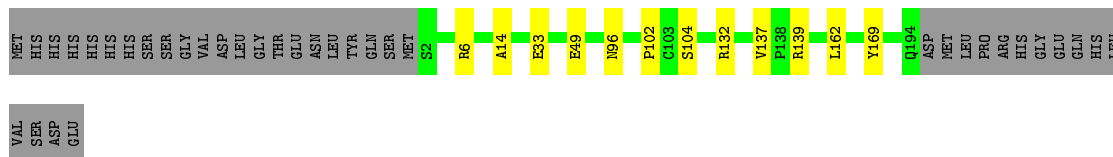
- Molecule 1: Flavin prenyltransferase UbiX

Chain G:  80% 15%




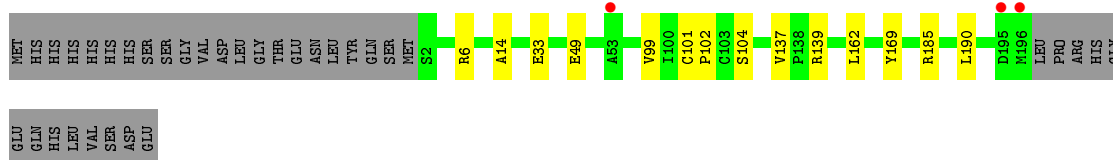
- Molecule 1: Flavin prenyltransferase UbiX

Chain H:  79% 5% 16%



- Molecule 1: Flavin prenyltransferase UbiX

Chain I:  79% 6% 15%



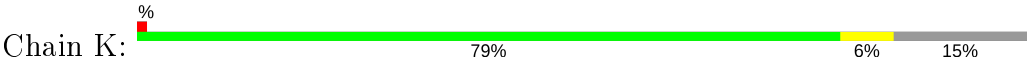
- Molecule 1: Flavin prenyltransferase UbiX

Chain J:  79% 5% 16%



GLU

- Molecule 1: Flavin prenyltransferase UbiX



LEU  
VAL  
SER  
ASP  
GLU

- Molecule 1: Flavin prenyltransferase UbiX



GLY  
GLU  
GLN  
HIS  
HIS  
LEU  
VAL  
SER  
ASP  
GLU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.53Å 164.93Å 102.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.40 – 2.39 115.40 – 2.39	Depositor EDS
% Data completeness (in resolution range)	100.0 (115.40-2.39) 92.7 (115.40-2.39)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, $R_{free}$	0.178 , 0.220 0.178 , 0.221	Depositor DCC
$R_{free}$ test set	2016 reflections (1.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtriage
Anisotropy	0.844	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18765	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PO4, FMN, ACT, HJN, HZZ

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	0.24	0/1475	0.40	0/2010
1	B	0.24	0/1501	0.40	0/2043
1	C	0.24	0/1464	0.40	0/1996
1	D	0.24	0/1523	0.40	0/2072
1	E	0.24	0/1488	0.40	0/2026
1	F	0.24	0/1491	0.40	0/2031
1	G	0.24	0/1487	0.40	0/2026
1	H	0.24	0/1460	0.39	0/1991
1	I	0.24	0/1480	0.40	0/2017
1	J	0.24	0/1468	0.40	0/2000
1	K	0.25	0/1488	0.41	0/2027
1	L	0.24	0/1464	0.40	0/1996
All	All	0.24	0/17789	0.40	0/24235

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 [i](#)

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	1428	0	1426	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1464	0	1474	9	0
1	C	1427	0	1431	8	0
1	D	1470	0	1484	10	0
1	E	1445	0	1463	6	0
1	F	1450	0	1455	9	0
1	G	1440	0	1435	5	0
1	H	1423	0	1425	7	0
1	I	1443	0	1444	9	0
1	J	1431	0	1442	8	0
1	K	1451	0	1462	8	0
1	L	1427	0	1431	9	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	G	15	0	0	0	0
2	H	15	0	0	0	0
2	I	15	0	0	0	0
2	J	15	0	0	0	0
2	K	15	0	0	0	0
2	L	15	0	0	0	0
3	A	31	0	19	0	0
3	B	31	0	19	0	0
3	D	31	0	19	0	0
3	E	31	0	19	0	0
3	F	31	0	19	0	0
3	H	31	0	19	0	0
3	J	31	0	19	0	0
3	K	31	0	19	0	0
3	L	31	0	19	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
4	F	4	0	3	0	0
4	G	4	0	3	0	0
4	H	4	0	3	0	0
4	I	4	0	3	0	0
4	J	4	0	3	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	1	0	0	0	0
6	C	41	0	0	0	0
6	G	41	0	0	1	0
6	I	41	0	0	0	0
7	D	5	0	0	0	0
7	E	5	0	0	0	0
7	F	5	0	0	0	0
8	A	68	0	0	0	0
8	B	79	0	0	0	0
8	C	74	0	0	0	0
8	D	97	0	0	0	0
8	E	74	0	0	1	0
8	F	66	0	0	1	0
8	G	77	0	0	0	0
8	H	73	0	0	0	0
8	I	59	0	0	0	0
8	J	71	0	0	1	0
8	K	71	0	0	0	0
8	L	70	0	0	0	0
All	All	18765	0	17564	83	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 83 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:D:185[A]:ARG:NH2	1:F:130:GLU:OE2	2.30	0.64
1:J:185:ARG:NH1	8:J:401:HOH:O	2.32	0.62
1:G:96:ASN:HA	1:G:132:ARG:HD3	1.84	0.59
1:E:96:ASN:HA	1:E:132:ARG:HD3	1.86	0.57
1:A:49:GLU:HG2	1:H:169:TYR:HA	1.86	0.57

There are no symmetry-related clashes.

## 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	193/230 (84%)	189 (98%)	4 (2%)	0	100	100
1	B	196/230 (85%)	191 (97%)	5 (3%)	0	100	100
1	C	192/230 (84%)	188 (98%)	4 (2%)	0	100	100
1	D	198/230 (86%)	194 (98%)	4 (2%)	0	100	100
1	E	194/230 (84%)	190 (98%)	4 (2%)	0	100	100
1	F	195/230 (85%)	190 (97%)	5 (3%)	0	100	100
1	G	195/230 (85%)	190 (97%)	5 (3%)	0	100	100
1	H	192/230 (84%)	188 (98%)	4 (2%)	0	100	100
1	I	194/230 (84%)	190 (98%)	4 (2%)	0	100	100
1	J	192/230 (84%)	188 (98%)	4 (2%)	0	100	100
1	K	195/230 (85%)	190 (97%)	5 (3%)	0	100	100
1	L	192/230 (84%)	188 (98%)	4 (2%)	0	100	100
All	All	2328/2760 (84%)	2276 (98%)	52 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	153/186 (82%)	150 (98%)	3 (2%)	55	74
1	B	157/186 (84%)	153 (98%)	4 (2%)	47	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	152/186 (82%)	151 (99%)	1 (1%)	84	92
1	D	159/186 (86%)	157 (99%)	2 (1%)	69	84
1	E	155/186 (83%)	150 (97%)	5 (3%)	39	59
1	F	155/186 (83%)	154 (99%)	1 (1%)	86	94
1	G	154/186 (83%)	152 (99%)	2 (1%)	69	84
1	H	151/186 (81%)	150 (99%)	1 (1%)	84	92
1	I	154/186 (83%)	153 (99%)	1 (1%)	86	94
1	J	153/186 (82%)	152 (99%)	1 (1%)	84	92
1	K	155/186 (83%)	154 (99%)	1 (1%)	86	94
1	L	152/186 (82%)	150 (99%)	2 (1%)	69	84
All	All	1850/2232 (83%)	1826 (99%)	24 (1%)	69	84

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	2	SER
1	E	185[A]	ARG
1	L	2	SER
1	E	85	MET
1	E	139	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	96	ASN
1	G	43	GLN
1	J	96	ASN
1	J	188	ASN
1	K	29	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 7 are monoatomic - leaving 31 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
7	PO4	E	302	-	4,4,4	0.92	0	6,6,6	0.40	0
2	HZZ	G	301	-	14,14,14	1.07	1 (7%)	17,18,18	1.40	4 (23%)
4	ACT	I	303	-	1,3,3	6.44	1 (100%)	0,3,3	0.00	-
3	FMN	H	301	-	31,33,33	1.47	6 (19%)	40,50,50	2.39	8 (20%)
3	FMN	J	301	-	31,33,33	1.48	6 (19%)	40,50,50	2.39	8 (20%)
2	HZZ	H	302	-	14,14,14	1.06	1 (7%)	17,18,18	1.43	4 (23%)
6	HJN	I	304	-	40,43,43	1.10	4 (10%)	48,63,63	2.14	9 (18%)
6	HJN	C	303	-	40,43,43	1.06	4 (10%)	48,63,63	2.09	8 (16%)
2	HZZ	L	302	-	14,14,14	1.07	1 (7%)	17,18,18	1.44	3 (17%)
4	ACT	F	302	-	1,3,3	6.90	1 (100%)	0,3,3	0.00	-
2	HZZ	C	301	-	14,14,14	1.07	1 (7%)	17,18,18	1.38	3 (17%)
2	HZZ	I	302	-	14,14,14	1.06	1 (7%)	17,18,18	1.48	3 (17%)
4	ACT	B	302	-	1,3,3	6.41	1 (100%)	0,3,3	0.00	-
4	ACT	J	302	-	1,3,3	6.54	1 (100%)	0,3,3	0.00	-
3	FMN	B	301	-	31,33,33	1.47	6 (19%)	40,50,50	2.39	8 (20%)
4	ACT	G	302	-	1,3,3	6.45	1 (100%)	0,3,3	0.00	-
6	HJN	G	303	-	40,43,43	1.10	4 (10%)	48,63,63	2.15	9 (18%)
3	FMN	E	301	-	31,33,33	1.48	6 (19%)	40,50,50	2.38	7 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	PO4	D	303	-	4,4,4	0.95	0	6,6,6	0.39	0
7	PO4	F	304	-	4,4,4	0.91	0	6,6,6	0.46	0
3	FMN	K	302	-	31,33,33	1.48	6 (19%)	40,50,50	2.39	8 (20%)
2	HZZ	B	303	-	14,14,14	1.07	1 (7%)	17,18,18	1.42	3 (17%)
3	FMN	A	302	-	31,33,33	1.48	6 (19%)	40,50,50	2.40	7 (17%)
3	FMN	D	302	-	31,33,33	1.46	6 (19%)	40,50,50	2.39	8 (20%)
4	ACT	C	302	-	1,3,3	6.40	1 (100%)	0,3,3	0.00	-
2	HZZ	K	301	-	14,14,14	1.07	1 (7%)	17,18,18	1.44	4 (23%)
2	HZZ	J	303	-	14,14,14	1.07	1 (7%)	17,18,18	1.44	4 (23%)
4	ACT	H	303	-	1,3,3	6.49	1 (100%)	0,3,3	0.00	-
2	HZZ	A	301	-	14,14,14	1.06	1 (7%)	17,18,18	1.45	4 (23%)
3	FMN	F	301	-	31,33,33	1.47	6 (19%)	40,50,50	2.38	7 (17%)
3	FMN	L	301	-	31,33,33	1.47	6 (19%)	40,50,50	2.39	7 (17%)

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	HZZ	K	301	-	-	3/13/13/13	-
6	HJN	I	304	-	-	6/29/29/29	0/3/3/3
2	HZZ	J	303	-	-	3/13/13/13	-
2	HZZ	G	301	-	-	5/13/13/13	-
3	FMN	J	301	-	-	0/18/18/18	0/3/3/3
3	FMN	B	301	-	-	1/18/18/18	0/3/3/3
2	HZZ	I	302	-	-	2/13/13/13	-
2	HZZ	A	301	-	-	3/13/13/13	-
2	HZZ	B	303	-	-	6/13/13/13	-
3	FMN	F	301	-	-	1/18/18/18	0/3/3/3
3	FMN	H	301	-	-	1/18/18/18	0/3/3/3
3	FMN	A	302	-	-	1/18/18/18	0/3/3/3
3	FMN	L	301	-	-	1/18/18/18	0/3/3/3
3	FMN	D	302	-	-	1/18/18/18	0/3/3/3
3	FMN	K	302	-	-	1/18/18/18	0/3/3/3
2	HZZ	C	301	-	-	1/13/13/13	-
2	HZZ	H	302	-	-	3/13/13/13	-
6	HJN	G	303	-	-	6/29/29/29	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	E	301	-	-	1/18/18/18	0/3/3/3
6	HJN	C	303	-	-	6/29/29/29	0/3/3/3
2	HZZ	L	302	-	-	3/13/13/13	-

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	302	ACT	CH3-C	6.90	1.57	1.48
4	J	302	ACT	CH3-C	6.54	1.57	1.48
4	H	303	ACT	CH3-C	6.49	1.57	1.48
4	G	302	ACT	CH3-C	6.45	1.57	1.48
4	I	303	ACT	CH3-C	6.44	1.56	1.48

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	303	HJN	C16-N3-C17	12.03	125.30	115.14
6	I	304	HJN	C16-N3-C17	12.01	125.28	115.14
6	C	303	HJN	C16-N3-C17	11.93	125.21	115.14
3	J	301	FMN	C4-N3-C2	11.83	125.13	115.14
3	A	302	FMN	C4-N3-C2	11.81	125.11	115.14

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	304	HJN	C19-C18-N2-C8
6	I	304	HJN	C19-C18-N2-C9
6	I	304	HJN	N2-C18-C19-C20
6	C	303	HJN	C19-C18-N2-C9
6	C	303	HJN	C18-C19-C20-C22

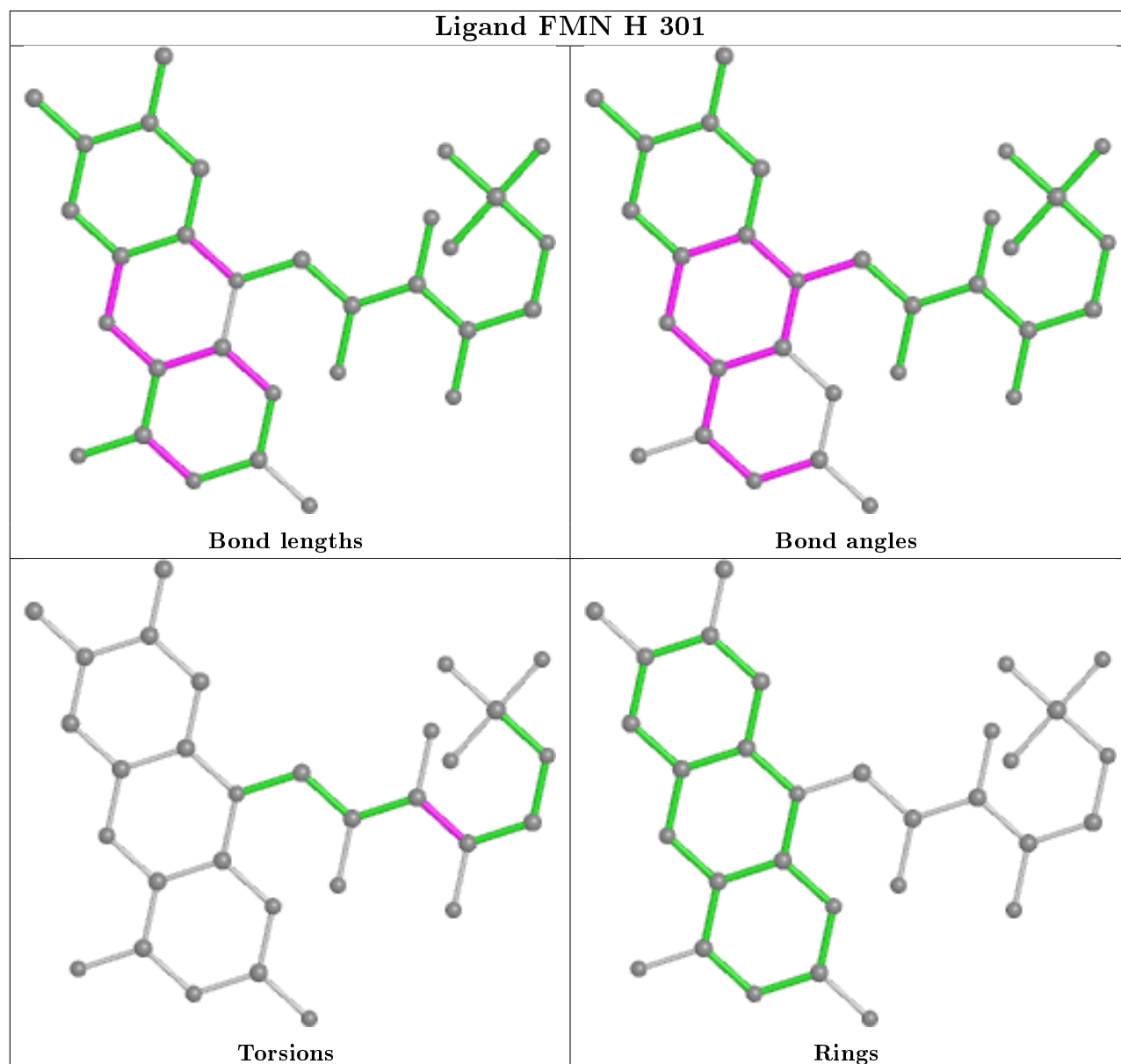
There are no ring outliers.

1 monomer is involved in 1 short contact:

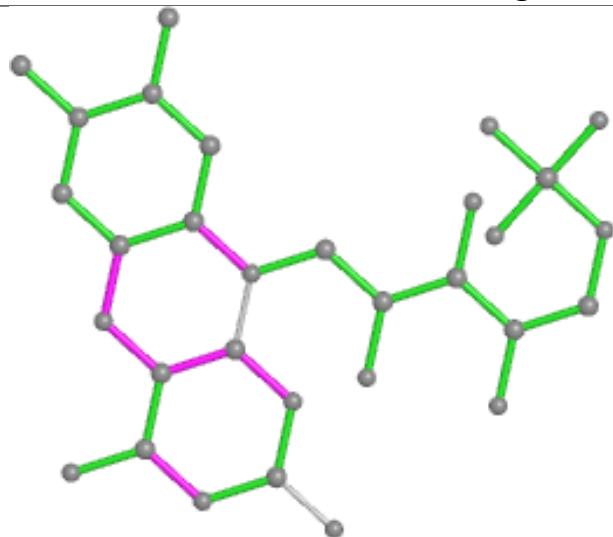
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	303	HJN	1	0

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

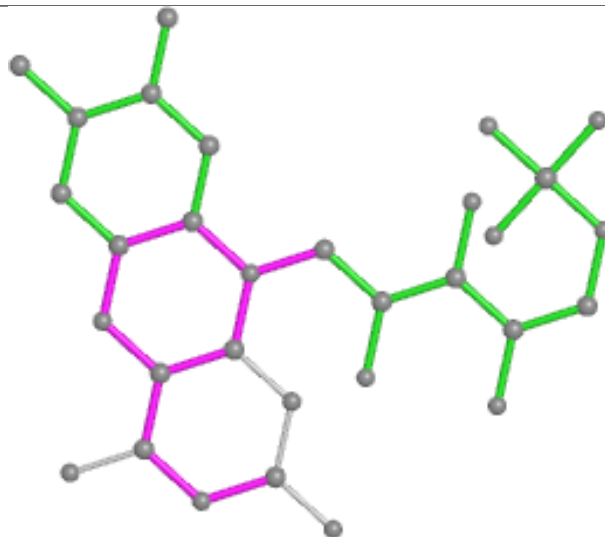
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



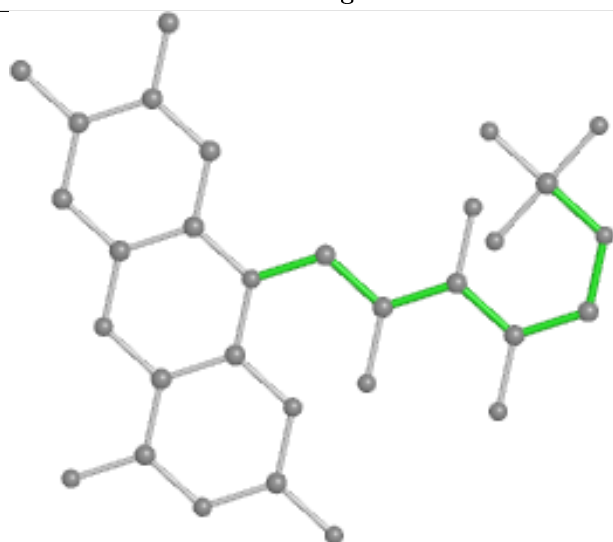
## Ligand FMN J 301



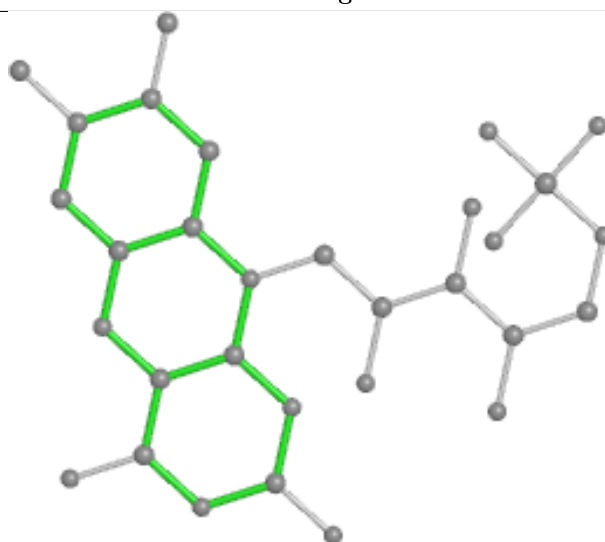
Bond lengths



Bond angles

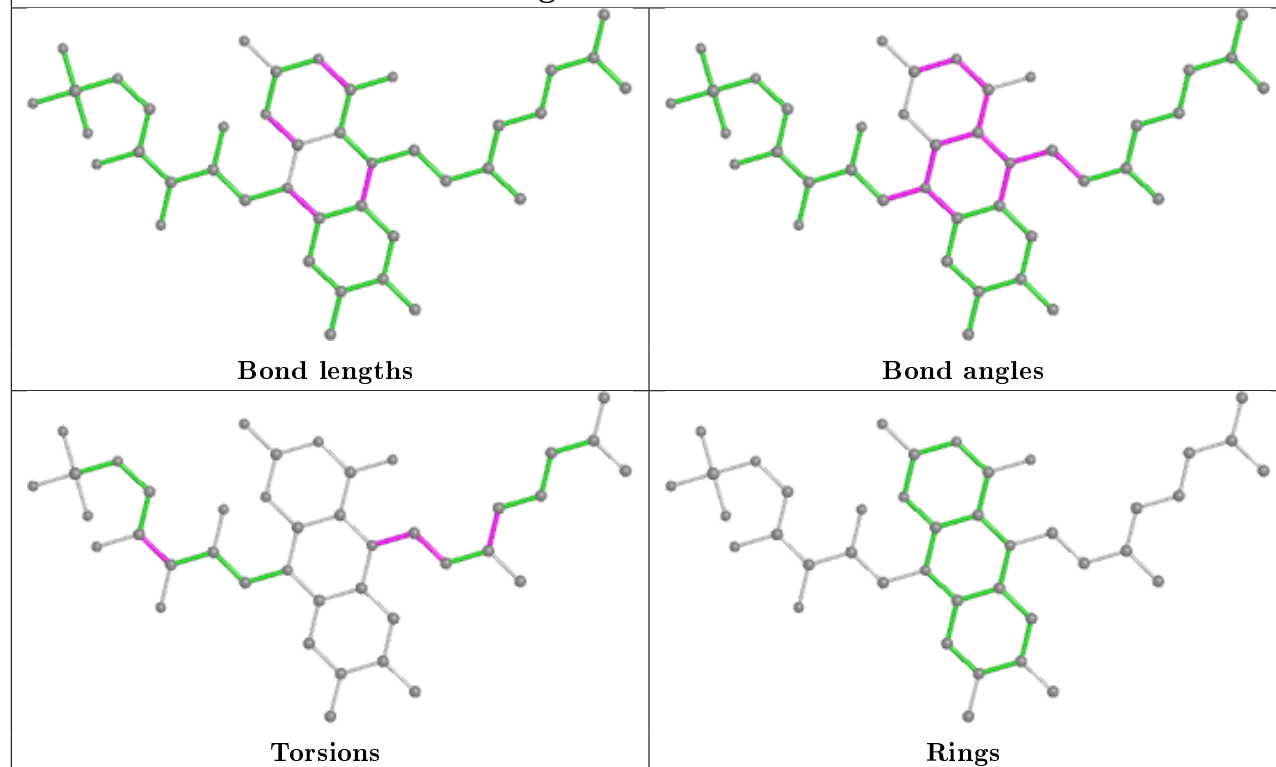


Torsions

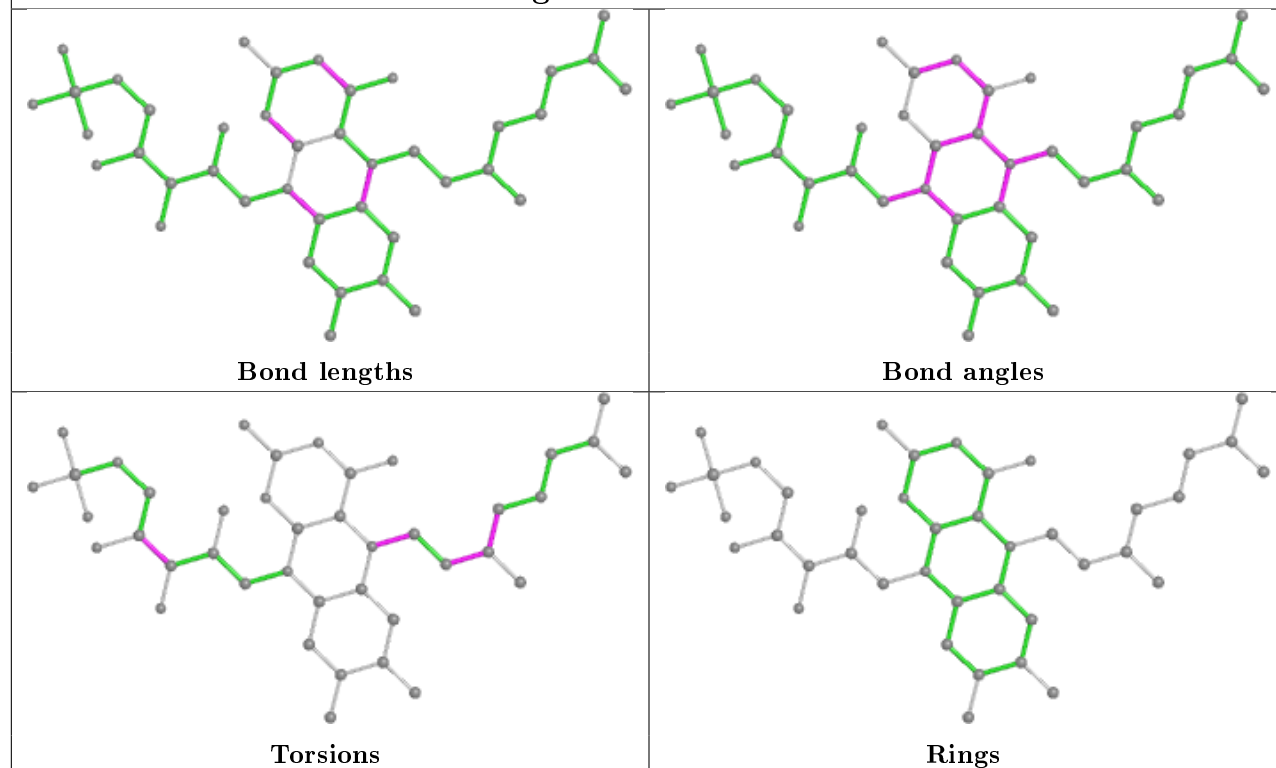


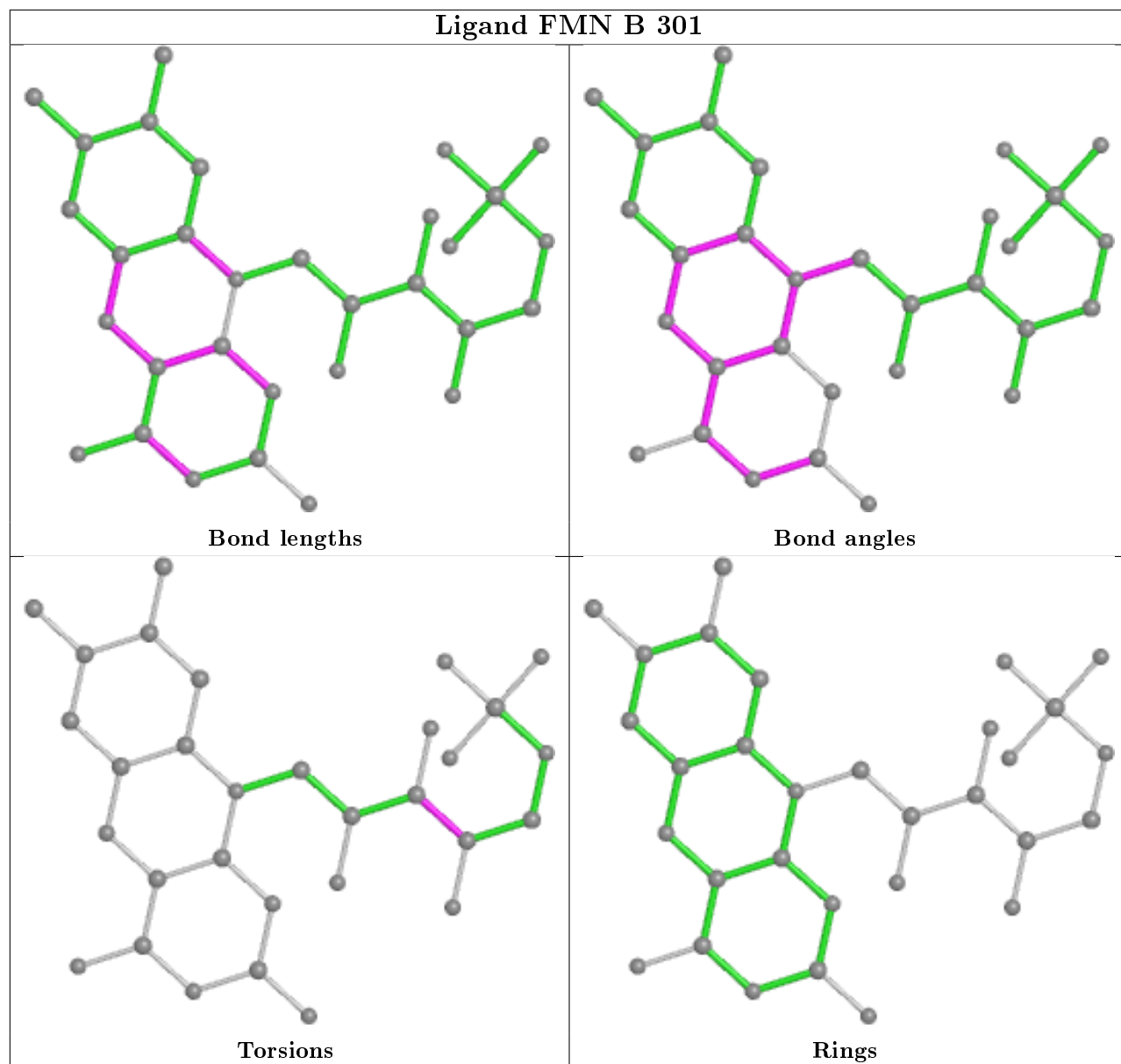
Rings

## Ligand HJN I 304

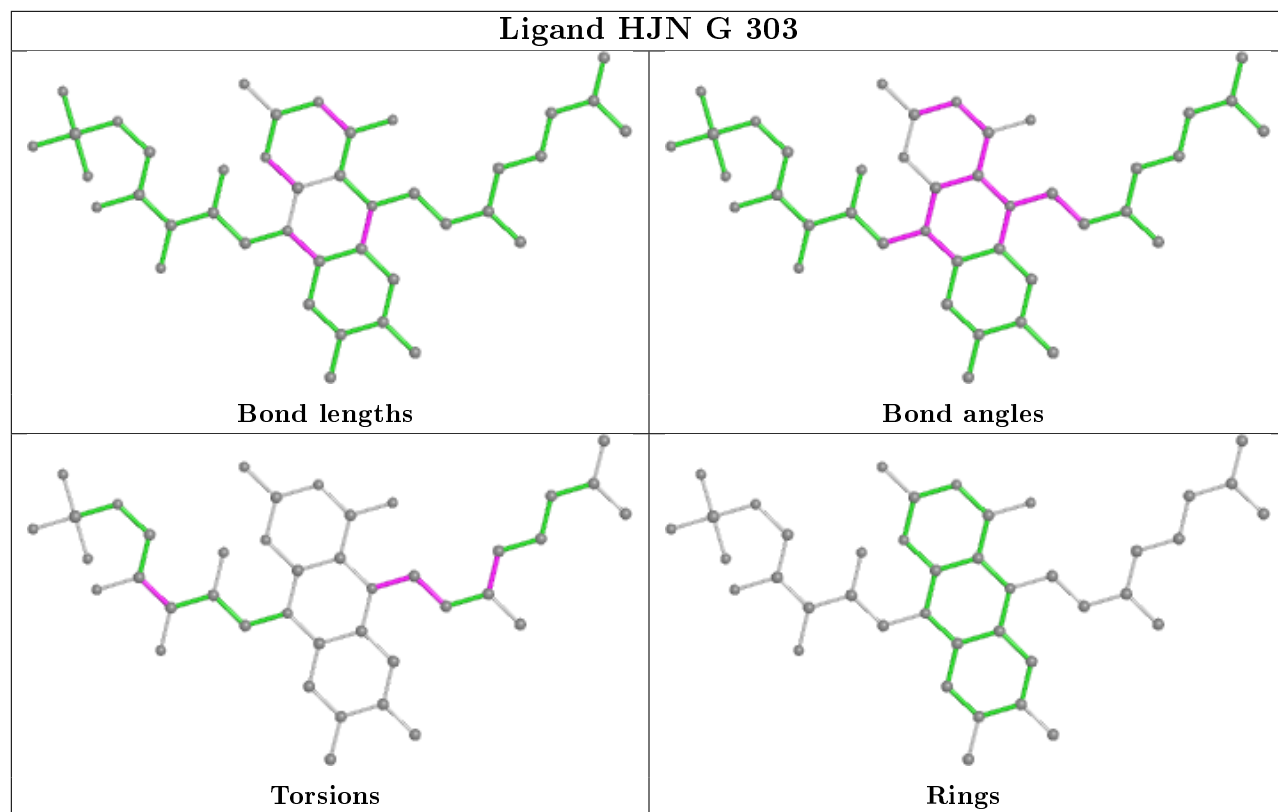


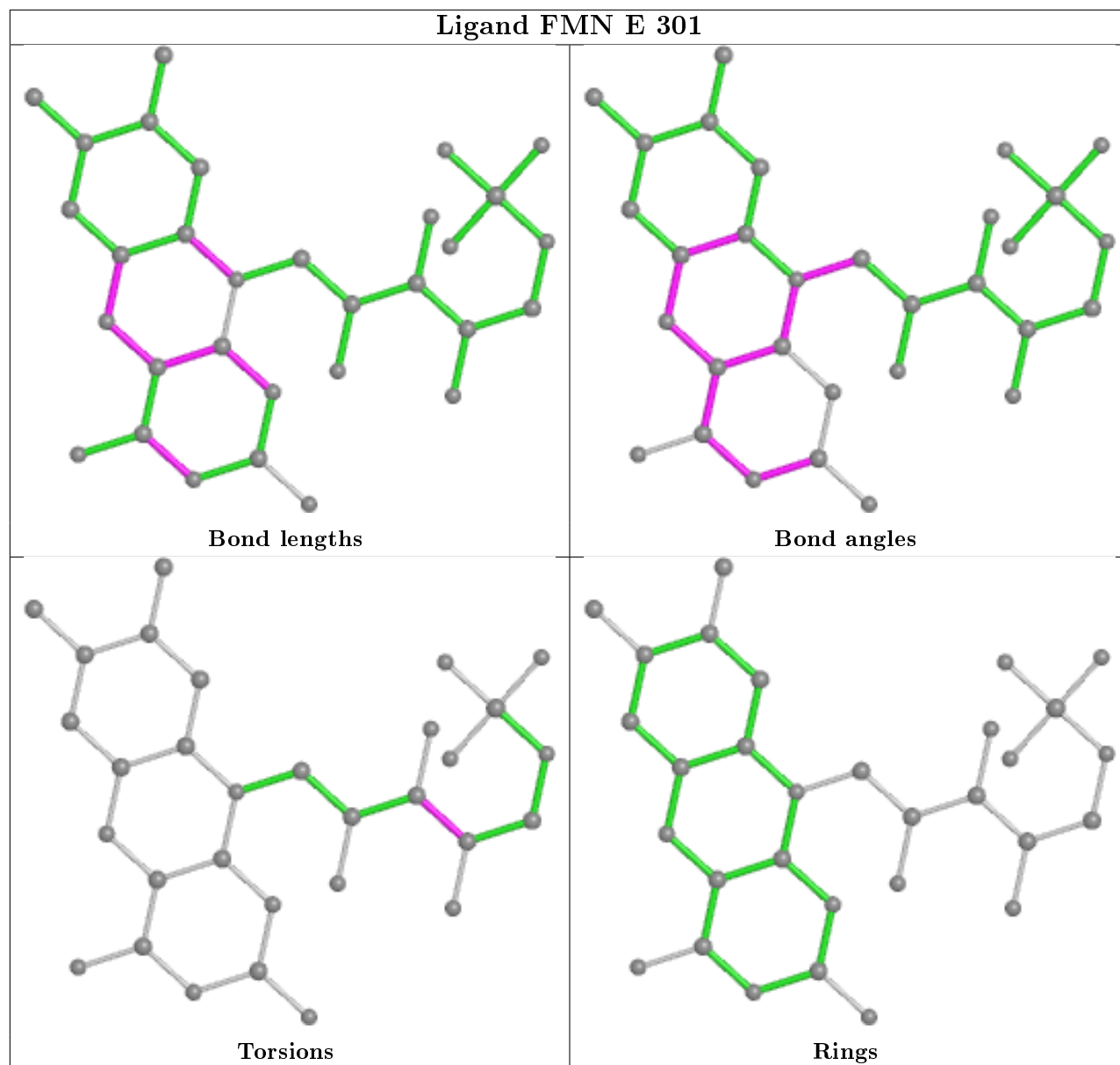
## Ligand HJN C 303

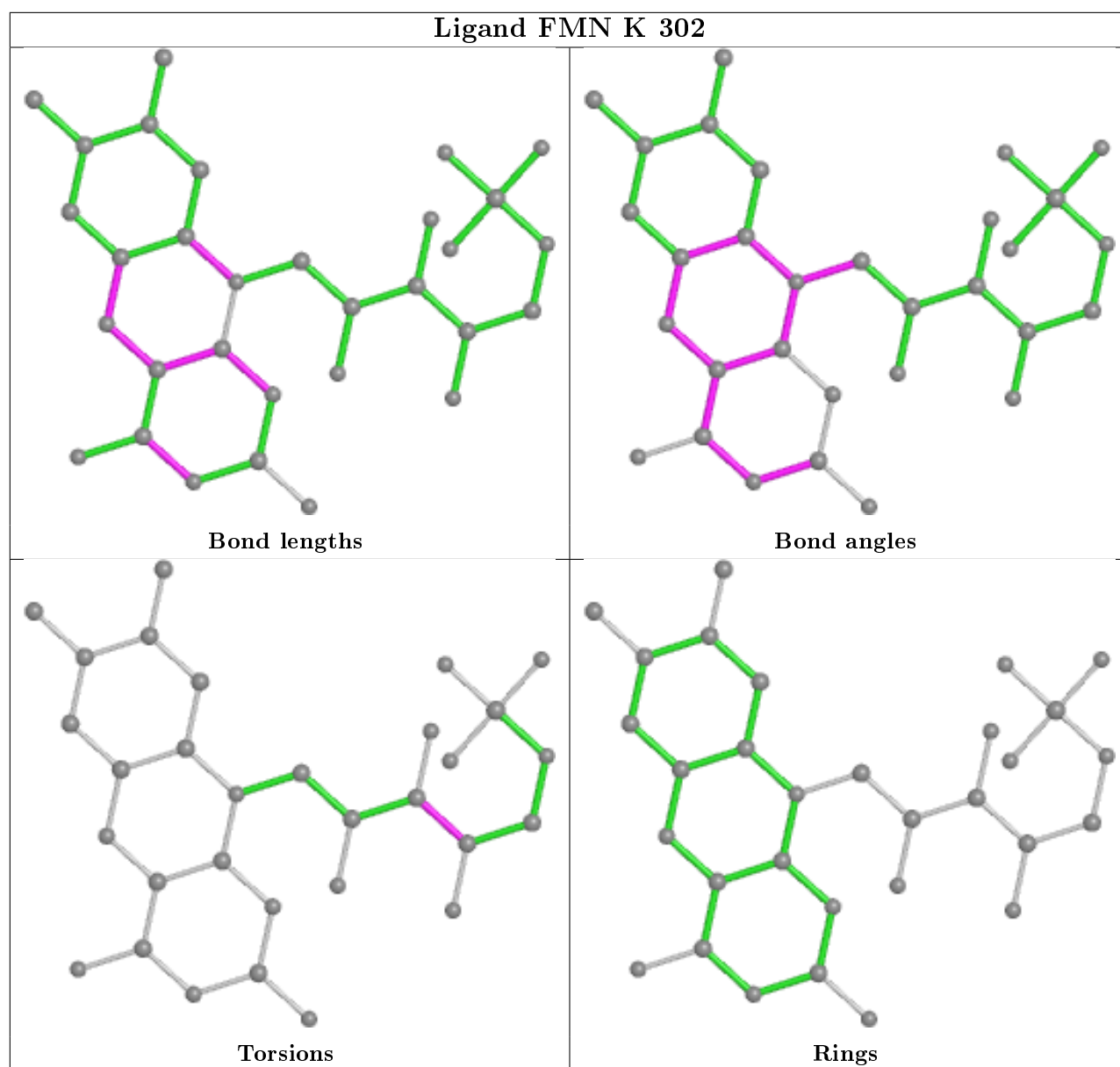


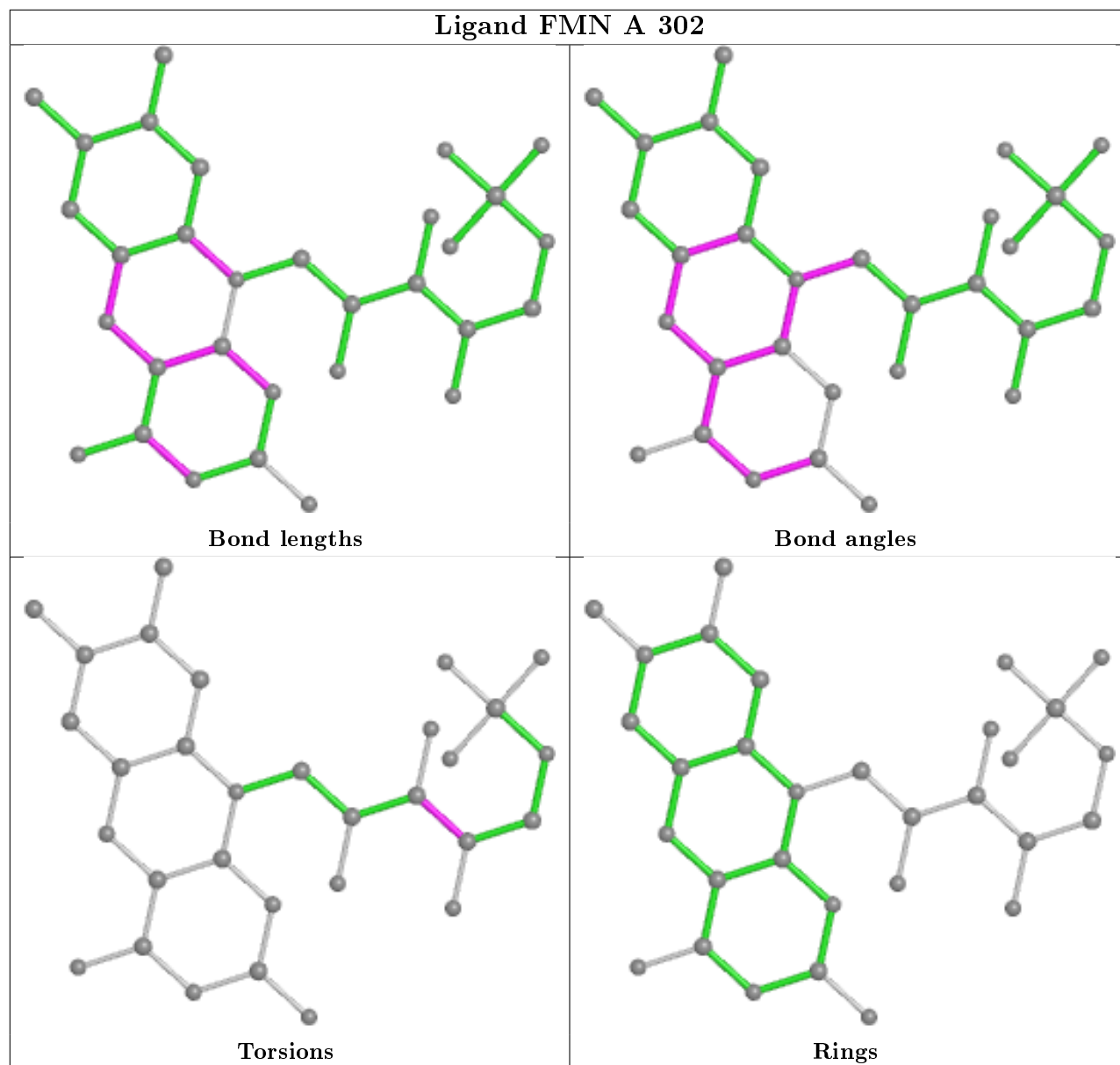


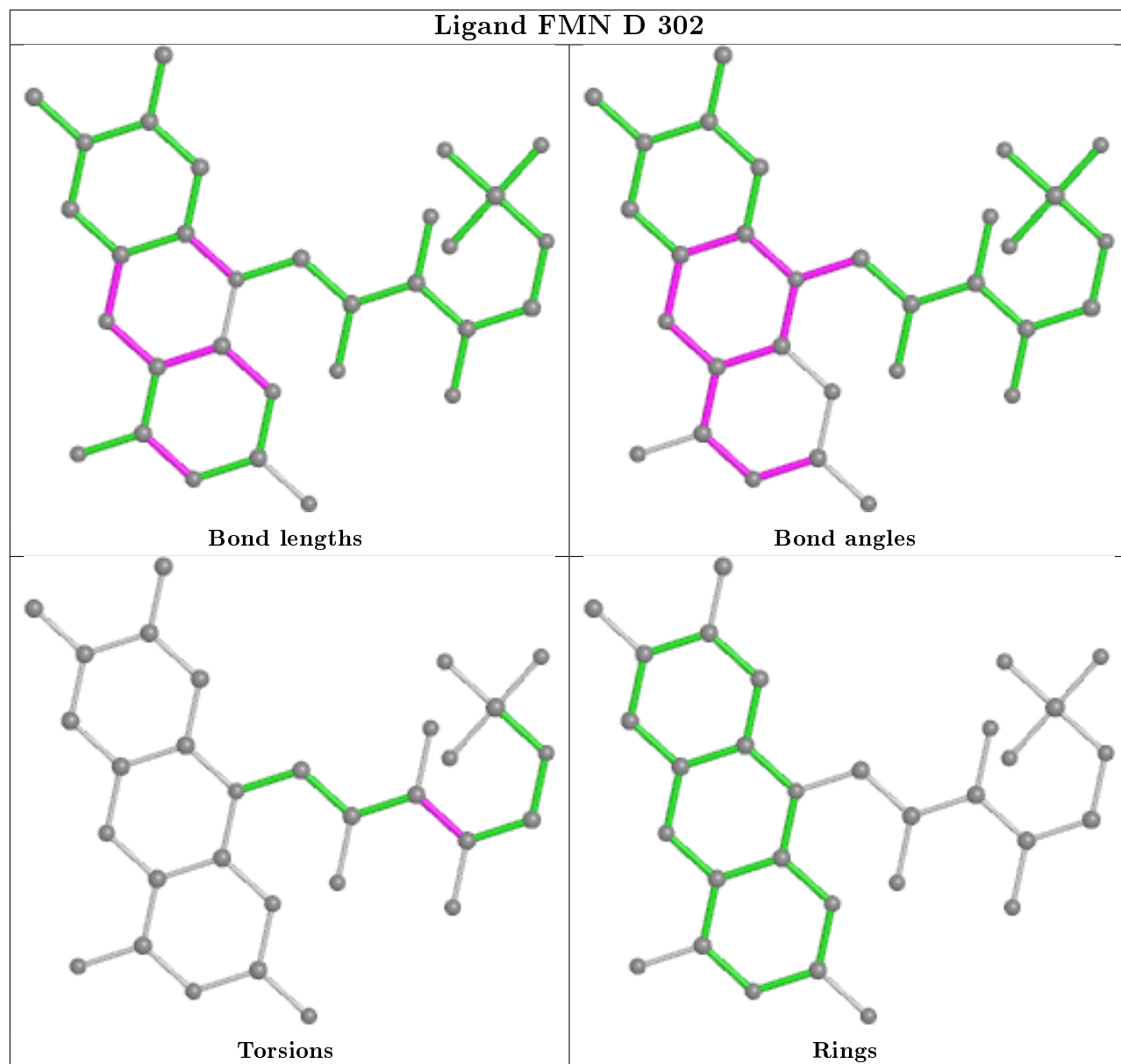


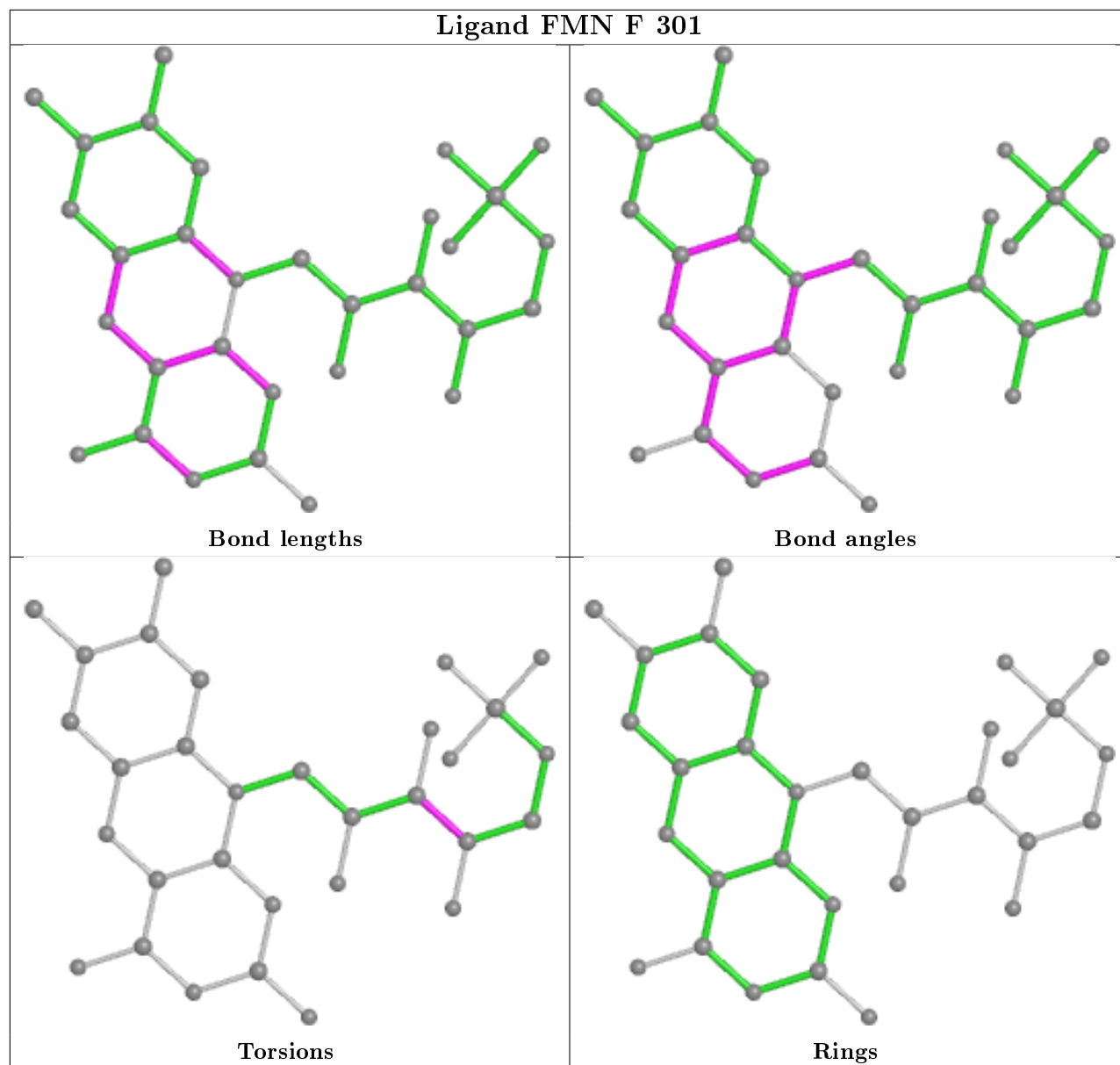


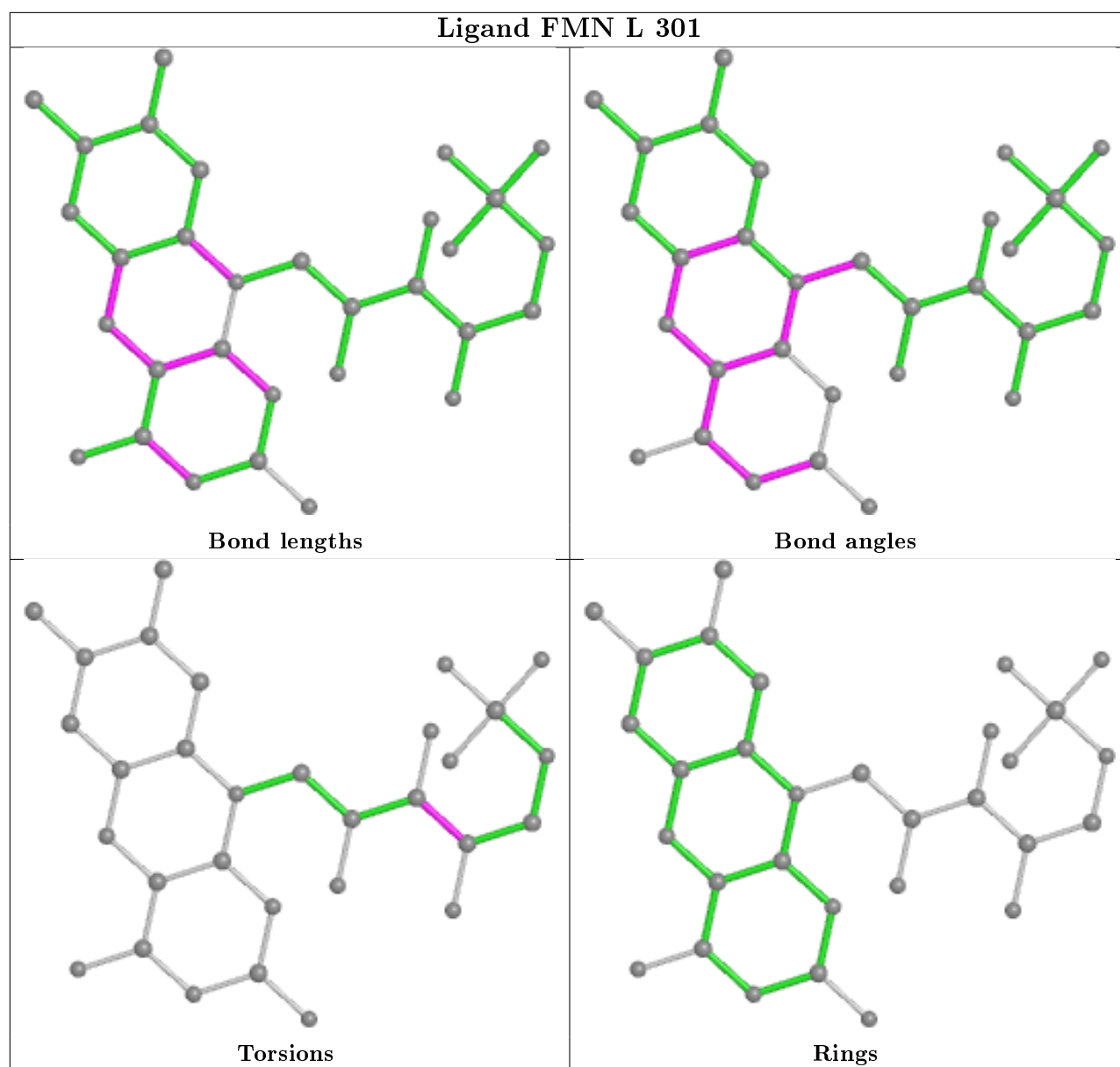












## 5.7 Other polymers [i](#)

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	193/230 (83%)	-0.28	1 (0%) 91 89	17, 29, 49, 67	0
1	B	196/230 (85%)	-0.24	2 (1%) 82 80	19, 30, 54, 103	0
1	C	193/230 (83%)	-0.26	0 100 100	20, 28, 51, 71	0
1	D	195/230 (84%)	-0.19	1 (0%) 91 89	18, 27, 49, 90	0
1	E	193/230 (83%)	-0.21	1 (0%) 91 89	20, 29, 50, 78	0
1	F	195/230 (84%)	-0.21	1 (0%) 91 89	19, 32, 57, 97	0
1	G	195/230 (84%)	-0.25	1 (0%) 91 89	18, 27, 52, 88	0
1	H	193/230 (83%)	-0.21	0 100 100	19, 30, 53, 83	0
1	I	195/230 (84%)	-0.20	3 (1%) 73 72	19, 33, 60, 92	0
1	J	193/230 (83%)	-0.23	0 100 100	20, 31, 54, 76	0
1	K	196/230 (85%)	-0.25	2 (1%) 82 80	21, 32, 56, 85	0
1	L	193/230 (83%)	-0.23	1 (0%) 91 89	19, 33, 60, 82	0
All	All	2330/2760 (84%)	-0.23	13 (0%) 89 88	17, 30, 55, 103	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	3.6
1	B	1	MET	3.3
1	F	196	MET	2.8
1	E	194	GLN	2.5
1	I	195	ASP	2.4

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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



## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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, 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.

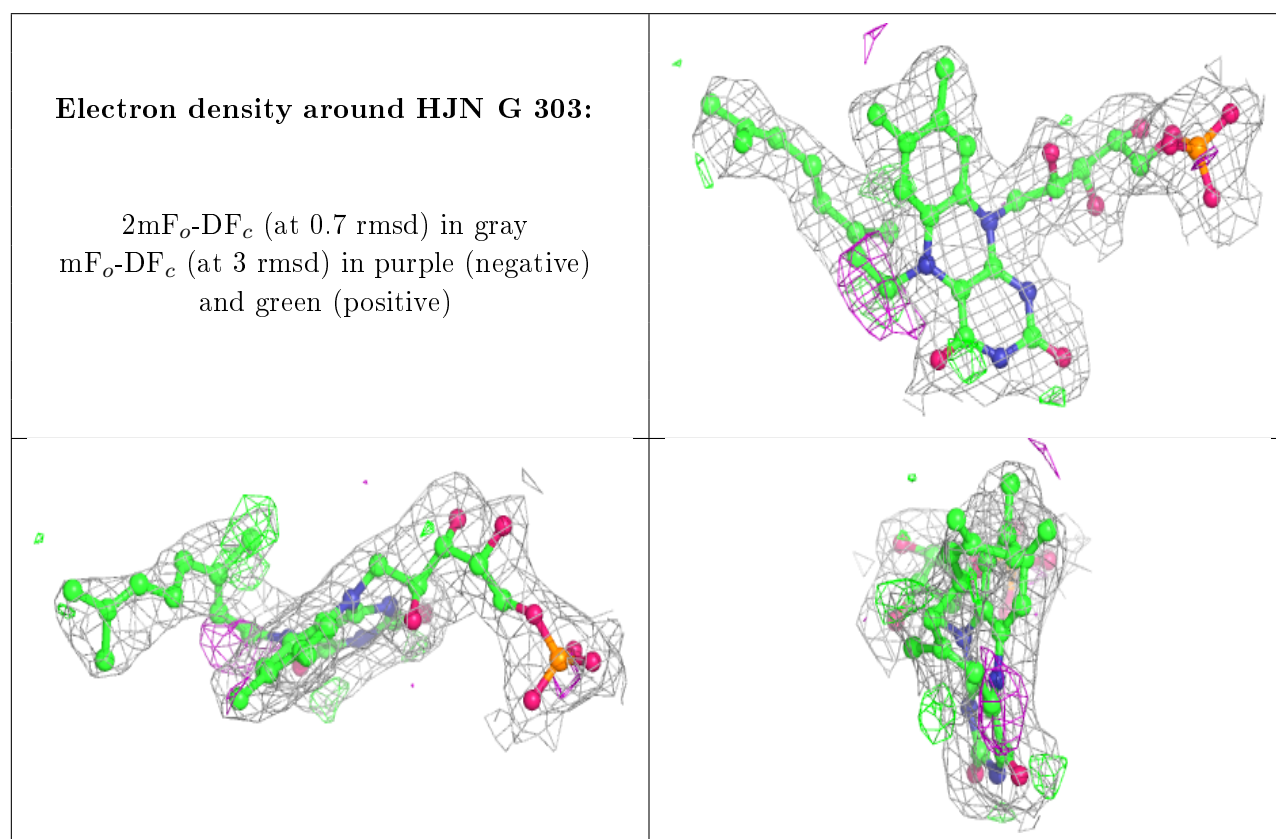
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NA	D	301	1/1	0.40	0.17	38,38,38,38	0
5	NA	J	304	1/1	0.47	0.15	48,48,48,48	0
5	NA	B	304	1/1	0.53	0.13	50,50,50,50	0
4	ACT	J	302	4/4	0.73	0.24	43,50,50,54	0
5	NA	F	303	1/1	0.78	0.20	47,47,47,47	0
4	ACT	H	303	4/4	0.82	0.18	42,43,46,51	0
5	NA	I	301	1/1	0.82	0.10	48,48,48,48	0
4	ACT	C	302	4/4	0.82	0.18	56,58,58,60	0
5	NA	G	304	1/1	0.83	0.21	72,72,72,72	0
4	ACT	F	302	4/4	0.84	0.20	38,46,47,49	0
4	ACT	G	302	4/4	0.84	0.21	41,45,47,48	0
4	ACT	B	302	4/4	0.86	0.20	46,47,47,49	0
5	NA	C	304	1/1	0.88	0.14	56,56,56,56	0
4	ACT	I	303	4/4	0.91	0.12	43,45,46,46	0
6	HJN	G	303	41/41	0.94	0.15	19,27,49,51	0
2	HZZ	B	303	15/15	0.94	0.19	26,34,51,52	0
2	HZZ	L	302	15/15	0.95	0.17	33,46,49,49	0
6	HJN	C	303	41/41	0.95	0.15	16,28,48,50	0
2	HZZ	C	301	15/15	0.95	0.19	29,37,52,55	0
2	HZZ	H	302	15/15	0.95	0.19	24,42,50,51	0
2	HZZ	I	302	15/15	0.95	0.18	33,44,51,51	0
6	HJN	I	304	41/41	0.95	0.14	19,31,51,52	0
2	HZZ	K	301	15/15	0.96	0.19	31,47,56,57	0
3	FMN	J	301	31/31	0.96	0.13	19,26,28,30	0
2	HZZ	A	301	15/15	0.96	0.17	27,40,55,56	0
3	FMN	F	301	31/31	0.96	0.12	25,28,32,35	0
2	HZZ	G	301	15/15	0.96	0.17	32,42,48,49	0
3	FMN	E	301	31/31	0.96	0.12	18,26,28,29	0
3	FMN	K	302	31/31	0.97	0.12	19,25,30,33	0
2	HZZ	J	303	15/15	0.97	0.20	27,42,49,50	0
7	PO4	D	303	5/5	0.97	0.14	26,28,33,39	0
3	FMN	A	302	31/31	0.97	0.12	21,26,33,34	0

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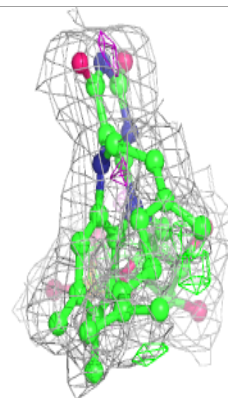
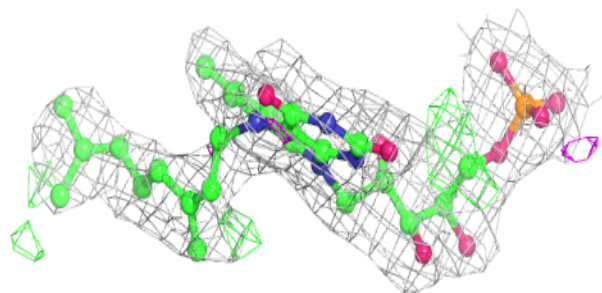
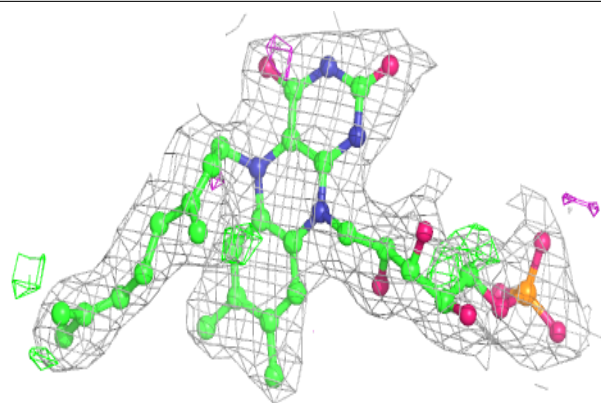
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FMN	D	302	31/31	0.97	0.14	17,26,30,32	0
3	FMN	L	301	31/31	0.97	0.12	22,30,32,33	0
3	FMN	B	301	31/31	0.97	0.12	20,25,31,32	0
3	FMN	H	301	31/31	0.97	0.12	19,24,29,29	0
7	PO4	E	302	5/5	0.98	0.11	21,26,29,33	0
7	PO4	F	304	5/5	0.99	0.11	28,30,33,33	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.

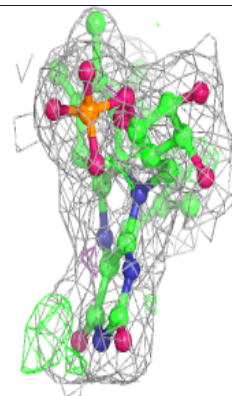
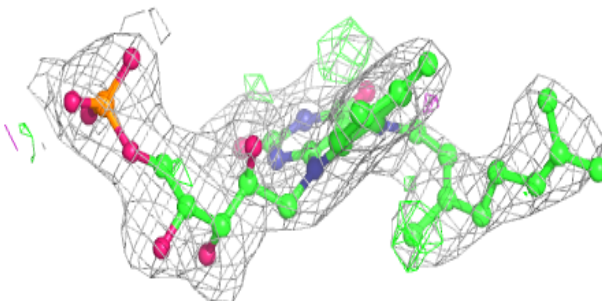
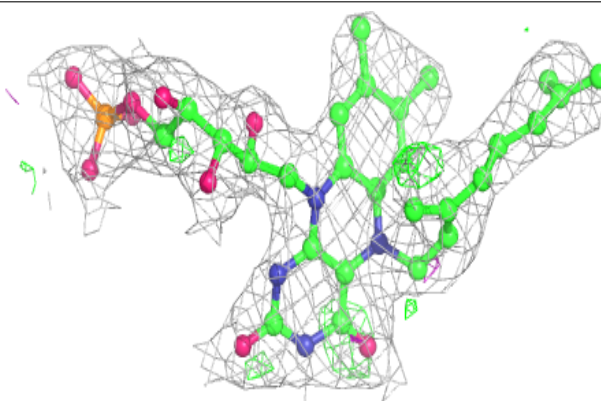


**Electron density around HJN C 303:**

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

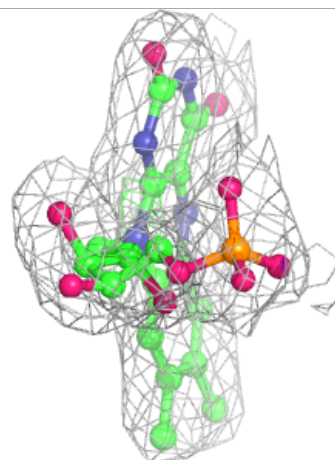
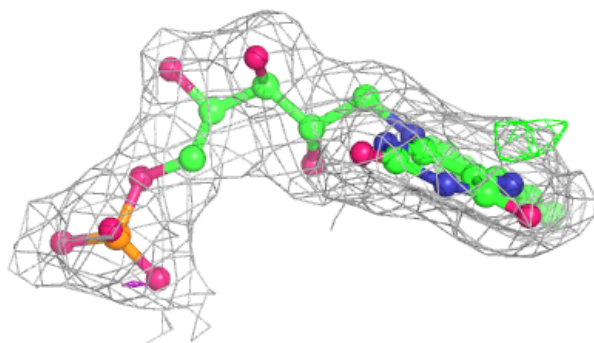
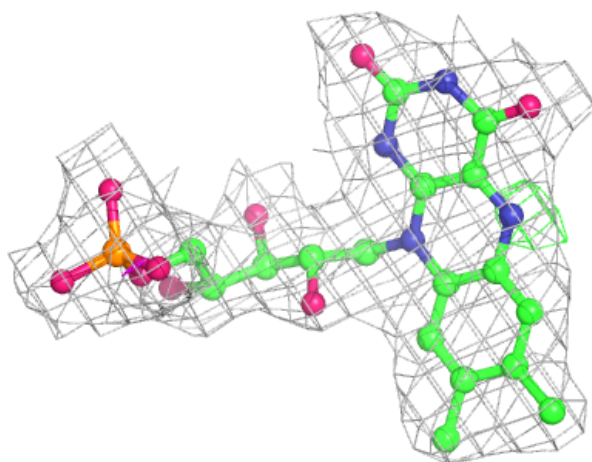
**Electron density around HJN I 304:**

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



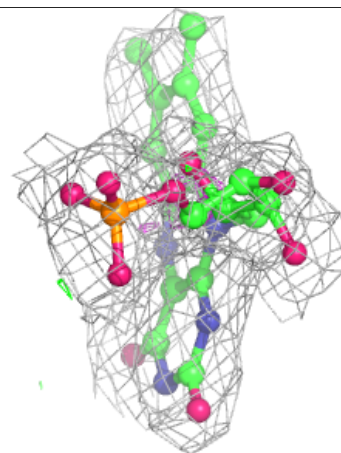
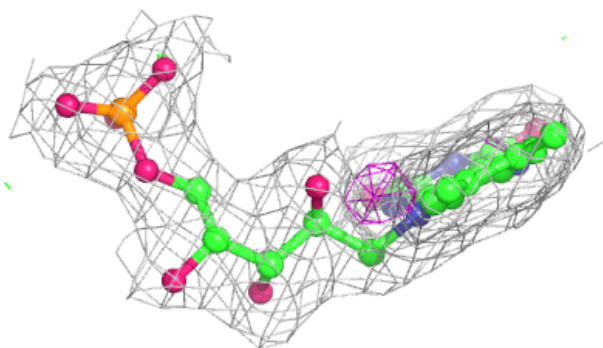
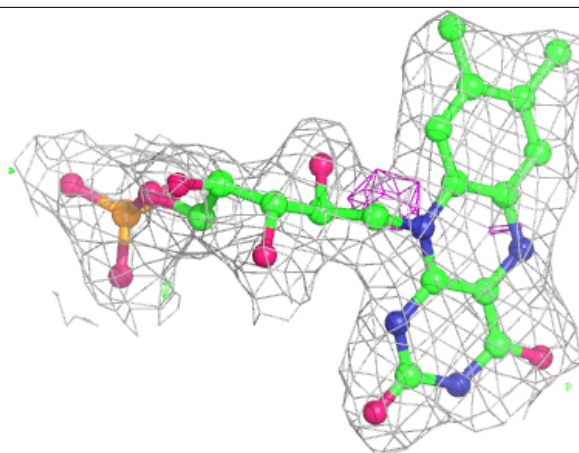
**Electron density around FMN J 301:**

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



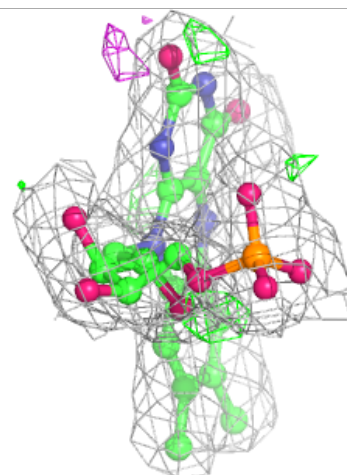
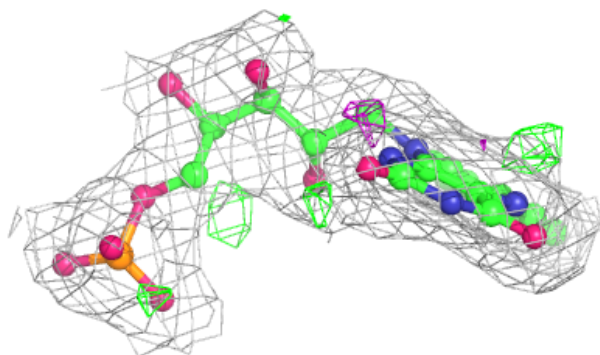
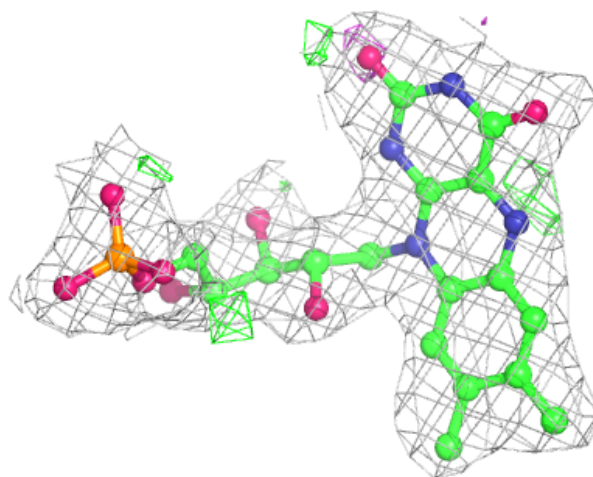
**Electron density around FMN F 301:**

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



**Electron density around FMN E 301:**

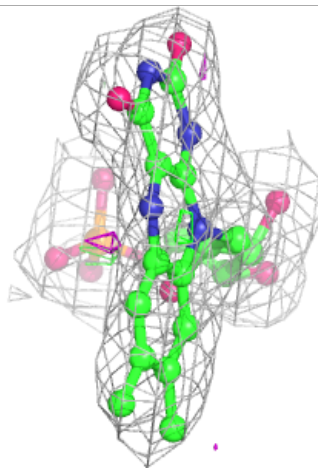
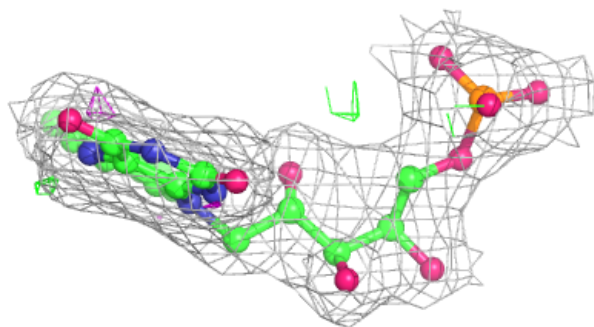
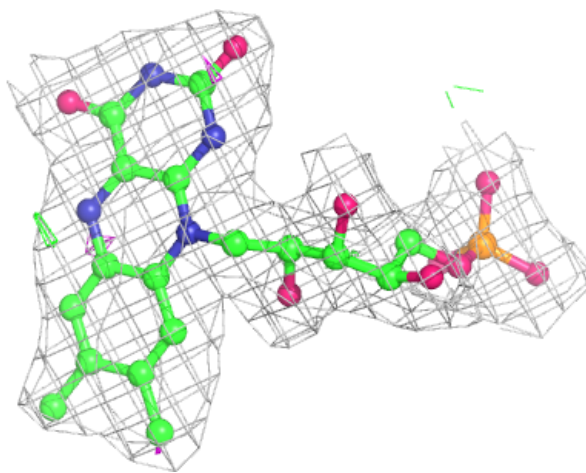
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





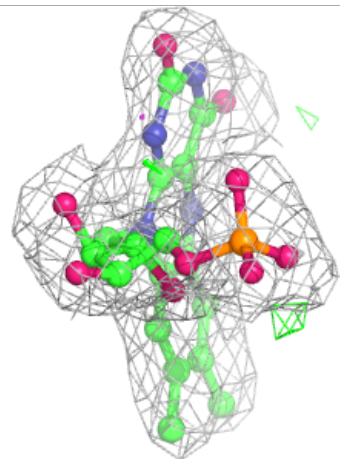
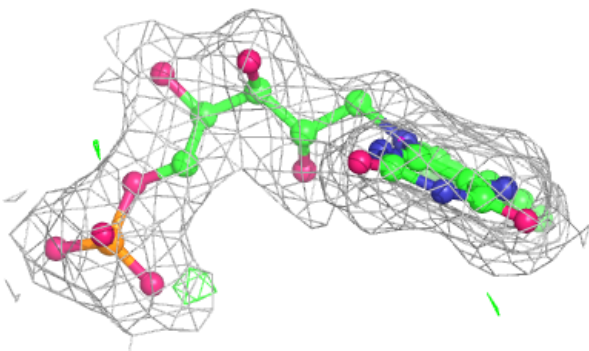
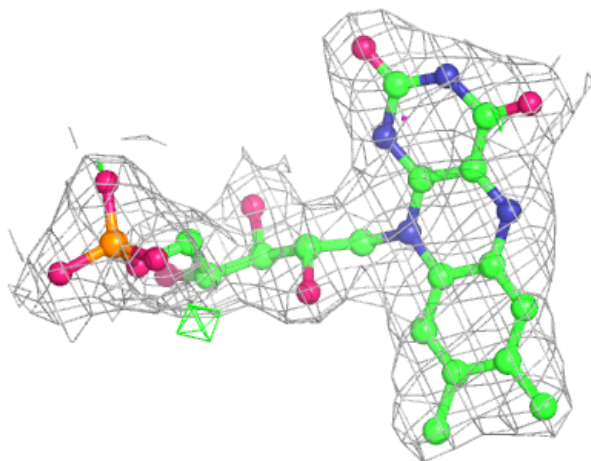
**Electron density around FMN K 302:**

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



**Electron density around FMN A 302:**

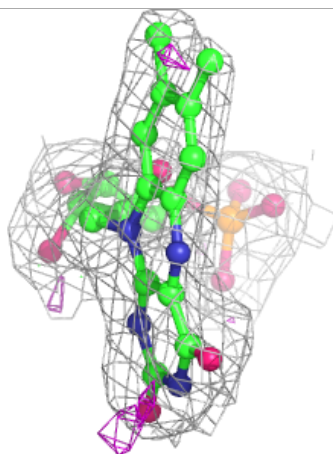
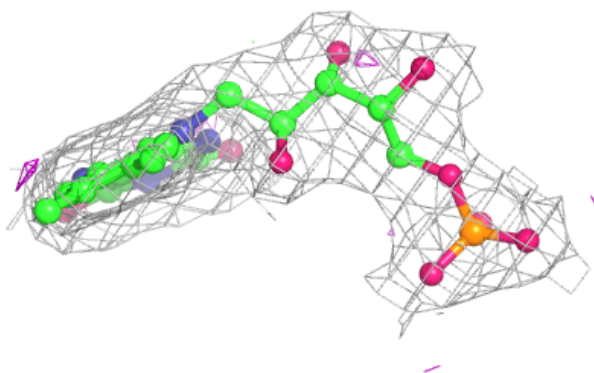
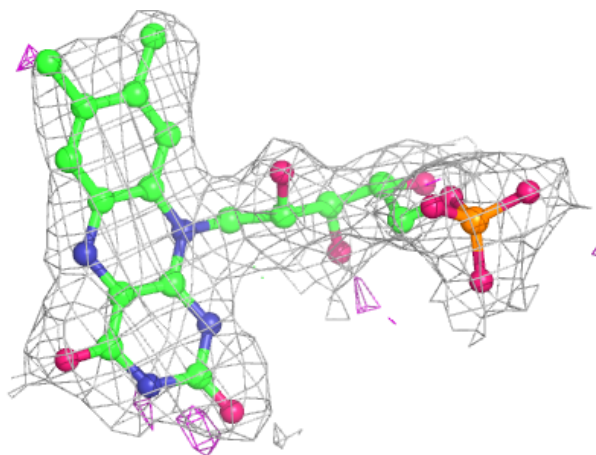
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





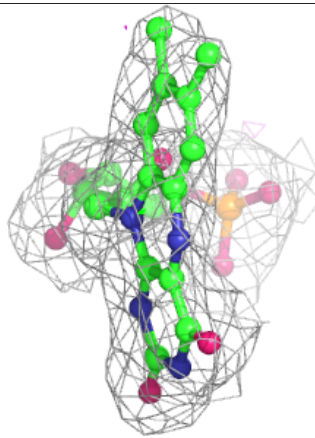
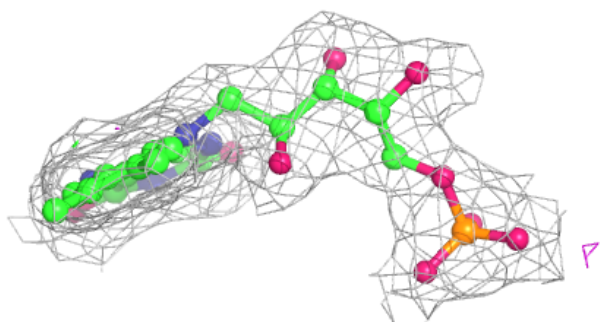
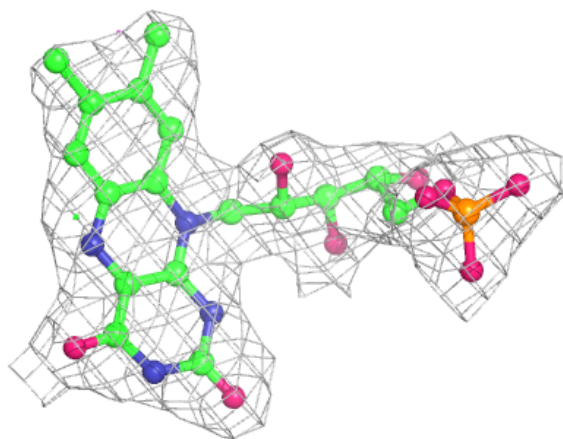
**Electron density around FMN D 302:**

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



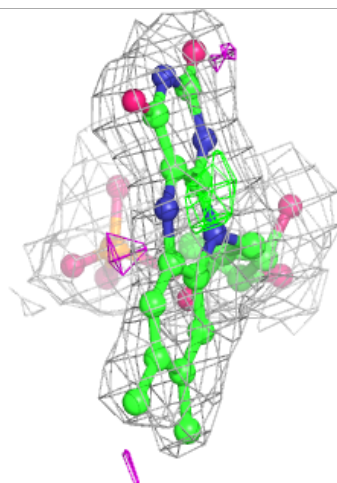
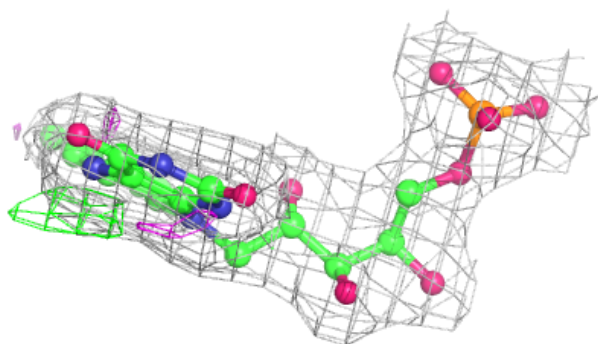
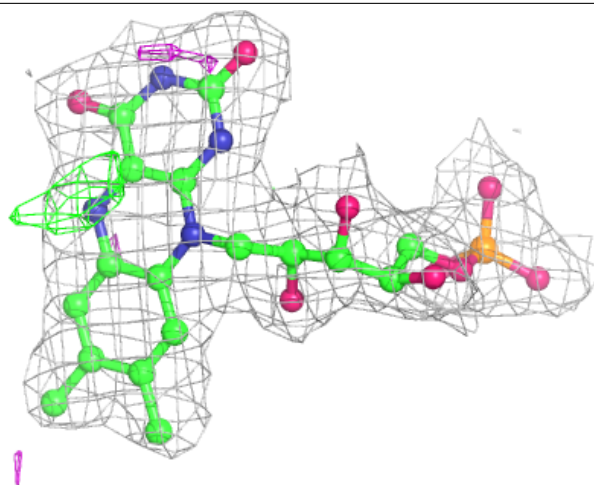
**Electron density around FMN L 301:**

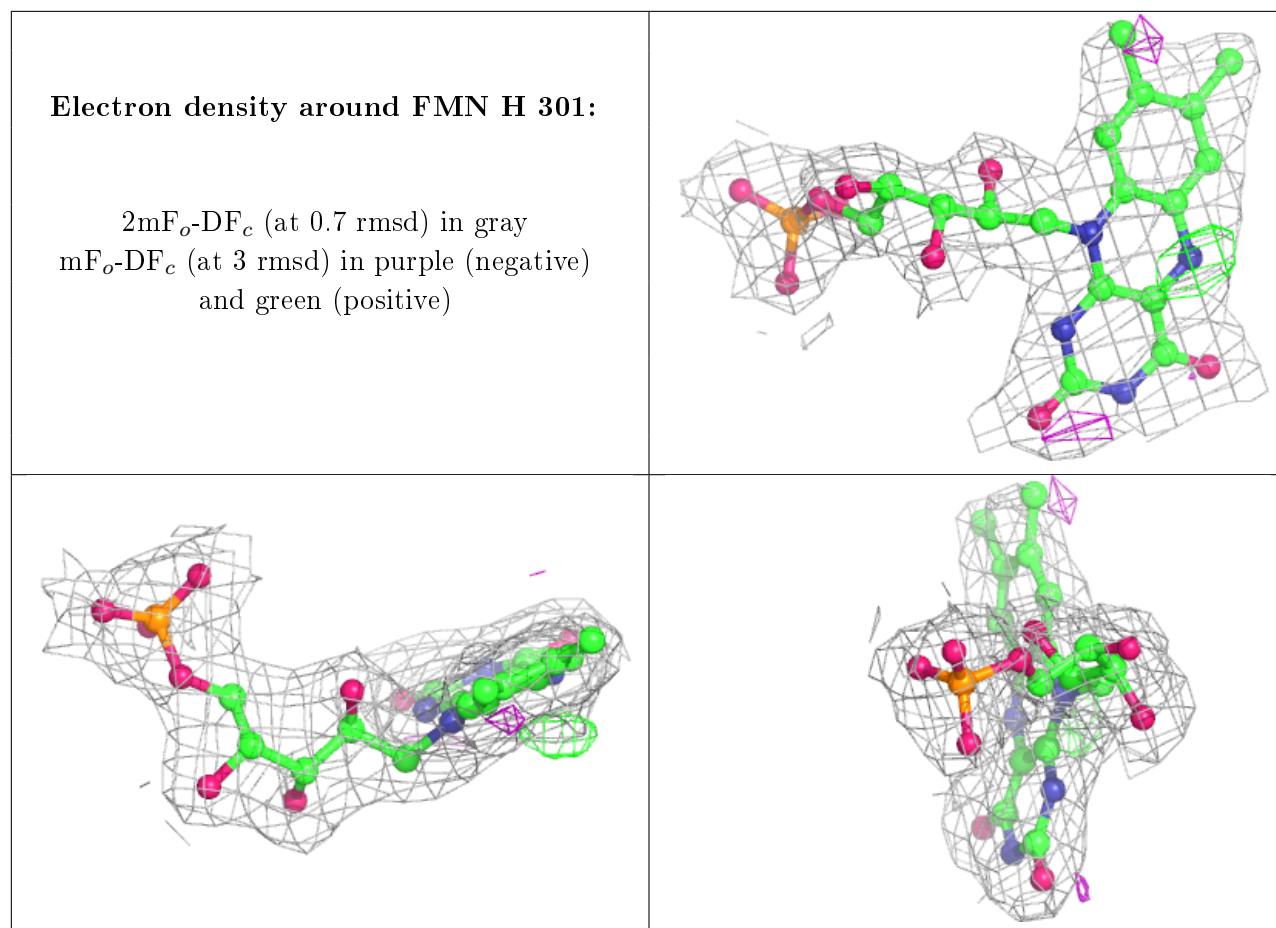
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FMN 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.