



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:42 PM UTC

PDB ID : 7CFU / pdb_00007cfu
Title : Crystal Structure of FMN-dependent Cysteine Decarboxylases SpaF
Authors : Li, J.; Lu, J.; Wang, H.; Zhu, J.
Deposited on : 2020-06-28
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

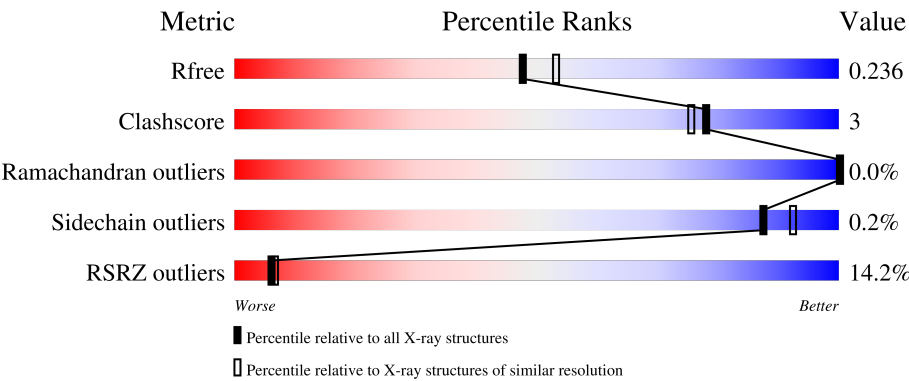
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	208	9% 76% 8% 16%
1	B	208	12% 78% 6% 16%
1	C	208	12% 79% 5% 16%
1	D	208	13% 79% 5% 16%
1	E	208	13% 78% 5% 16%

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Mol	Chain	Length	Quality of chain
1	F	208	
1	G	208	
1	H	208	
1	I	208	
1	J	208	
1	K	208	
1	L	208	
1	M	208	
1	N	208	
1	O	208	
1	P	208	
1	Q	208	
1	R	208	
1	S	208	
1	T	208	
1	U	208	
1	V	208	
1	W	208	
1	X	208	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33215 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 DNA/pantothenate metabolism flavoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	S	175	Total	C	N	O	S	0	0	0
			1274	812	229	226	7			
1	H	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	P	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	A	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	B	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	C	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	D	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	E	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	G	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	I	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	J	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	K	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	L	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	M	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	N	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	Q	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	R	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	T	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	U	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	V	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	W	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			
1	X	175	Total	C	N	O	S	0	0	0
			1281	812	229	233	7			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	LEU	-	expression tag	UNP A0A1R1S5L5
F	2	VAL	-	expression tag	UNP A0A1R1S5L5
F	3	PRO	-	expression tag	UNP A0A1R1S5L5
F	4	ARG	-	expression tag	UNP A0A1R1S5L5
F	5	GLY	-	expression tag	UNP A0A1R1S5L5
F	6	SER	-	expression tag	UNP A0A1R1S5L5
F	7	HIS	-	expression tag	UNP A0A1R1S5L5
S	1	LEU	-	expression tag	UNP A0A1R1S5L5
S	2	VAL	-	expression tag	UNP A0A1R1S5L5
S	3	PRO	-	expression tag	UNP A0A1R1S5L5
S	4	ARG	-	expression tag	UNP A0A1R1S5L5
S	5	GLY	-	expression tag	UNP A0A1R1S5L5
S	6	SER	-	expression tag	UNP A0A1R1S5L5
S	7	HIS	-	expression tag	UNP A0A1R1S5L5
H	1	LEU	-	expression tag	UNP A0A1R1S5L5
H	2	VAL	-	expression tag	UNP A0A1R1S5L5
H	3	PRO	-	expression tag	UNP A0A1R1S5L5
H	4	ARG	-	expression tag	UNP A0A1R1S5L5
H	5	GLY	-	expression tag	UNP A0A1R1S5L5
H	6	SER	-	expression tag	UNP A0A1R1S5L5
H	7	HIS	-	expression tag	UNP A0A1R1S5L5
P	1	LEU	-	expression tag	UNP A0A1R1S5L5
P	2	VAL	-	expression tag	UNP A0A1R1S5L5

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Chain	Residue	Modelled	Actual	Comment	Reference
P	3	PRO	-	expression tag	UNP A0A1R1S5L5
P	4	ARG	-	expression tag	UNP A0A1R1S5L5
P	5	GLY	-	expression tag	UNP A0A1R1S5L5
P	6	SER	-	expression tag	UNP A0A1R1S5L5
P	7	HIS	-	expression tag	UNP A0A1R1S5L5
A	1	LEU	-	expression tag	UNP A0A1R1S5L5
A	2	VAL	-	expression tag	UNP A0A1R1S5L5
A	3	PRO	-	expression tag	UNP A0A1R1S5L5
A	4	ARG	-	expression tag	UNP A0A1R1S5L5
A	5	GLY	-	expression tag	UNP A0A1R1S5L5
A	6	SER	-	expression tag	UNP A0A1R1S5L5
A	7	HIS	-	expression tag	UNP A0A1R1S5L5
B	1	LEU	-	expression tag	UNP A0A1R1S5L5
B	2	VAL	-	expression tag	UNP A0A1R1S5L5
B	3	PRO	-	expression tag	UNP A0A1R1S5L5
B	4	ARG	-	expression tag	UNP A0A1R1S5L5
B	5	GLY	-	expression tag	UNP A0A1R1S5L5
B	6	SER	-	expression tag	UNP A0A1R1S5L5
B	7	HIS	-	expression tag	UNP A0A1R1S5L5
C	1	LEU	-	expression tag	UNP A0A1R1S5L5
C	2	VAL	-	expression tag	UNP A0A1R1S5L5
C	3	PRO	-	expression tag	UNP A0A1R1S5L5
C	4	ARG	-	expression tag	UNP A0A1R1S5L5
C	5	GLY	-	expression tag	UNP A0A1R1S5L5
C	6	SER	-	expression tag	UNP A0A1R1S5L5
C	7	HIS	-	expression tag	UNP A0A1R1S5L5
D	1	LEU	-	expression tag	UNP A0A1R1S5L5
D	2	VAL	-	expression tag	UNP A0A1R1S5L5
D	3	PRO	-	expression tag	UNP A0A1R1S5L5
D	4	ARG	-	expression tag	UNP A0A1R1S5L5
D	5	GLY	-	expression tag	UNP A0A1R1S5L5
D	6	SER	-	expression tag	UNP A0A1R1S5L5
D	7	HIS	-	expression tag	UNP A0A1R1S5L5
E	1	LEU	-	expression tag	UNP A0A1R1S5L5
E	2	VAL	-	expression tag	UNP A0A1R1S5L5
E	3	PRO	-	expression tag	UNP A0A1R1S5L5
E	4	ARG	-	expression tag	UNP A0A1R1S5L5
E	5	GLY	-	expression tag	UNP A0A1R1S5L5
E	6	SER	-	expression tag	UNP A0A1R1S5L5
E	7	HIS	-	expression tag	UNP A0A1R1S5L5
G	1	LEU	-	expression tag	UNP A0A1R1S5L5
G	2	VAL	-	expression tag	UNP A0A1R1S5L5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	3	PRO	-	expression tag	UNP A0A1R1S5L5
G	4	ARG	-	expression tag	UNP A0A1R1S5L5
G	5	GLY	-	expression tag	UNP A0A1R1S5L5
G	6	SER	-	expression tag	UNP A0A1R1S5L5
G	7	HIS	-	expression tag	UNP A0A1R1S5L5
I	1	LEU	-	expression tag	UNP A0A1R1S5L5
I	2	VAL	-	expression tag	UNP A0A1R1S5L5
I	3	PRO	-	expression tag	UNP A0A1R1S5L5
I	4	ARG	-	expression tag	UNP A0A1R1S5L5
I	5	GLY	-	expression tag	UNP A0A1R1S5L5
I	6	SER	-	expression tag	UNP A0A1R1S5L5
I	7	HIS	-	expression tag	UNP A0A1R1S5L5
J	1	LEU	-	expression tag	UNP A0A1R1S5L5
J	2	VAL	-	expression tag	UNP A0A1R1S5L5
J	3	PRO	-	expression tag	UNP A0A1R1S5L5
J	4	ARG	-	expression tag	UNP A0A1R1S5L5
J	5	GLY	-	expression tag	UNP A0A1R1S5L5
J	6	SER	-	expression tag	UNP A0A1R1S5L5
J	7	HIS	-	expression tag	UNP A0A1R1S5L5
K	1	LEU	-	expression tag	UNP A0A1R1S5L5
K	2	VAL	-	expression tag	UNP A0A1R1S5L5
K	3	PRO	-	expression tag	UNP A0A1R1S5L5
K	4	ARG	-	expression tag	UNP A0A1R1S5L5
K	5	GLY	-	expression tag	UNP A0A1R1S5L5
K	6	SER	-	expression tag	UNP A0A1R1S5L5
K	7	HIS	-	expression tag	UNP A0A1R1S5L5
L	1	LEU	-	expression tag	UNP A0A1R1S5L5
L	2	VAL	-	expression tag	UNP A0A1R1S5L5
L	3	PRO	-	expression tag	UNP A0A1R1S5L5
L	4	ARG	-	expression tag	UNP A0A1R1S5L5
L	5	GLY	-	expression tag	UNP A0A1R1S5L5
L	6	SER	-	expression tag	UNP A0A1R1S5L5
L	7	HIS	-	expression tag	UNP A0A1R1S5L5
M	1	LEU	-	expression tag	UNP A0A1R1S5L5
M	2	VAL	-	expression tag	UNP A0A1R1S5L5
M	3	PRO	-	expression tag	UNP A0A1R1S5L5
M	4	ARG	-	expression tag	UNP A0A1R1S5L5
M	5	GLY	-	expression tag	UNP A0A1R1S5L5
M	6	SER	-	expression tag	UNP A0A1R1S5L5
M	7	HIS	-	expression tag	UNP A0A1R1S5L5
N	1	LEU	-	expression tag	UNP A0A1R1S5L5
N	2	VAL	-	expression tag	UNP A0A1R1S5L5

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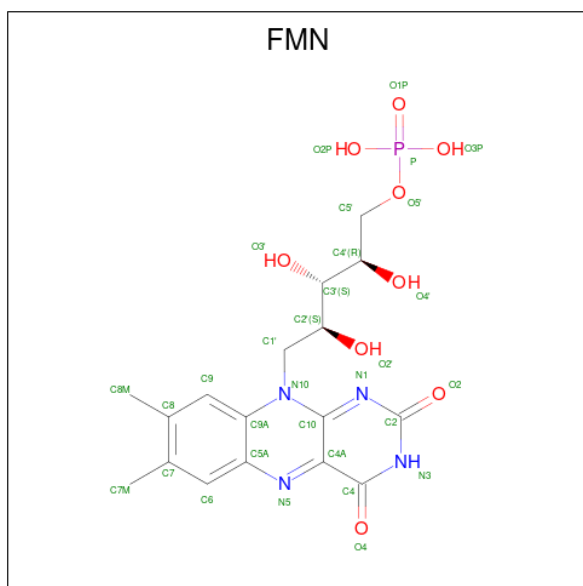
Chain	Residue	Modelled	Actual	Comment	Reference
N	3	PRO	-	expression tag	UNP A0A1R1S5L5
N	4	ARG	-	expression tag	UNP A0A1R1S5L5
N	5	GLY	-	expression tag	UNP A0A1R1S5L5
N	6	SER	-	expression tag	UNP A0A1R1S5L5
N	7	HIS	-	expression tag	UNP A0A1R1S5L5
O	1	LEU	-	expression tag	UNP A0A1R1S5L5
O	2	VAL	-	expression tag	UNP A0A1R1S5L5
O	3	PRO	-	expression tag	UNP A0A1R1S5L5
O	4	ARG	-	expression tag	UNP A0A1R1S5L5
O	5	GLY	-	expression tag	UNP A0A1R1S5L5
O	6	SER	-	expression tag	UNP A0A1R1S5L5
O	7	HIS	-	expression tag	UNP A0A1R1S5L5
Q	1	LEU	-	expression tag	UNP A0A1R1S5L5
Q	2	VAL	-	expression tag	UNP A0A1R1S5L5
Q	3	PRO	-	expression tag	UNP A0A1R1S5L5
Q	4	ARG	-	expression tag	UNP A0A1R1S5L5
Q	5	GLY	-	expression tag	UNP A0A1R1S5L5
Q	6	SER	-	expression tag	UNP A0A1R1S5L5
Q	7	HIS	-	expression tag	UNP A0A1R1S5L5
R	1	LEU	-	expression tag	UNP A0A1R1S5L5
R	2	VAL	-	expression tag	UNP A0A1R1S5L5
R	3	PRO	-	expression tag	UNP A0A1R1S5L5
R	4	ARG	-	expression tag	UNP A0A1R1S5L5
R	5	GLY	-	expression tag	UNP A0A1R1S5L5
R	6	SER	-	expression tag	UNP A0A1R1S5L5
R	7	HIS	-	expression tag	UNP A0A1R1S5L5
T	1	LEU	-	expression tag	UNP A0A1R1S5L5
T	2	VAL	-	expression tag	UNP A0A1R1S5L5
T	3	PRO	-	expression tag	UNP A0A1R1S5L5
T	4	ARG	-	expression tag	UNP A0A1R1S5L5
T	5	GLY	-	expression tag	UNP A0A1R1S5L5
T	6	SER	-	expression tag	UNP A0A1R1S5L5
T	7	HIS	-	expression tag	UNP A0A1R1S5L5
U	1	LEU	-	expression tag	UNP A0A1R1S5L5
U	2	VAL	-	expression tag	UNP A0A1R1S5L5
U	3	PRO	-	expression tag	UNP A0A1R1S5L5
U	4	ARG	-	expression tag	UNP A0A1R1S5L5
U	5	GLY	-	expression tag	UNP A0A1R1S5L5
U	6	SER	-	expression tag	UNP A0A1R1S5L5
U	7	HIS	-	expression tag	UNP A0A1R1S5L5
V	1	LEU	-	expression tag	UNP A0A1R1S5L5
V	2	VAL	-	expression tag	UNP A0A1R1S5L5

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Chain	Residue	Modelled	Actual	Comment	Reference
V	3	PRO	-	expression tag	UNP A0A1R1S5L5
V	4	ARG	-	expression tag	UNP A0A1R1S5L5
V	5	GLY	-	expression tag	UNP A0A1R1S5L5
V	6	SER	-	expression tag	UNP A0A1R1S5L5
V	7	HIS	-	expression tag	UNP A0A1R1S5L5
W	1	LEU	-	expression tag	UNP A0A1R1S5L5
W	2	VAL	-	expression tag	UNP A0A1R1S5L5
W	3	PRO	-	expression tag	UNP A0A1R1S5L5
W	4	ARG	-	expression tag	UNP A0A1R1S5L5
W	5	GLY	-	expression tag	UNP A0A1R1S5L5
W	6	SER	-	expression tag	UNP A0A1R1S5L5
W	7	HIS	-	expression tag	UNP A0A1R1S5L5
X	1	LEU	-	expression tag	UNP A0A1R1S5L5
X	2	VAL	-	expression tag	UNP A0A1R1S5L5
X	3	PRO	-	expression tag	UNP A0A1R1S5L5
X	4	ARG	-	expression tag	UNP A0A1R1S5L5
X	5	GLY	-	expression tag	UNP A0A1R1S5L5
X	6	SER	-	expression tag	UNP A0A1R1S5L5
X	7	HIS	-	expression tag	UNP A0A1R1S5L5

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	S	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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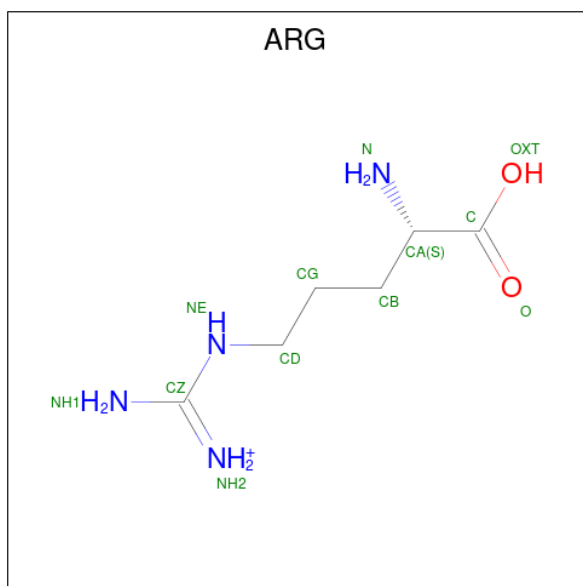
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	P	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	B	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	C	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	D	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	E	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	G	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	I	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	J	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	K	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	L	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	M	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	N	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	O	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	Q	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	R	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	T	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	U	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	V	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	W	1	Total 31	C 17	N 4	O 9	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	X	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	S	1	Total	C	N	O	0	0
			11	6	4	1		

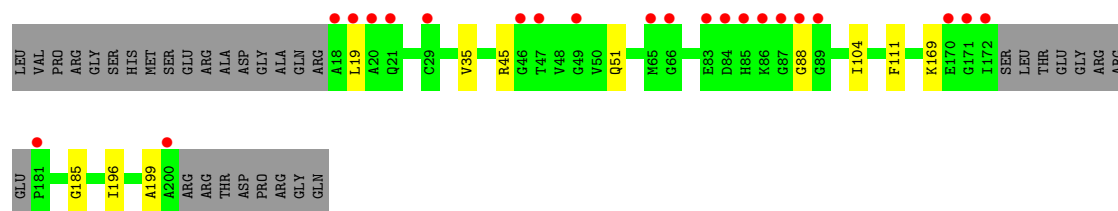
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	69	Total	O	0	0
			69	69		
4	S	80	Total	O	0	0
			80	80		
4	H	87	Total	O	0	0
			87	87		
4	P	80	Total	O	0	0
			80	80		
4	A	71	Total	O	0	0
			71	71		
4	B	82	Total	O	0	0
			82	82		
4	C	78	Total	O	0	0
			78	78		

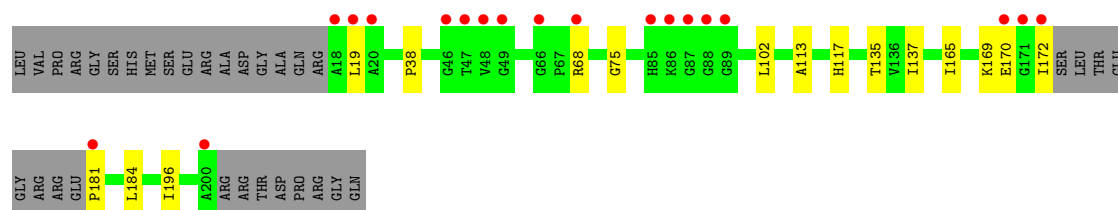
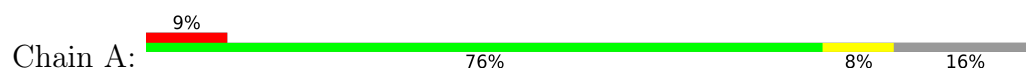
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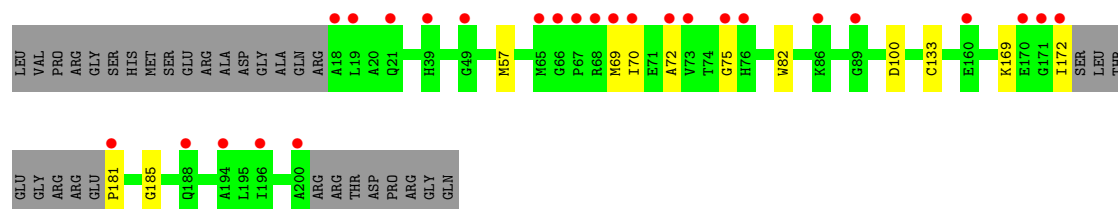
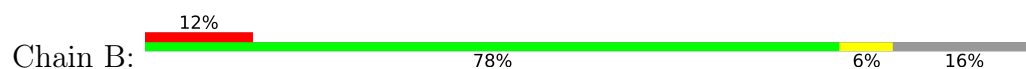
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	85	Total 85	O 85	0	0
4	E	75	Total 75	O 75	0	0
4	G	73	Total 73	O 73	0	0
4	I	78	Total 78	O 78	0	0
4	J	61	Total 61	O 61	0	0
4	K	60	Total 60	O 60	0	0
4	L	66	Total 66	O 66	0	0
4	M	59	Total 59	O 59	0	0
4	N	61	Total 61	O 61	0	0
4	O	69	Total 69	O 69	0	0
4	Q	75	Total 75	O 75	0	0
4	R	74	Total 74	O 74	0	0
4	T	59	Total 59	O 59	0	0
4	U	64	Total 64	O 64	0	0
4	V	68	Total 68	O 68	0	0
4	W	74	Total 74	O 74	0	0
4	X	75	Total 75	O 75	0	0



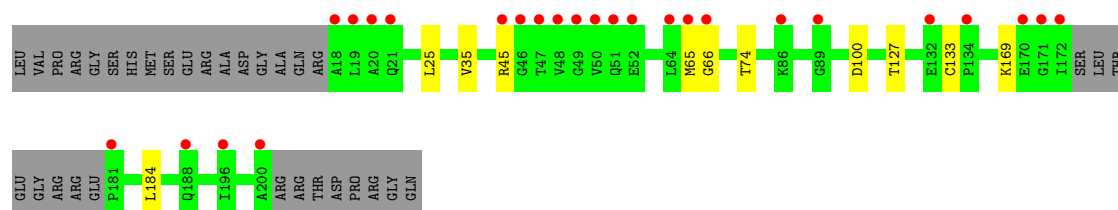
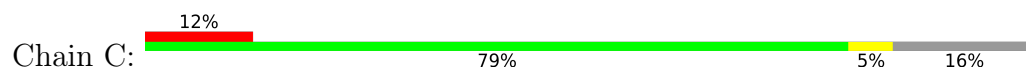
● Molecule 1: DNA/pantothenate metabolism flavoprotein



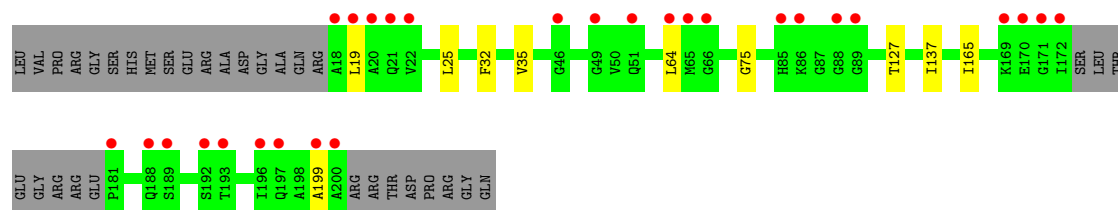
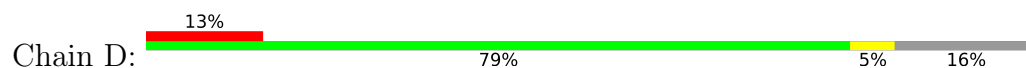
● Molecule 1: DNA/pantothenate metabolism flavoprotein



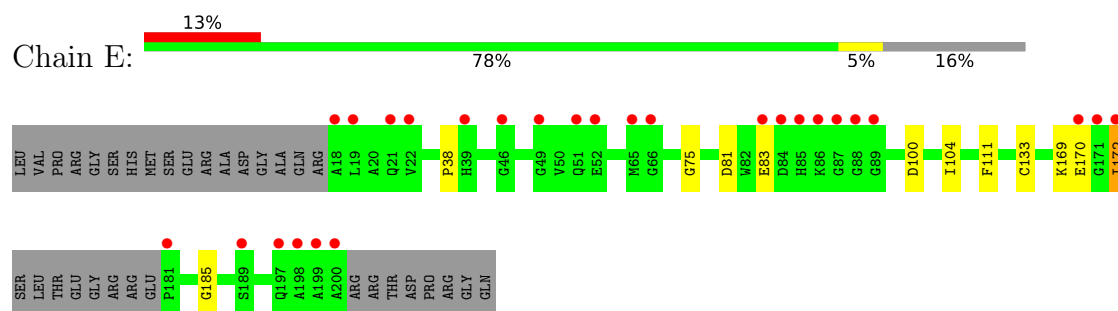
● Molecule 1: DNA/pantothenate metabolism flavoprotein



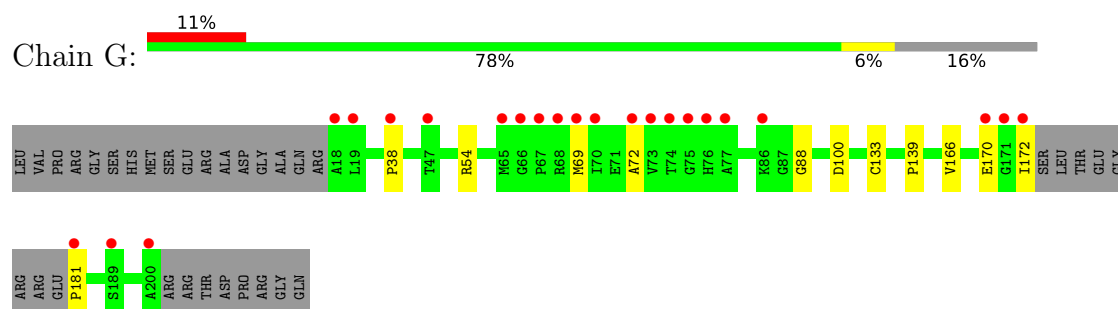
● Molecule 1: DNA/pantothenate metabolism flavoprotein



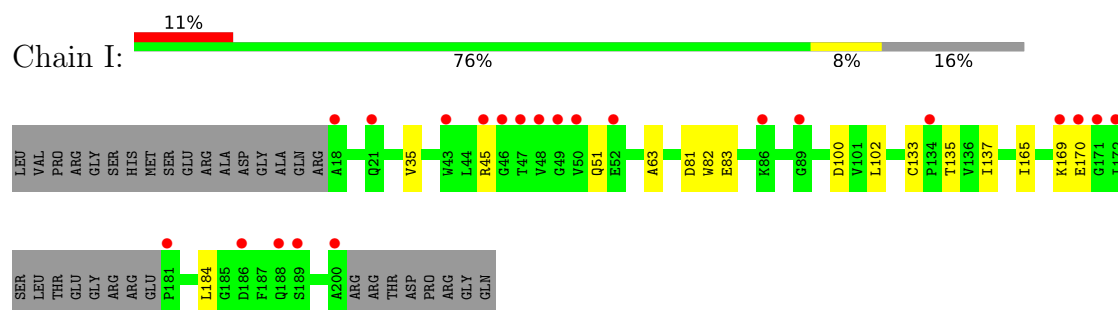
- Molecule 1: DNA/pantothenate metabolism flavoprotein



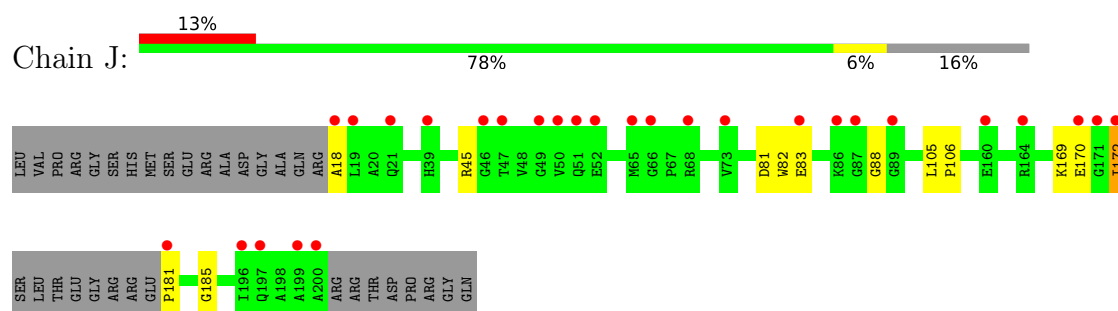
- Molecule 1: DNA/pantothenate metabolism flavoprotein



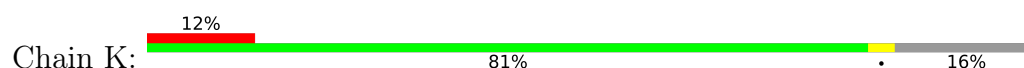
- Molecule 1: DNA/pantothenate metabolism flavoprotein



- Molecule 1: DNA/pantothenate metabolism flavoprotein

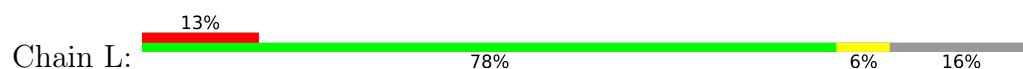


- Molecule 1: DNA/pantothenate metabolism flavoprotein

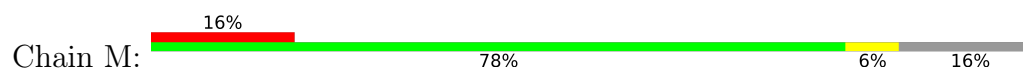




• Molecule 1: DNA/pantothenate metabolism flavoprotein



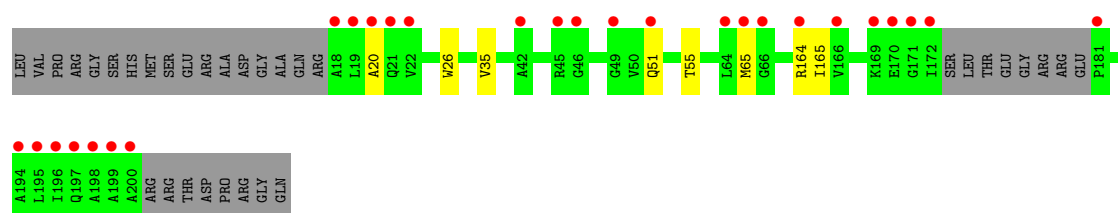
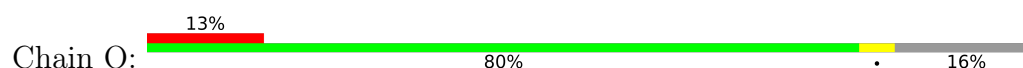
• Molecule 1: DNA/pantothenate metabolism flavoprotein



• Molecule 1: DNA/pantothenate metabolism flavoprotein

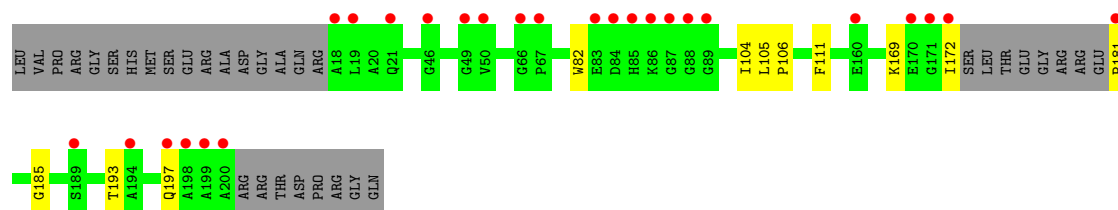


• Molecule 1: DNA/pantothenate metabolism flavoprotein



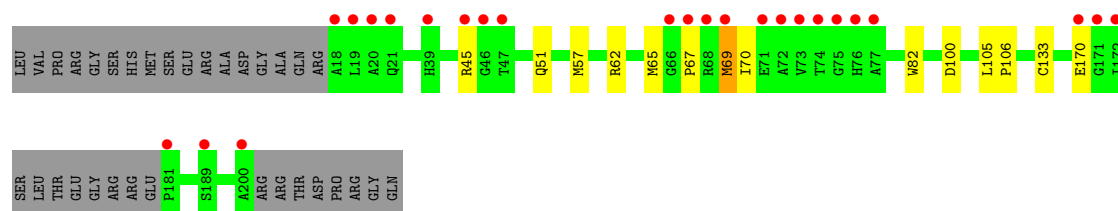
- Molecule 1: DNA/pantothenate metabolism flavoprotein

Chain Q: 



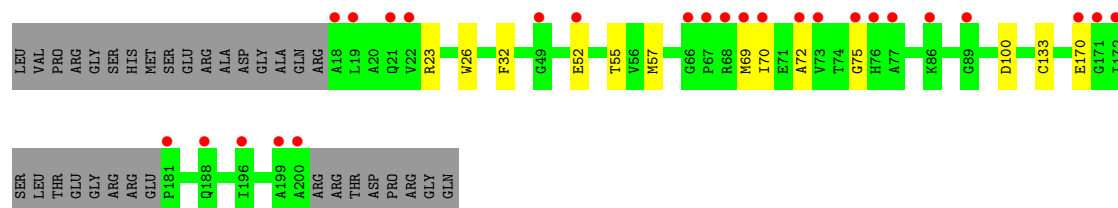
- Molecule 1: DNA/pantothenate metabolism flavoprotein

Chain R: 



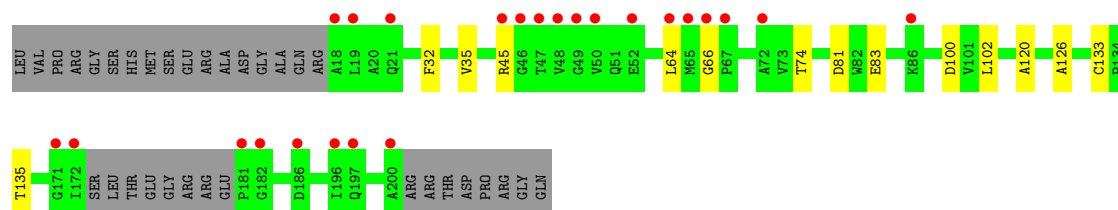
- Molecule 1: DNA/pantothenate metabolism flavoprotein

Chain T: 



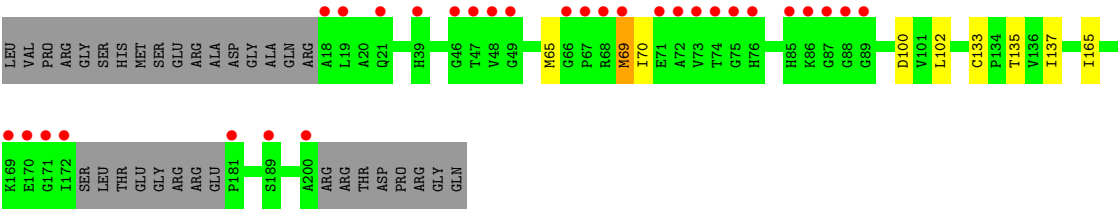
- Molecule 1: DNA/pantothenate metabolism flavoprotein

Chain U: 

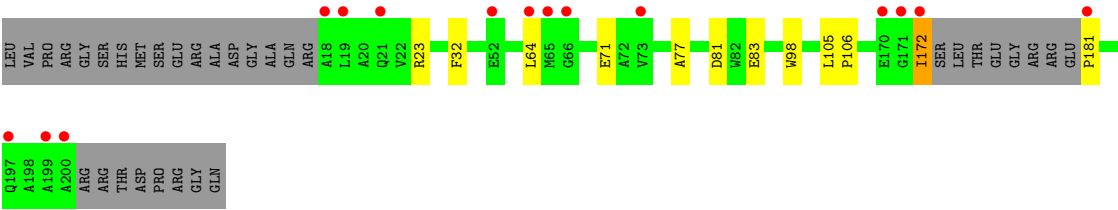
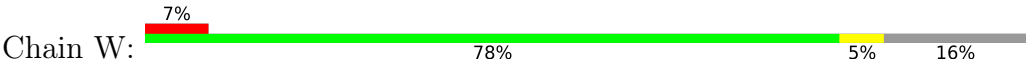


- Molecule 1: DNA/pantothenate metabolism flavoprotein

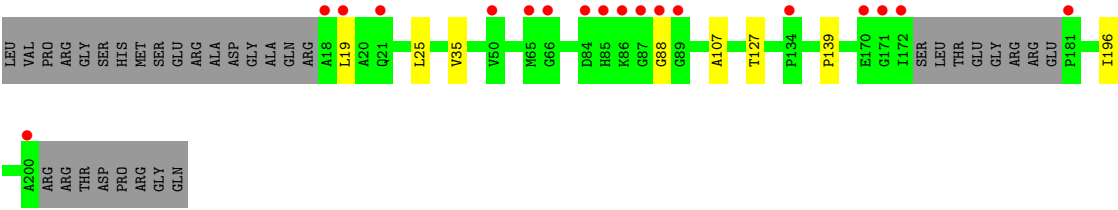
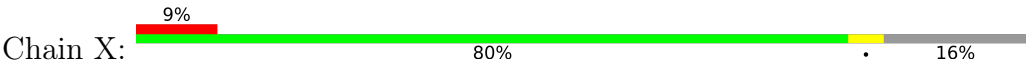
Chain V: 



● Molecule 1: DNA/pantothenate metabolism flavoprotein



● Molecule 1: DNA/pantothenate metabolism flavoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.63Å 189.61Å 185.35Å 90.00° 92.52° 90.00°	Depositor
Resolution (Å)	48.96 – 2.15 48.96 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.96-2.15) 97.5 (48.96-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.14_3235	Depositor
R, R_{free}	0.203 , 0.235 0.204 , 0.236	Depositor DCC
R_{free} test set	17331 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.079 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33215	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8442e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: FMN

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	0/1307	0.43	0/1786
1	B	0.23	0/1307	0.41	0/1786
1	C	0.23	0/1307	0.41	0/1786
1	D	0.23	0/1307	0.43	0/1786
1	E	0.23	0/1307	0.42	0/1786
1	F	0.23	0/1307	0.43	0/1786
1	G	0.25	0/1307	0.44	0/1786
1	H	0.24	0/1307	0.43	0/1786
1	I	0.22	0/1307	0.41	0/1786
1	J	0.23	0/1307	0.41	0/1786
1	K	0.22	0/1307	0.41	0/1786
1	L	0.22	0/1307	0.40	0/1786
1	M	0.21	0/1307	0.41	0/1786
1	N	0.21	0/1307	0.39	0/1786
1	O	0.23	0/1307	0.43	0/1786
1	P	0.23	0/1307	0.42	0/1786
1	Q	0.23	0/1307	0.41	0/1786
1	R	0.23	0/1307	0.42	0/1786
1	S	0.23	0/1300	0.45	0/1772
1	T	0.22	0/1307	0.41	0/1786
1	U	0.22	0/1307	0.40	0/1786
1	V	0.23	0/1307	0.42	0/1786
1	W	0.24	0/1307	0.43	0/1786
1	X	0.23	0/1307	0.43	0/1786
All	All	0.23	0/31361	0.42	0/42850

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1281	0	1291	11	0
1	B	1281	0	1291	9	0
1	C	1281	0	1291	5	0
1	D	1281	0	1291	7	0
1	E	1281	0	1291	12	0
1	F	1281	0	1291	11	0
1	G	1281	0	1291	12	0
1	H	1281	0	1291	13	0
1	I	1281	0	1291	10	0
1	J	1281	0	1291	10	0
1	K	1281	0	1291	4	0
1	L	1281	0	1291	7	0
1	M	1281	0	1291	9	0
1	N	1281	0	1291	7	0
1	O	1281	0	1291	5	0
1	P	1281	0	1291	7	0
1	Q	1281	0	1291	6	0
1	R	1281	0	1291	11	0
1	S	1274	0	1291	9	0
1	T	1281	0	1291	11	0
1	U	1281	0	1291	9	0
1	V	1281	0	1291	6	0
1	W	1281	0	1291	7	0
1	X	1281	0	1291	6	0
2	A	31	0	19	1	0
2	B	31	0	19	0	0
2	C	31	0	19	0	0
2	D	31	0	19	0	0
2	E	31	0	19	0	0
2	F	31	0	19	1	0
2	G	31	0	19	1	0
2	H	31	0	19	0	0
2	I	31	0	19	1	0
2	J	31	0	19	1	0
2	K	31	0	19	2	0
2	L	31	0	19	1	0
2	M	31	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	31	0	19	1	0
2	O	31	0	19	1	0
2	P	31	0	19	0	0
2	Q	31	0	19	1	0
2	R	31	0	19	0	0
2	S	31	0	19	0	0
2	T	31	0	19	0	0
2	U	31	0	19	0	0
2	V	31	0	19	0	0
2	W	31	0	19	0	0
2	X	31	0	19	0	0
3	S	11	0	12	1	0
4	A	71	0	0	0	0
4	B	82	0	0	0	0
4	C	78	0	0	0	0
4	D	85	0	0	0	0
4	E	75	0	0	0	0
4	F	69	0	0	0	0
4	G	73	0	0	1	0
4	H	87	0	0	0	0
4	I	78	0	0	0	0
4	J	61	0	0	2	0
4	K	60	0	0	0	0
4	L	66	0	0	0	0
4	M	59	0	0	0	0
4	N	61	0	0	0	0
4	O	69	0	0	1	0
4	P	80	0	0	0	0
4	Q	75	0	0	0	0
4	R	74	0	0	1	0
4	S	80	0	0	1	0
4	T	59	0	0	0	0
4	U	64	0	0	0	0
4	V	68	0	0	0	0
4	W	74	0	0	0	0
4	X	75	0	0	0	0
All	All	33215	0	31452	174	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 3.

All (174) 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:68:ARG:HH12	1:E:83:GLU:HG3	1.36	0.90
1:R:65:MET:HB3	1:R:69:MET:HE2	1.58	0.84
1:V:69:MET:HE3	1:V:70:ILE:HG13	1.61	0.82
1:R:69:MET:HE3	1:R:70:ILE:HG13	1.61	0.81
1:F:68:ARG:HH22	1:E:83:GLU:HA	1.48	0.77
1:V:65:MET:HB3	1:V:69:MET:HE2	1.66	0.77
1:U:45:ARG:NH2	1:U:74:THR:O	2.18	0.77
1:C:45:ARG:NH2	1:C:74:THR:O	2.19	0.75
1:O:164:ARG:NH1	1:O:165:ILE:O	2.24	0.70
1:B:69:MET:HE2	1:W:64:LEU:HB3	1.75	0.69
1:J:45:ARG:NH2	4:J:401:HOH:O	2.25	0.68
1:R:62:ARG:HG3	1:R:67:PRO:HB3	1.75	0.66
1:A:172:ILE:HA	1:A:181:PRO:HG2	1.81	0.62
1:I:45:ARG:NH1	1:I:51:GLN:O	2.30	0.62
1:S:164:ARG:NH2	4:S:401:HOH:O	2.33	0.61
1:F:68:ARG:NH2	1:E:83:GLU:HA	2.16	0.61
1:P:45:ARG:NH1	1:P:51:GLN:O	2.32	0.61
1:H:32:PHE:HE1	1:T:72:ALA:HB1	1.66	0.60
1:H:64:LEU:HB3	1:T:69:MET:HE2	1.84	0.58
1:F:69:MET:HE2	1:D:64:LEU:HB3	1.84	0.58
1:B:172:ILE:HA	1:B:181:PRO:HG2	1.86	0.57
1:L:169:LYS:HE2	1:L:184:LEU:O	2.05	0.57
1:F:68:ARG:NH1	1:E:83:GLU:HG3	2.16	0.56
1:O:164:ARG:NH1	4:O:401:HOH:O	2.37	0.55
1:Q:172:ILE:HA	1:Q:181:PRO:HG2	1.89	0.55
1:L:172:ILE:HA	1:L:181:PRO:HG2	1.88	0.55
1:W:172:ILE:HA	1:W:181:PRO:HG2	1.90	0.55
1:G:54:ARG:NH1	4:G:404:HOH:O	2.35	0.53
1:M:172:ILE:HA	1:M:181:PRO:HG2	1.90	0.52
1:I:102:LEU:O	1:I:135:THR:HA	2.09	0.52
1:R:62:ARG:NH2	4:R:405:HOH:O	2.42	0.52
1:K:23:ARG:HG2	1:K:52:GLU:OE1	2.10	0.52
1:U:81:ASP:HB3	1:U:83:GLU:OE1	2.11	0.51
1:A:19:LEU:HD21	1:A:196:ILE:HG13	1.91	0.51
1:E:81:ASP:HB3	1:E:83:GLU:OE1	2.11	0.50
1:S:172:ILE:HG12	1:S:181:PRO:HG2	1.92	0.50
1:H:72:ALA:HB1	1:T:32:PHE:HE1	1.76	0.50
1:L:62:ARG:HG3	1:L:67:PRO:HD3	1.93	0.50
1:J:18:ALA:N	4:J:405:HOH:O	2.45	0.50
1:S:170:GLU:N	1:S:170:GLU:OE1	2.46	0.49
1:A:170:GLU:N	1:A:170:GLU:OE1	2.46	0.49
1:L:82:TRP:CZ2	2:N:301:FMN:H3'	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:57:MET:SD	1:T:70:ILE:HD12	2.53	0.48
1:S:102:LEU:O	1:S:135:THR:HA	2.14	0.48
1:T:170:GLU:N	1:T:170:GLU:OE1	2.47	0.48
1:S:25:LEU:HD21	1:S:127:THR:HG21	1.96	0.48
1:R:170:GLU:N	1:R:170:GLU:OE1	2.47	0.48
1:R:65:MET:HB3	1:R:69:MET:CE	2.39	0.47
1:B:72:ALA:HB1	1:W:32:PHE:HE1	1.80	0.47
1:H:23:ARG:HD2	1:H:98:TRP:NE1	2.30	0.47
1:A:75:GLY:HA2	1:J:88:GLY:N	2.28	0.47
1:H:169:LYS:HE2	1:H:184:LEU:O	2.15	0.47
1:G:170:GLU:N	1:G:170:GLU:OE1	2.48	0.47
1:A:137:ILE:HB	1:A:165:ILE:HD13	1.97	0.47
1:B:169:LYS:HG3	1:B:185:GLY:HA2	1.97	0.46
1:K:100:ASP:O	1:K:133:CYS:HB2	2.16	0.46
1:P:88:GLY:CA	1:T:75:GLY:HA2	2.46	0.46
1:W:23:ARG:HD2	1:W:98:TRP:NE1	2.30	0.46
1:X:19:LEU:HD21	1:X:196:ILE:HA	1.98	0.46
2:F:301:FMN:H3'	1:H:82:TRP:CZ2	2.51	0.46
1:P:169:LYS:HG3	1:P:185:GLY:HA2	1.98	0.46
1:E:170:GLU:OE2	1:E:172:ILE:HG13	2.16	0.46
1:M:25:LEU:HD21	1:M:127:THR:HG21	1.97	0.46
1:A:169:LYS:HE2	1:A:184:LEU:O	2.16	0.46
1:G:172:ILE:HA	1:G:181:PRO:HG2	1.97	0.46
1:W:81:ASP:HB3	1:W:83:GLU:OE1	2.15	0.46
1:E:75:GLY:HA2	1:N:88:GLY:N	2.31	0.46
1:F:137:ILE:HB	1:F:165:ILE:HD13	1.98	0.45
1:O:20:ALA:HB1	1:O:51:GLN:NE2	2.30	0.45
1:A:170:GLU:HG2	1:A:170:GLU:O	2.17	0.45
2:L:301:FMN:H3'	1:M:82:TRP:CZ2	2.51	0.45
1:T:23:ARG:HG2	1:T:52:GLU:OE1	2.17	0.45
2:Q:301:FMN:H3'	1:R:82:TRP:CZ2	2.51	0.45
1:Q:193:THR:O	1:Q:197:GLN:HG3	2.17	0.45
1:G:69:MET:HE2	1:U:64:LEU:HB3	1.98	0.45
1:G:88:GLY:N	1:M:75:GLY:HA2	2.32	0.45
1:L:25:LEU:HD21	1:L:127:THR:HG21	1.99	0.45
1:A:38:PRO:HG2	1:I:35:VAL:HB	1.97	0.45
1:H:25:LEU:HD21	1:H:127:THR:HG21	1.99	0.45
1:B:57:MET:SD	1:B:70:ILE:HD12	2.56	0.45
1:C:35:VAL:HA	1:C:65:MET:SD	2.57	0.44
1:G:38:PRO:HG2	1:U:35:VAL:HB	1.97	0.44
1:N:170:GLU:N	1:N:170:GLU:OE1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:32:PHE:CE1	1:T:72:ALA:HB1	2.50	0.44
1:H:88:GLY:N	1:D:75:GLY:HA2	2.32	0.44
1:V:69:MET:HE3	1:V:70:ILE:CG1	2.38	0.44
1:P:104:ILE:HG13	1:P:111:PHE:CZ	2.52	0.44
1:I:81:ASP:HB3	1:I:83:GLU:OE1	2.17	0.44
2:I:301:FMN:H3'	1:J:82:TRP:CZ2	2.53	0.44
1:T:100:ASP:O	1:T:133:CYS:HB2	2.18	0.44
1:S:75:GLY:HA2	1:M:88:GLY:N	2.33	0.44
1:P:19:LEU:HD23	1:P:199:ALA:HB2	2.00	0.44
1:G:72:ALA:HB1	1:U:32:PHE:HE1	1.83	0.44
1:F:38:PRO:HG2	1:D:35:VAL:HB	2.00	0.43
1:J:170:GLU:OE1	1:J:170:GLU:N	2.51	0.43
1:U:100:ASP:O	1:U:133:CYS:HB2	2.18	0.43
1:D:19:LEU:HD23	1:D:199:ALA:HB2	2.00	0.43
1:J:105:LEU:HA	1:J:106:PRO:HA	1.88	0.43
1:B:75:GLY:HA2	1:X:88:GLY:CA	2.49	0.43
1:D:137:ILE:HB	1:D:165:ILE:HD13	2.00	0.43
1:O:26:TRP:O	1:O:55:THR:HA	2.19	0.43
1:Q:169:LYS:HG3	1:Q:185:GLY:HA2	2.00	0.43
1:S:198:ALA:O	3:S:301:ARG:N	2.52	0.43
1:L:105:LEU:HA	1:L:106:PRO:HA	1.88	0.43
1:R:45:ARG:NH1	1:R:51:GLN:O	2.49	0.43
1:H:35:VAL:CG1	1:T:69:MET:HG2	2.49	0.43
1:J:172:ILE:HA	1:J:181:PRO:HG2	2.00	0.43
1:H:81:ASP:HB3	1:H:83:GLU:OE1	2.19	0.43
1:V:102:LEU:O	1:V:135:THR:HA	2.19	0.43
1:F:100:ASP:O	1:F:133:CYS:HB2	2.19	0.42
1:A:68:ARG:NH1	1:I:63:ALA:HB1	2.34	0.42
1:A:113:ALA:O	1:A:117:HIS:HD2	2.02	0.42
1:N:57:MET:SD	1:N:70:ILE:HD12	2.59	0.42
1:R:57:MET:SD	1:R:70:ILE:HD12	2.59	0.42
1:G:100:ASP:O	1:G:133:CYS:HB2	2.19	0.42
1:I:82:TRP:CZ2	2:K:301:FMN:H3'	2.54	0.42
1:E:169:LYS:HG3	1:E:185:GLY:HA2	2.01	0.42
1:X:107:ALA:O	1:X:139:PRO:HA	2.19	0.42
1:H:57:MET:SD	1:H:70:ILE:HD12	2.60	0.42
1:P:35:VAL:HB	1:N:38:PRO:HG2	2.00	0.42
2:K:301:FMN:H9	2:K:301:FMN:H1'1	1.84	0.42
1:O:35:VAL:HA	1:O:65:MET:SD	2.60	0.42
1:R:100:ASP:O	1:R:133:CYS:HB2	2.20	0.42
1:G:170:GLU:O	1:G:170:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:100:ASP:O	1:I:133:CYS:HB2	2.19	0.42
1:B:100:ASP:O	1:B:133:CYS:HB2	2.19	0.42
1:E:104:ILE:HG13	1:E:111:PHE:CZ	2.55	0.42
1:T:26:TRP:O	1:T:55:THR:HA	2.20	0.41
1:P:19:LEU:HD21	1:P:196:ILE:HA	2.02	0.41
1:I:137:ILE:HB	1:I:165:ILE:HD13	2.02	0.41
1:I:169:LYS:HE2	1:I:184:LEU:O	2.20	0.41
1:L:137:ILE:HB	1:L:165:ILE:HD13	2.00	0.41
1:G:88:GLY:CA	1:M:75:GLY:HA2	2.51	0.41
1:M:100:ASP:O	1:M:133:CYS:HB2	2.21	0.41
1:U:120:ALA:HB1	1:U:126:ALA:HA	2.02	0.41
1:C:169:LYS:HE2	1:C:184:LEU:O	2.21	0.41
2:G:301:FMN:HM81	2:G:301:FMN:HM73	1.91	0.41
1:I:170:GLU:OE1	1:I:170:GLU:N	2.53	0.41
1:J:169:LYS:HG3	1:J:185:GLY:HA2	2.02	0.41
1:K:38:PRO:HG2	1:X:35:VAL:HB	2.02	0.41
1:F:72:ALA:HB1	1:D:32:PHE:HE1	1.85	0.41
1:S:89:GLY:O	1:S:90:ALA:HB3	2.21	0.41
1:A:102:LEU:O	1:A:135:THR:HA	2.21	0.41
1:J:81:ASP:HB3	1:J:83:GLU:OE1	2.20	0.41
1:M:102:LEU:O	1:M:135:THR:HA	2.20	0.41
2:O:301:FMN:H3'	1:Q:82:TRP:CZ2	2.56	0.41
1:D:25:LEU:HD21	1:D:127:THR:HG21	2.02	0.41
1:E:100:ASP:O	1:E:133:CYS:HB2	2.21	0.41
1:J:105:LEU:C	1:J:105:LEU:HD23	2.46	0.41
1:N:105:LEU:HA	1:N:106:PRO:HA	1.88	0.41
1:N:172:ILE:HA	1:N:181:PRO:HG2	2.03	0.41
1:U:102:LEU:O	1:U:135:THR:HA	2.21	0.41
1:V:137:ILE:HB	1:V:165:ILE:HD13	2.03	0.41
1:H:35:VAL:HA	1:H:65:MET:SD	2.61	0.41
1:B:75:GLY:HA2	1:X:88:GLY:HA3	2.03	0.41
1:Q:105:LEU:HA	1:Q:106:PRO:HA	1.95	0.41
1:X:25:LEU:HD21	1:X:127:THR:HG21	2.02	0.41
1:F:68:ARG:HH22	1:E:83:GLU:CA	2.25	0.40
2:M:301:FMN:H9	2:M:301:FMN:H1'1	1.84	0.40
1:E:38:PRO:HG2	1:M:35:VAL:HB	2.03	0.40
1:F:102:LEU:O	1:F:135:THR:HA	2.21	0.40
1:S:100:ASP:O	1:S:133:CYS:HB2	2.22	0.40
1:C:100:ASP:O	1:C:133:CYS:HB2	2.20	0.40
1:R:105:LEU:HA	1:R:106:PRO:HA	1.85	0.40
1:W:71:GLU:HB2	1:W:77:ALA:HA	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:MET:HG2	1:U:35:VAL:CG1	2.51	0.40
1:G:139:PRO:HD2	1:G:166:VAL:O	2.22	0.40
1:Q:104:ILE:HG13	1:Q:111:PHE:CZ	2.56	0.40
2:A:301:FMN:H3'	1:B:82:TRP:CZ2	2.57	0.40
1:C:25:LEU:HD21	1:C:127:THR:HG21	2.03	0.40
2:J:301:FMN:H3'	1:K:82:TRP:CZ2	2.56	0.40
1:N:100:ASP:O	1:N:133:CYS:HB2	2.22	0.40
1:V:100:ASP:O	1:V:133:CYS:HB2	2.22	0.40
1:W:105:LEU:HA	1:W:106:PRO:HA	1.94	0.40

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	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	B	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	C	171/208 (82%)	164 (96%)	6 (4%)	1 (1%)	21	15
1	D	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	E	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	F	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	G	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	H	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	I	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	J	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	K	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	L	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	M	171/208 (82%)	164 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	O	171/208 (82%)	165 (96%)	6 (4%)	0	100	100
1	P	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	Q	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	R	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	S	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	T	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	U	171/208 (82%)	164 (96%)	6 (4%)	1 (1%)	21	15
1	V	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	W	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
1	X	171/208 (82%)	164 (96%)	7 (4%)	0	100	100
All	All	4104/4992 (82%)	3937 (96%)	165 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	66	GLY
1	U	66	GLY

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	127/154 (82%)	127 (100%)	0	100	100
1	B	127/154 (82%)	127 (100%)	0	100	100
1	C	127/154 (82%)	127 (100%)	0	100	100
1	D	127/154 (82%)	127 (100%)	0	100	100
1	E	127/154 (82%)	126 (99%)	1 (1%)	73	79
1	F	127/154 (82%)	127 (100%)	0	100	100
1	G	127/154 (82%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	127/154 (82%)	127 (100%)	0	100	100
1	I	127/154 (82%)	127 (100%)	0	100	100
1	J	127/154 (82%)	126 (99%)	1 (1%)	73	79
1	K	127/154 (82%)	127 (100%)	0	100	100
1	L	127/154 (82%)	127 (100%)	0	100	100
1	M	127/154 (82%)	127 (100%)	0	100	100
1	N	127/154 (82%)	127 (100%)	0	100	100
1	O	127/154 (82%)	127 (100%)	0	100	100
1	P	127/154 (82%)	127 (100%)	0	100	100
1	Q	127/154 (82%)	127 (100%)	0	100	100
1	R	127/154 (82%)	126 (99%)	1 (1%)	73	79
1	S	127/154 (82%)	126 (99%)	1 (1%)	73	79
1	T	127/154 (82%)	127 (100%)	0	100	100
1	U	127/154 (82%)	127 (100%)	0	100	100
1	V	127/154 (82%)	126 (99%)	1 (1%)	73	79
1	W	127/154 (82%)	126 (99%)	1 (1%)	73	79
1	X	127/154 (82%)	127 (100%)	0	100	100
All	All	3048/3696 (82%)	3042 (100%)	6 (0%)	87	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	83	GLU
1	E	172	ILE
1	J	172	ILE
1	R	69	MET
1	V	69	MET
1	W	172	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	157	GLN
1	H	41	ASN
1	A	41	ASN

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Mol	Chain	Res	Type
1	L	41	ASN
1	M	41	ASN
1	V	76	HIS
1	W	41	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 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	FMN	S	302	-	33,33,33	1.06	2 (6%)	48,50,50	1.23	6 (12%)
2	FMN	V	301	-	33,33,33	1.02	2 (6%)	48,50,50	1.23	5 (10%)
2	FMN	T	301	-	33,33,33	1.01	2 (6%)	48,50,50	1.19	8 (16%)
2	FMN	F	301	-	33,33,33	0.97	2 (6%)	48,50,50	1.24	6 (12%)
2	FMN	L	301	-	33,33,33	1.01	2 (6%)	48,50,50	1.27	6 (12%)
2	FMN	X	301	-	33,33,33	1.04	2 (6%)	48,50,50	1.16	6 (12%)
2	FMN	H	301	-	33,33,33	1.04	2 (6%)	48,50,50	1.21	7 (14%)
2	FMN	D	301	-	33,33,33	1.06	2 (6%)	48,50,50	1.25	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	C	301	-	33,33,33	1.00	2 (6%)	48,50,50	1.23	6 (12%)
2	FMN	I	301	-	33,33,33	1.05	2 (6%)	48,50,50	1.31	6 (12%)
2	FMN	W	301	-	33,33,33	1.04	2 (6%)	48,50,50	1.22	7 (14%)
2	FMN	U	301	-	33,33,33	1.02	2 (6%)	48,50,50	1.29	8 (16%)
2	FMN	G	301	-	33,33,33	0.98	2 (6%)	48,50,50	1.23	6 (12%)
2	FMN	R	301	-	33,33,33	0.97	2 (6%)	48,50,50	1.23	6 (12%)
2	FMN	P	301	-	33,33,33	1.02	2 (6%)	48,50,50	1.17	6 (12%)
2	FMN	M	301	-	33,33,33	1.04	2 (6%)	48,50,50	1.24	8 (16%)
2	FMN	B	301	-	33,33,33	1.07	2 (6%)	48,50,50	1.17	7 (14%)
2	FMN	Q	301	-	33,33,33	1.03	2 (6%)	48,50,50	1.22	7 (14%)
2	FMN	E	301	-	33,33,33	1.02	2 (6%)	48,50,50	1.23	7 (14%)
3	ARG	S	301	-	9,10,11	0.47	0	5,11,13	0.31	0
2	FMN	J	301	-	33,33,33	1.01	2 (6%)	48,50,50	1.20	7 (14%)
2	FMN	N	301	-	33,33,33	1.02	2 (6%)	48,50,50	1.31	8 (16%)
2	FMN	K	301	-	33,33,33	1.03	2 (6%)	48,50,50	1.28	6 (12%)
2	FMN	O	301	-	33,33,33	1.06	2 (6%)	48,50,50	1.23	8 (16%)
2	FMN	A	301	-	33,33,33	0.99	1 (3%)	48,50,50	1.29	5 (10%)

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	FMN	S	302	-	-	3/18/18/18	0/3/3/3
2	FMN	V	301	-	-	3/18/18/18	0/3/3/3
2	FMN	T	301	-	-	3/18/18/18	0/3/3/3
2	FMN	F	301	-	-	3/18/18/18	0/3/3/3
2	FMN	L	301	-	-	3/18/18/18	0/3/3/3
2	FMN	X	301	-	-	3/18/18/18	0/3/3/3
2	FMN	H	301	-	-	3/18/18/18	0/3/3/3
2	FMN	D	301	-	-	3/18/18/18	0/3/3/3
2	FMN	C	301	-	-	3/18/18/18	0/3/3/3
2	FMN	I	301	-	-	3/18/18/18	0/3/3/3
2	FMN	W	301	-	-	3/18/18/18	0/3/3/3
2	FMN	U	301	-	-	3/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	G	301	-	-	3/18/18/18	0/3/3/3
2	FMN	R	301	-	-	3/18/18/18	0/3/3/3
2	FMN	P	301	-	-	3/18/18/18	0/3/3/3
2	FMN	M	301	-	-	3/18/18/18	0/3/3/3
2	FMN	B	301	-	-	3/18/18/18	0/3/3/3
2	FMN	Q	301	-	-	3/18/18/18	0/3/3/3
2	FMN	E	301	-	-	3/18/18/18	0/3/3/3
3	ARG	S	301	-	-	1/8/9/11	-
2	FMN	J	301	-	-	3/18/18/18	0/3/3/3
2	FMN	N	301	-	-	3/18/18/18	0/3/3/3
2	FMN	K	301	-	-	3/18/18/18	0/3/3/3
2	FMN	O	301	-	-	3/18/18/18	0/3/3/3
2	FMN	A	301	-	-	3/18/18/18	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	302	FMN	C4A-N5	4.06	1.39	1.30
2	B	301	FMN	C4A-N5	3.93	1.39	1.30
2	O	301	FMN	C4A-N5	3.91	1.39	1.30
2	D	301	FMN	C4A-N5	3.89	1.39	1.30
2	V	301	FMN	C4A-N5	3.83	1.39	1.30
2	Q	301	FMN	C4A-N5	3.83	1.39	1.30
2	P	301	FMN	C4A-N5	3.79	1.38	1.30
2	H	301	FMN	C4A-N5	3.79	1.38	1.30
2	T	301	FMN	C4A-N5	3.78	1.38	1.30
2	I	301	FMN	C4A-N5	3.78	1.38	1.30
2	W	301	FMN	C4A-N5	3.78	1.38	1.30
2	U	301	FMN	C4A-N5	3.77	1.38	1.30
2	X	301	FMN	C4A-N5	3.76	1.38	1.30
2	A	301	FMN	C4A-N5	3.71	1.38	1.30
2	N	301	FMN	C4A-N5	3.70	1.38	1.30
2	M	301	FMN	C4A-N5	3.69	1.38	1.30
2	K	301	FMN	C4A-N5	3.67	1.38	1.30
2	E	301	FMN	C4A-N5	3.66	1.38	1.30
2	G	301	FMN	C4A-N5	3.61	1.38	1.30
2	C	301	FMN	C4A-N5	3.53	1.38	1.30
2	J	301	FMN	C4A-N5	3.50	1.38	1.30
2	R	301	FMN	C4A-N5	3.46	1.38	1.30
2	F	301	FMN	C4A-N5	3.41	1.38	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	301	FMN	C4A-N5	3.36	1.38	1.30
2	B	301	FMN	C10-N1	2.80	1.38	1.33
2	E	301	FMN	C10-N1	2.76	1.38	1.33
2	P	301	FMN	C10-N1	2.73	1.38	1.33
2	X	301	FMN	C10-N1	2.73	1.38	1.33
2	S	302	FMN	C10-N1	2.71	1.38	1.33
2	W	301	FMN	C10-N1	2.66	1.38	1.33
2	D	301	FMN	C10-N1	2.63	1.38	1.33
2	T	301	FMN	C10-N1	2.58	1.38	1.33
2	H	301	FMN	C10-N1	2.55	1.38	1.33
2	O	301	FMN	C10-N1	2.50	1.38	1.33
2	J	301	FMN	C10-N1	2.44	1.38	1.33
2	L	301	FMN	C10-N1	2.39	1.38	1.33
2	U	301	FMN	C10-N1	2.38	1.38	1.33
2	C	301	FMN	C10-N1	2.33	1.37	1.33
2	Q	301	FMN	C10-N1	2.31	1.37	1.33
2	N	301	FMN	C10-N1	2.27	1.37	1.33
2	M	301	FMN	C10-N1	2.27	1.37	1.33
2	K	301	FMN	C10-N1	2.20	1.37	1.33
2	R	301	FMN	C10-N1	2.20	1.37	1.33
2	V	301	FMN	C10-N1	2.19	1.37	1.33
2	F	301	FMN	C10-N1	2.14	1.37	1.33
2	I	301	FMN	C10-N1	2.10	1.37	1.33
2	G	301	FMN	C10-N1	2.00	1.37	1.33

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	301	FMN	C4-N3-C2	-3.47	119.48	125.64
2	A	301	FMN	C4A-C10-N10	3.43	121.39	116.48
2	V	301	FMN	C4-N3-C2	-3.31	119.77	125.64
2	F	301	FMN	C4-N3-C2	-3.29	119.81	125.64
2	N	301	FMN	C4-N3-C2	-3.16	120.03	125.64
2	D	301	FMN	C4-N3-C2	-3.13	120.09	125.64
2	R	301	FMN	C4-N3-C2	-3.11	120.11	125.64
2	L	301	FMN	C4-N3-C2	-3.09	120.16	125.64
2	G	301	FMN	C4A-C10-N10	3.06	120.87	116.48
2	S	302	FMN	C4-N3-C2	-3.02	120.28	125.64
2	C	301	FMN	C4-N3-C2	-2.99	120.34	125.64
2	V	301	FMN	C4A-C10-N10	2.99	120.76	116.48
2	G	301	FMN	C4-N3-C2	-2.95	120.41	125.64
2	N	301	FMN	C4A-C10-N10	2.94	120.69	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	301	FMN	C4A-C10-N10	2.94	120.69	116.48
2	A	301	FMN	C4-N3-C2	-2.92	120.45	125.64
2	U	301	FMN	C4-N3-C2	-2.92	120.45	125.64
2	K	301	FMN	C4A-C10-N10	2.91	120.65	116.48
2	S	302	FMN	C4A-C4-N3	2.88	120.57	113.25
2	E	301	FMN	C9A-C5A-N5	-2.84	119.44	122.45
2	J	301	FMN	C4A-C10-N10	2.81	120.51	116.48
2	U	301	FMN	C4A-C10-N10	2.81	120.51	116.48
2	O	301	FMN	C5A-C9A-N10	2.81	120.51	117.97
2	F	301	FMN	C4A-C10-N10	2.80	120.49	116.48
2	I	301	FMN	C4A-C4-N3	2.78	120.33	113.25
2	A	301	FMN	C4-C4A-N5	2.77	122.04	118.21
2	M	301	FMN	C4-N3-C2	-2.76	120.74	125.64
2	A	301	FMN	C10-C4A-N5	-2.76	119.17	124.81
2	K	301	FMN	C4-N3-C2	-2.76	120.74	125.64
2	L	301	FMN	O4-C4-C4A	-2.75	119.26	126.53
2	W	301	FMN	C4A-C10-N10	2.74	120.41	116.48
2	S	302	FMN	C9A-C5A-N5	-2.74	119.55	122.45
2	P	301	FMN	C4-N3-C2	-2.73	120.79	125.64
2	V	301	FMN	C4A-C4-N3	2.72	120.19	113.25
2	X	301	FMN	C4-N3-C2	-2.70	120.85	125.64
2	I	301	FMN	C4A-C10-N10	2.69	120.33	116.48
2	D	301	FMN	C4A-C4-N3	2.68	120.07	113.25
2	J	301	FMN	C4-N3-C2	-2.68	120.88	125.64
2	K	301	FMN	C10-C4A-N5	-2.68	119.34	124.81
2	Q	301	FMN	C4-N3-C2	-2.67	120.90	125.64
2	R	301	FMN	C9A-C5A-N5	-2.67	119.62	122.45
2	E	301	FMN	C4-N3-C2	-2.66	120.91	125.64
2	B	301	FMN	C9A-C5A-N5	-2.66	119.63	122.45
2	W	301	FMN	C10-C4A-N5	-2.65	119.40	124.81
2	M	301	FMN	C4A-C10-N10	2.65	120.27	116.48
2	C	301	FMN	C4A-C10-N10	2.64	120.27	116.48
2	N	301	FMN	O4-C4-C4A	-2.64	119.56	126.53
2	Q	301	FMN	C9A-C5A-N5	-2.64	119.66	122.45
2	O	301	FMN	C4A-C10-N10	2.64	120.26	116.48
2	I	301	FMN	O4-C4-C4A	-2.63	119.59	126.53
2	N	301	FMN	C4A-C4-N3	2.63	119.94	113.25
2	A	301	FMN	C4A-C4-N3	2.62	119.92	113.25
2	O	301	FMN	C4-N3-C2	-2.61	121.00	125.64
2	J	301	FMN	C10-C4A-N5	-2.61	119.49	124.81
2	K	301	FMN	C9A-C5A-N5	-2.60	119.70	122.45
2	E	301	FMN	O4-C4-C4A	-2.59	119.69	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	301	FMN	O4-C4-C4A	-2.59	119.71	126.53
2	O	301	FMN	O4-C4-C4A	-2.58	119.72	126.53
2	D	301	FMN	O4-C4-C4A	-2.58	119.72	126.53
2	C	301	FMN	C4A-C4-N3	2.58	119.81	113.25
2	M	301	FMN	C9A-C5A-N5	-2.57	119.72	122.45
2	L	301	FMN	C4A-C4-N3	2.57	119.80	113.25
2	H	301	FMN	C4A-C10-N10	2.56	120.15	116.48
2	E	301	FMN	C4A-C4-N3	2.56	119.76	113.25
2	M	301	FMN	C10-C4A-N5	-2.54	119.63	124.81
2	C	301	FMN	C10-C4A-N5	-2.53	119.64	124.81
2	F	301	FMN	C4A-C4-N3	2.53	119.69	113.25
2	L	301	FMN	C4A-C10-N10	2.53	120.10	116.48
2	B	301	FMN	C5A-C9A-N10	2.52	120.25	117.97
2	U	301	FMN	C4A-C4-N3	2.52	119.67	113.25
2	W	301	FMN	C4-C4A-N5	2.52	121.69	118.21
2	H	301	FMN	C4-N3-C2	-2.52	121.17	125.64
2	O	301	FMN	C4A-C4-N3	2.52	119.66	113.25
2	V	301	FMN	O4-C4-C4A	-2.51	119.89	126.53
2	D	301	FMN	C4A-C10-N10	2.51	120.08	116.48
2	H	301	FMN	O4-C4-C4A	-2.51	119.92	126.53
2	F	301	FMN	C10-C4A-N5	-2.50	119.70	124.81
2	X	301	FMN	C9A-C5A-N5	-2.50	119.80	122.45
2	G	301	FMN	C4A-C4-N3	2.50	119.61	113.25
2	I	301	FMN	C9A-C5A-N5	-2.50	119.81	122.45
2	S	302	FMN	C10-C4A-N5	-2.49	119.72	124.81
2	Q	301	FMN	C5A-C9A-N10	2.49	120.22	117.97
2	X	301	FMN	C4A-C4-N3	2.49	119.59	113.25
2	O	301	FMN	O3P-P-O5'	2.48	113.15	106.67
2	Q	301	FMN	O4-C4-C4A	-2.48	120.00	126.53
2	V	301	FMN	C10-C4A-N5	-2.47	119.77	124.81
2	T	301	FMN	C10-C4A-N5	-2.46	119.78	124.81
2	I	301	FMN	C10-C4A-N5	-2.46	119.78	124.81
2	P	301	FMN	O4-C4-C4A	-2.46	120.05	126.53
2	W	301	FMN	C9A-C5A-N5	-2.45	119.86	122.45
2	U	301	FMN	C9A-C5A-N5	-2.44	119.86	122.45
2	S	302	FMN	C4A-C10-N10	2.44	119.97	116.48
2	G	301	FMN	C10-C4A-N5	-2.44	119.83	124.81
2	R	301	FMN	C4A-C10-N10	2.44	119.97	116.48
2	R	301	FMN	C4A-C4-N3	2.43	119.45	113.25
2	C	301	FMN	O4-C4-C4A	-2.43	120.11	126.53
2	R	301	FMN	C10-C4A-N5	-2.42	119.87	124.81
2	M	301	FMN	C4A-C4-N3	2.41	119.39	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	FMN	C9A-C5A-N5	-2.41	119.90	122.45
2	J	301	FMN	C4A-C4-N3	2.40	119.38	113.25
2	D	301	FMN	C10-C4A-N5	-2.40	119.91	124.81
2	N	301	FMN	C10-C4A-N5	-2.40	119.91	124.81
2	R	301	FMN	O4-C4-C4A	-2.39	120.21	126.53
2	T	301	FMN	C4-N3-C2	-2.39	121.39	125.64
2	H	301	FMN	C4A-C4-N3	2.38	119.31	113.25
2	N	301	FMN	C9A-C5A-N5	-2.38	119.93	122.45
2	L	301	FMN	C9A-C5A-N5	-2.37	119.94	122.45
2	T	301	FMN	C4A-C4-N3	2.37	119.29	113.25
2	P	301	FMN	C4A-C4-N3	2.36	119.26	113.25
2	U	301	FMN	C10-C4A-N5	-2.36	119.99	124.81
2	P	301	FMN	C9A-C5A-N5	-2.35	119.96	122.45
2	S	302	FMN	C4-C4A-N5	2.35	121.46	118.21
2	P	301	FMN	C4A-C10-N10	2.35	119.85	116.48
2	Q	301	FMN	C4A-C4-N3	2.35	119.23	113.25
2	Q	301	FMN	C10-C4A-N5	-2.35	120.02	124.81
2	K	301	FMN	C4A-C4-N3	2.34	119.22	113.25
2	U	301	FMN	C5A-C9A-N10	2.33	120.07	117.97
2	K	301	FMN	C4-C4A-N5	2.33	121.42	118.21
2	Q	301	FMN	C4A-C10-N10	2.32	119.81	116.48
2	X	301	FMN	C10-C4A-N5	-2.32	120.07	124.81
2	H	301	FMN	C10-C4A-N5	-2.32	120.08	124.81
2	E	301	FMN	C10-C4A-N5	-2.31	120.09	124.81
2	T	301	FMN	C9A-C5A-N5	-2.30	120.01	122.45
2	W	301	FMN	C4A-C4-N3	2.30	119.10	113.25
2	B	301	FMN	C4A-C10-N10	2.30	119.77	116.48
2	L	301	FMN	C10-C4A-N5	-2.29	120.12	124.81
2	B	301	FMN	C10-C4A-N5	-2.29	120.14	124.81
2	G	301	FMN	O4-C4-C4A	-2.29	120.50	126.53
2	M	301	FMN	C4-C4A-N5	2.27	121.35	118.21
2	B	301	FMN	C4A-C4-N3	2.27	119.04	113.25
2	P	301	FMN	C10-C4A-N5	-2.27	120.18	124.81
2	X	301	FMN	C4A-C10-N10	2.27	119.73	116.48
2	F	301	FMN	O4-C4-C4A	-2.27	120.55	126.53
2	W	301	FMN	C4-N3-C2	-2.26	121.62	125.64
2	M	301	FMN	C5A-C9A-N10	2.26	120.01	117.97
2	H	301	FMN	C9A-C5A-N5	-2.25	120.06	122.45
2	T	301	FMN	C4-C4A-N5	2.25	121.31	118.21
2	B	301	FMN	C4-N3-C2	-2.25	121.65	125.64
2	O	301	FMN	C9A-C5A-N5	-2.24	120.08	122.45
2	C	301	FMN	C9A-C5A-N5	-2.22	120.09	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	301	FMN	O4-C4-C4A	-2.20	120.72	126.53
2	E	301	FMN	C5A-C9A-N10	2.20	119.96	117.97
2	T	301	FMN	C5A-C9A-N10	2.19	119.94	117.97
2	X	301	FMN	O4-C4-C4A	-2.16	120.83	126.53
2	T	301	FMN	O4-C4-C4A	-2.16	120.83	126.53
2	N	301	FMN	C4-C4A-N5	2.13	121.15	118.21
2	H	301	FMN	C5A-C9A-N10	2.13	119.89	117.97
2	E	301	FMN	C4A-C10-N10	2.12	119.52	116.48
2	U	301	FMN	O3P-P-O5'	2.11	112.17	106.67
2	M	301	FMN	O4-C4-C4A	-2.11	120.97	126.53
2	W	301	FMN	O4-C4-C4A	-2.10	121.00	126.53
2	G	301	FMN	C9A-C5A-N5	-2.08	120.25	122.45
2	B	301	FMN	O4-C4-C4A	-2.07	121.06	126.53
2	J	301	FMN	C4-C4A-N5	2.07	121.07	118.21
2	F	301	FMN	C9A-C5A-N5	-2.06	120.27	122.45
2	N	301	FMN	C5A-C9A-N10	2.05	119.82	117.97
2	J	301	FMN	C9A-C5A-N5	-2.03	120.30	122.45
2	O	301	FMN	C10-C4A-N5	-2.00	120.72	124.81

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	301	FMN	C5'-O5'-P-O2P
2	S	302	FMN	C5'-O5'-P-O2P
2	H	301	FMN	C5'-O5'-P-O2P
2	P	301	FMN	C5'-O5'-P-O2P
2	P	301	FMN	C5'-O5'-P-O3P
2	A	301	FMN	C5'-O5'-P-O2P
2	B	301	FMN	C5'-O5'-P-O2P
2	C	301	FMN	C5'-O5'-P-O2P
2	C	301	FMN	C5'-O5'-P-O3P
2	D	301	FMN	C5'-O5'-P-O2P
2	D	301	FMN	C5'-O5'-P-O3P
2	E	301	FMN	C5'-O5'-P-O2P
2	G	301	FMN	C5'-O5'-P-O2P
2	G	301	FMN	C5'-O5'-P-O3P
2	I	301	FMN	C5'-O5'-P-O2P
2	J	301	FMN	C5'-O5'-P-O2P
2	K	301	FMN	C5'-O5'-P-O2P
2	L	301	FMN	C5'-O5'-P-O2P
2	M	301	FMN	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
2	M	301	FMN	C5'-O5'-P-O3P
2	N	301	FMN	C5'-O5'-P-O2P
2	N	301	FMN	C5'-O5'-P-O3P
2	O	301	FMN	C5'-O5'-P-O2P
2	O	301	FMN	C5'-O5'-P-O3P
2	Q	301	FMN	C5'-O5'-P-O2P
2	R	301	FMN	C5'-O5'-P-O2P
2	R	301	FMN	C5'-O5'-P-O3P
2	T	301	FMN	C5'-O5'-P-O2P
2	U	301	FMN	C5'-O5'-P-O2P
2	U	301	FMN	C5'-O5'-P-O3P
2	V	301	FMN	C5'-O5'-P-O2P
2	V	301	FMN	C5'-O5'-P-O3P
2	W	301	FMN	C5'-O5'-P-O2P
2	W	301	FMN	C5'-O5'-P-O3P
2	X	301	FMN	C5'-O5'-P-O2P
2	X	301	FMN	C5'-O5'-P-O3P
3	S	301	ARG	NE-CD-CG-CB
2	F	301	FMN	C5'-O5'-P-O1P
2	S	302	FMN	C5'-O5'-P-O1P
2	H	301	FMN	C5'-O5'-P-O1P
2	P	301	FMN	C5'-O5'-P-O1P
2	A	301	FMN	C5'-O5'-P-O1P
2	B	301	FMN	C5'-O5'-P-O1P
2	C	301	FMN	C5'-O5'-P-O1P
2	D	301	FMN	C5'-O5'-P-O1P
2	E	301	FMN	C5'-O5'-P-O1P
2	G	301	FMN	C5'-O5'-P-O1P
2	I	301	FMN	C5'-O5'-P-O1P
2	J	301	FMN	C5'-O5'-P-O1P
2	K	301	FMN	C5'-O5'-P-O1P
2	L	301	FMN	C5'-O5'-P-O1P
2	M	301	FMN	C5'-O5'-P-O1P
2	N	301	FMN	C5'-O5'-P-O1P
2	O	301	FMN	C5'-O5'-P-O1P
2	Q	301	FMN	C5'-O5'-P-O1P
2	R	301	FMN	C5'-O5'-P-O1P
2	T	301	FMN	C5'-O5'-P-O1P
2	U	301	FMN	C5'-O5'-P-O1P
2	V	301	FMN	C5'-O5'-P-O1P
2	W	301	FMN	C5'-O5'-P-O1P
2	X	301	FMN	C5'-O5'-P-O1P

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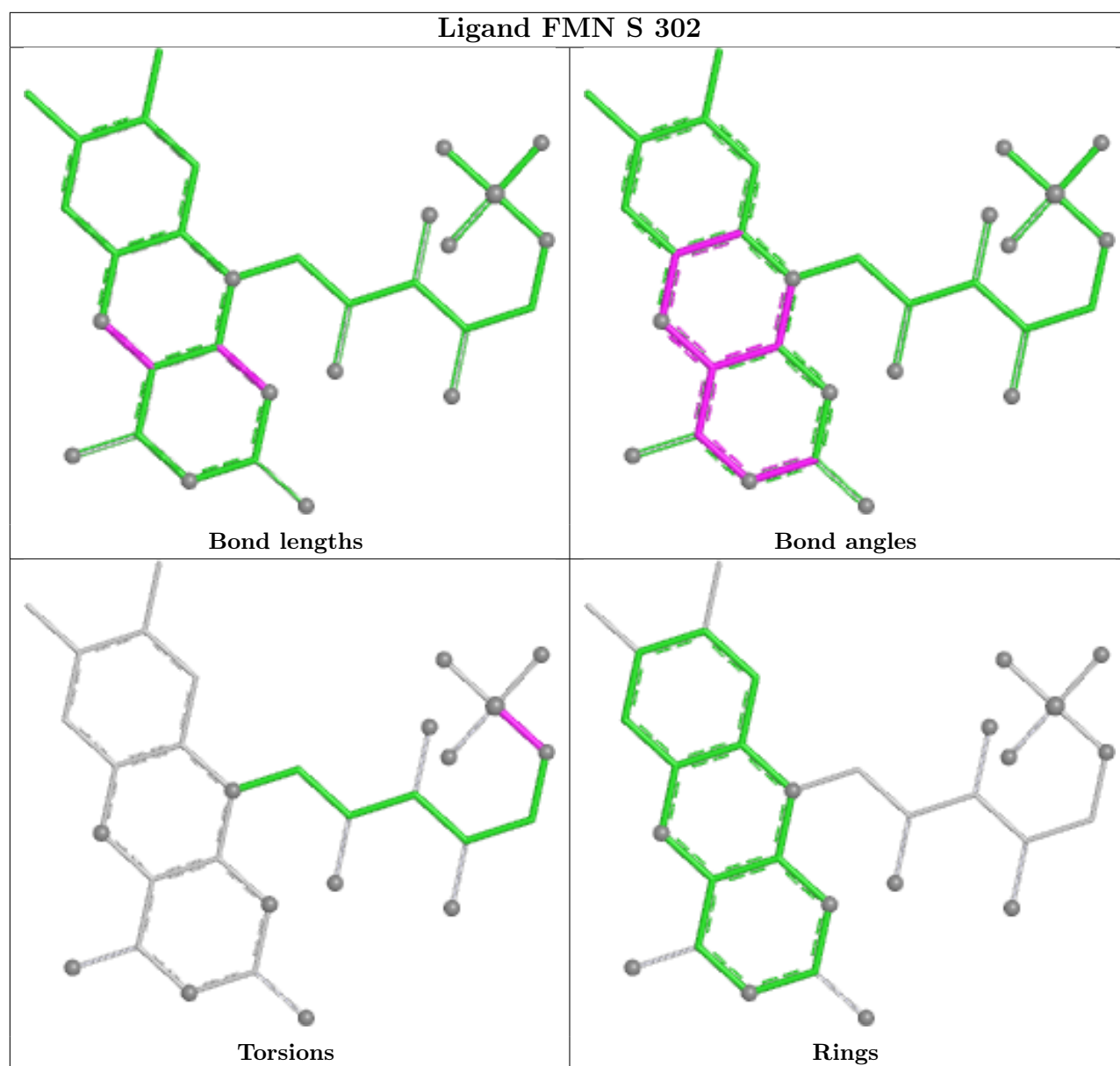
Mol	Chain	Res	Type	Atoms
2	F	301	FMN	C5'-O5'-P-O3P
2	S	302	FMN	C5'-O5'-P-O3P
2	H	301	FMN	C5'-O5'-P-O3P
2	A	301	FMN	C5'-O5'-P-O3P
2	B	301	FMN	C5'-O5'-P-O3P
2	E	301	FMN	C5'-O5'-P-O3P
2	I	301	FMN	C5'-O5'-P-O3P
2	J	301	FMN	C5'-O5'-P-O3P
2	K	301	FMN	C5'-O5'-P-O3P
2	L	301	FMN	C5'-O5'-P-O3P
2	Q	301	FMN	C5'-O5'-P-O3P
2	T	301	FMN	C5'-O5'-P-O3P

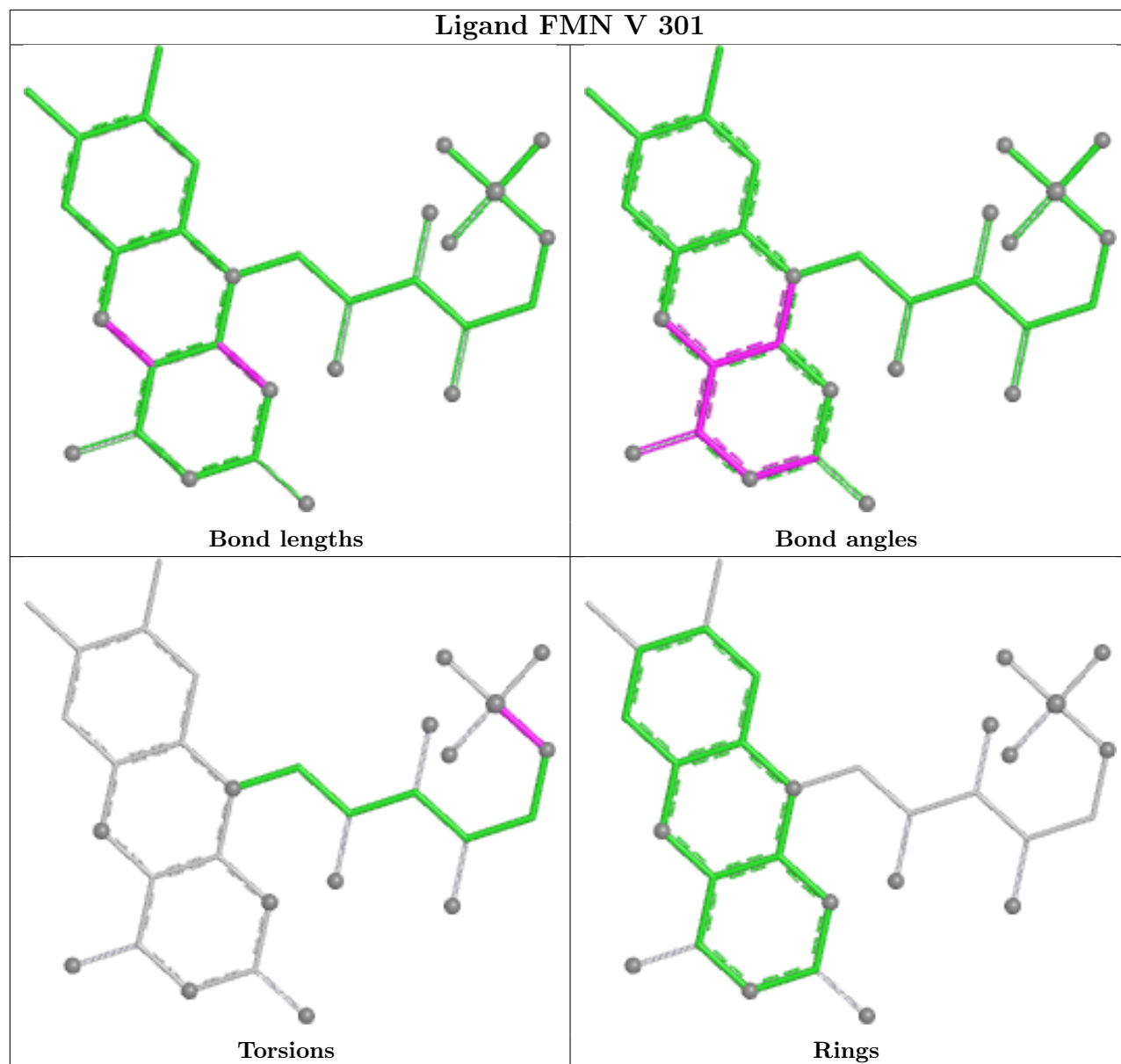
There are no ring outliers.

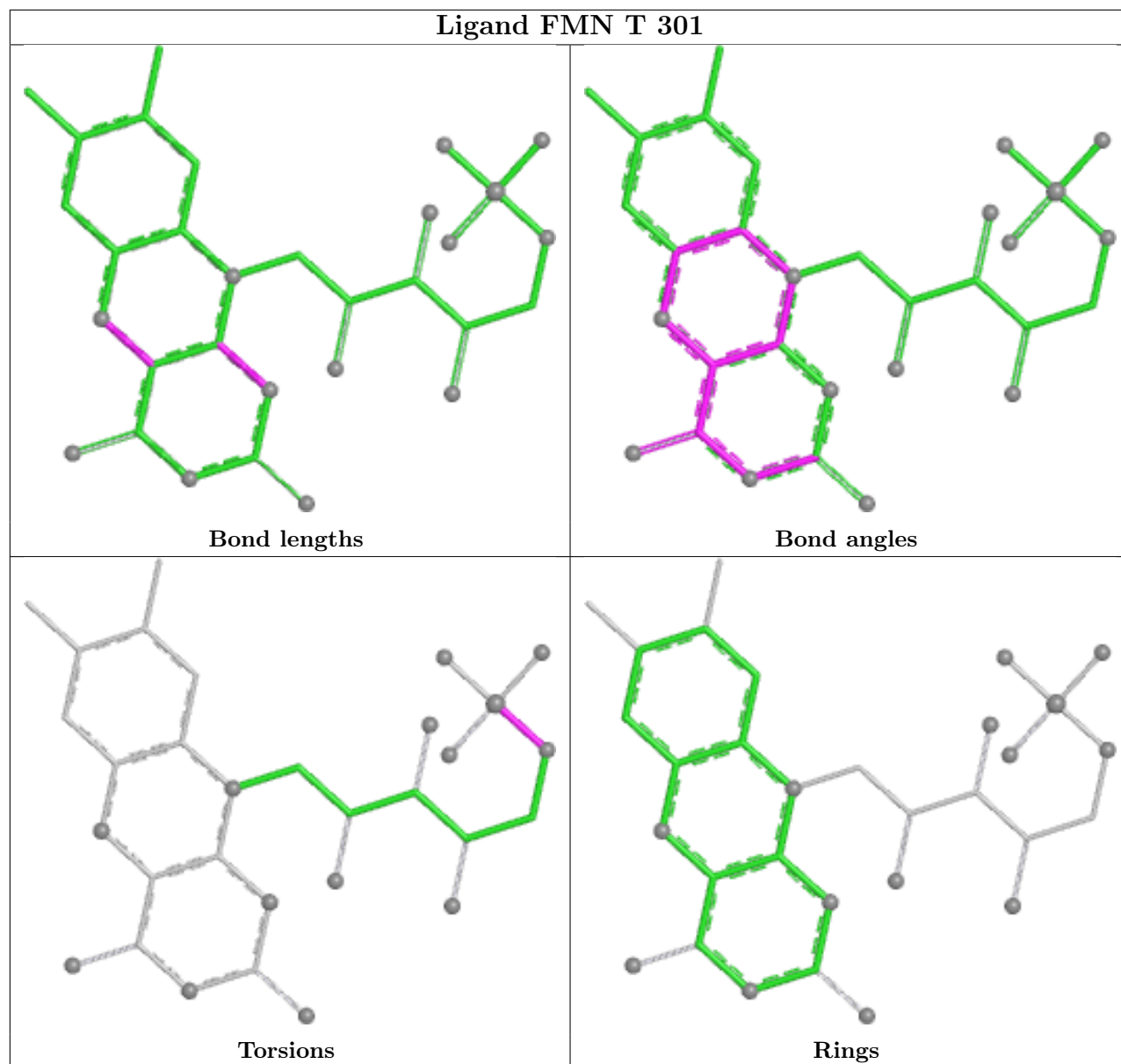
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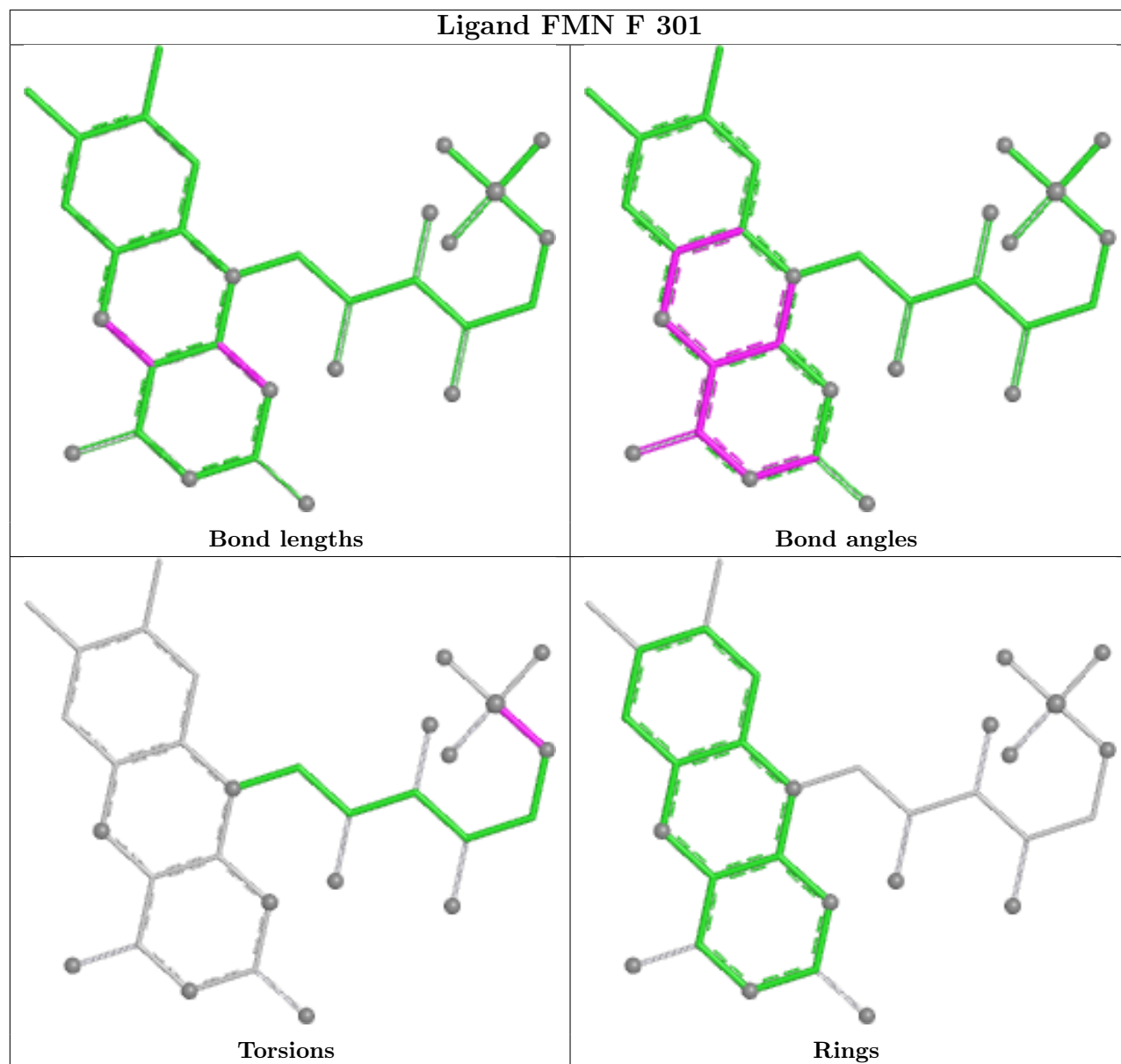
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	FMN	1	0
2	L	301	FMN	1	0
2	I	301	FMN	1	0
2	G	301	FMN	1	0
2	M	301	FMN	1	0
2	Q	301	FMN	1	0
3	S	301	ARG	1	0
2	J	301	FMN	1	0
2	N	301	FMN	1	0
2	K	301	FMN	2	0
2	O	301	FMN	1	0
2	A	301	FMN	1	0

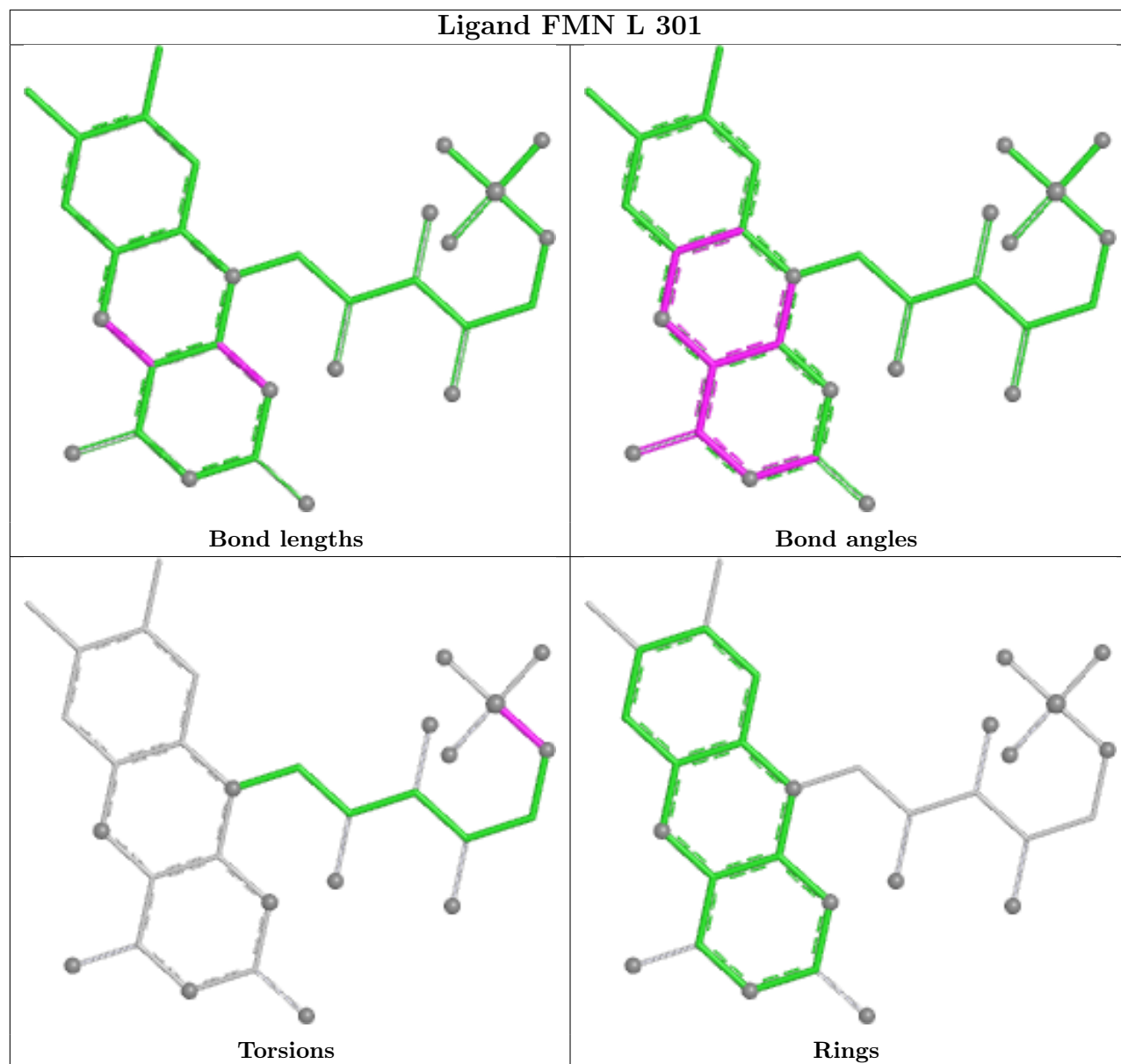
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

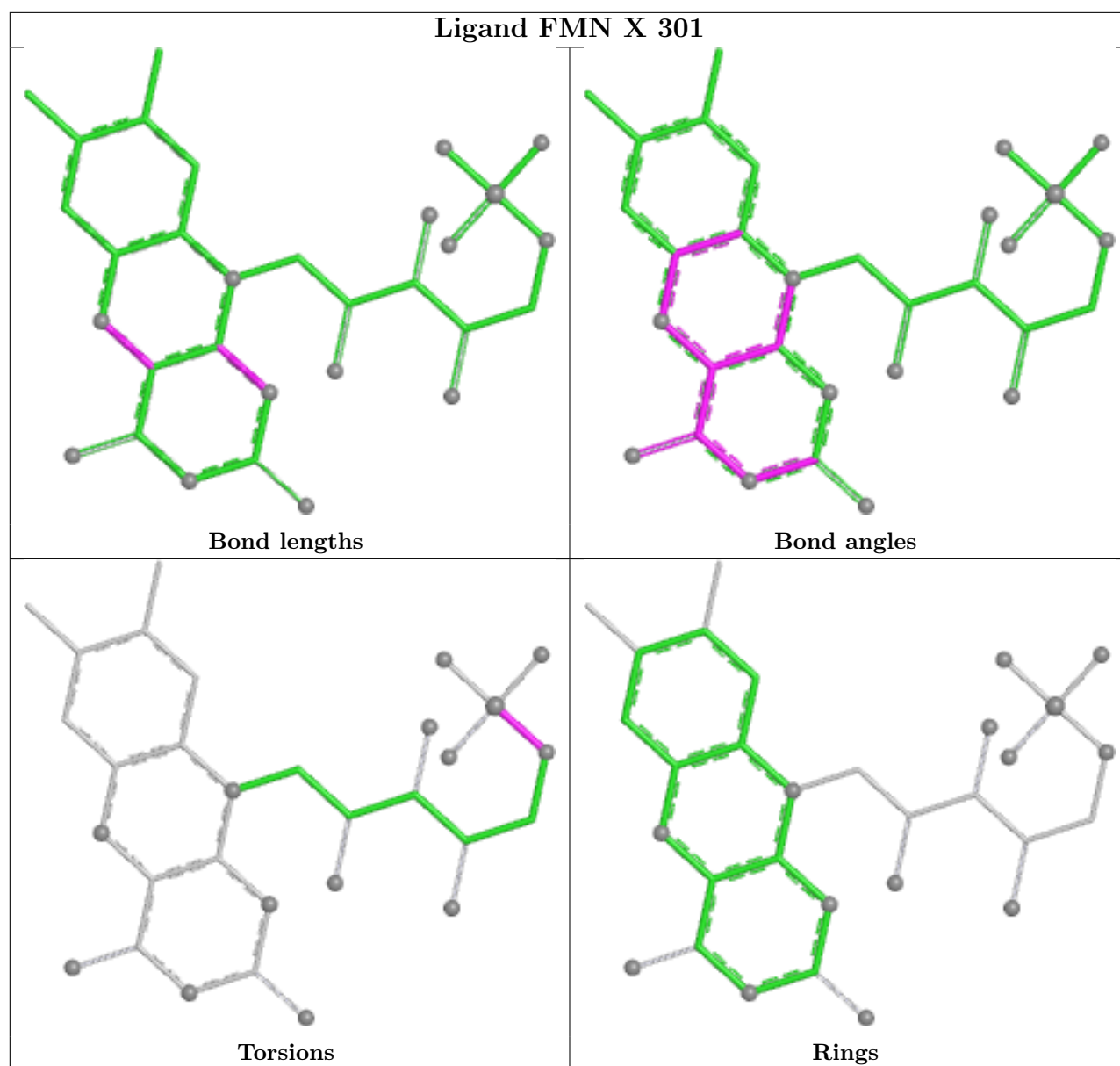


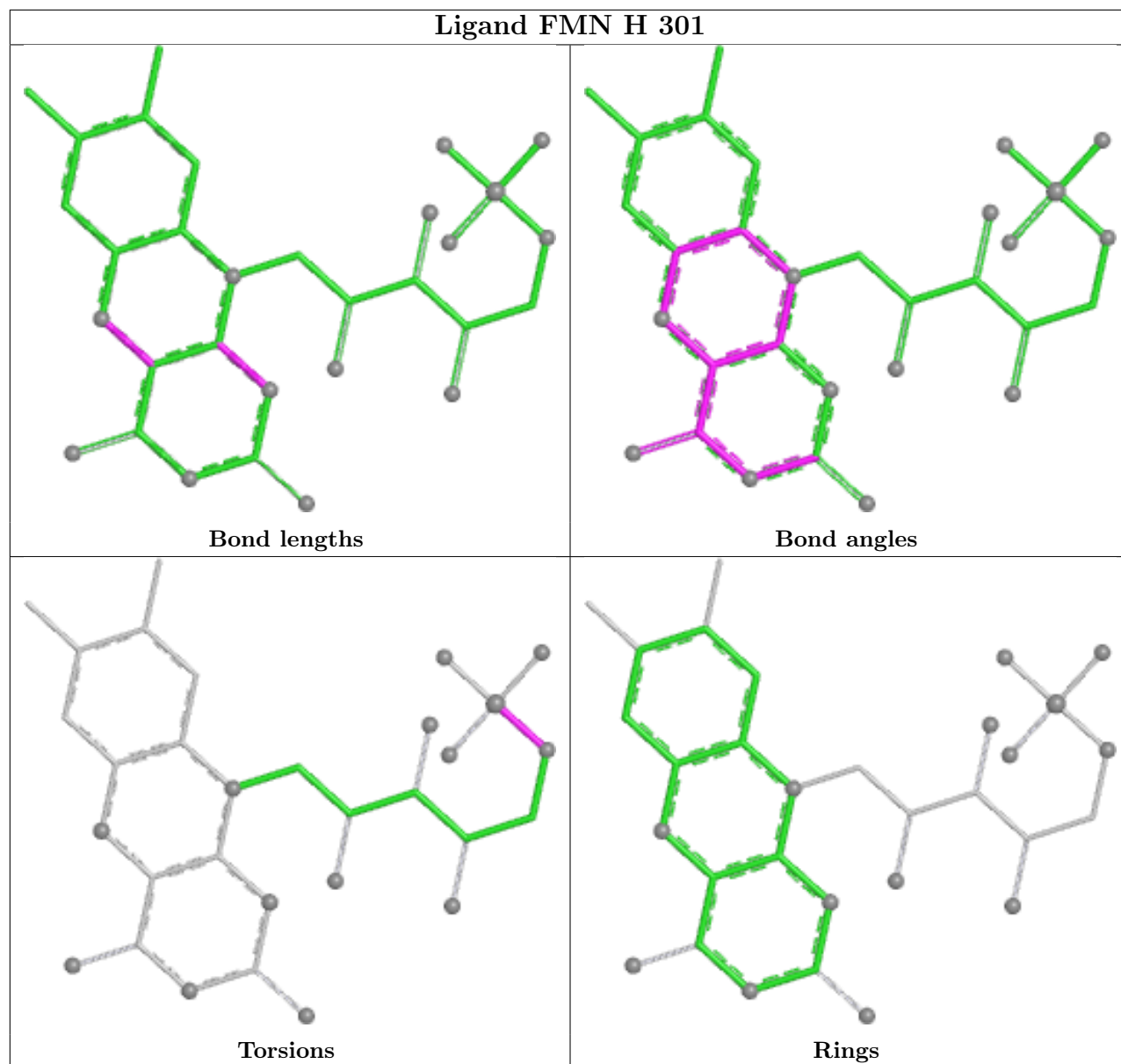


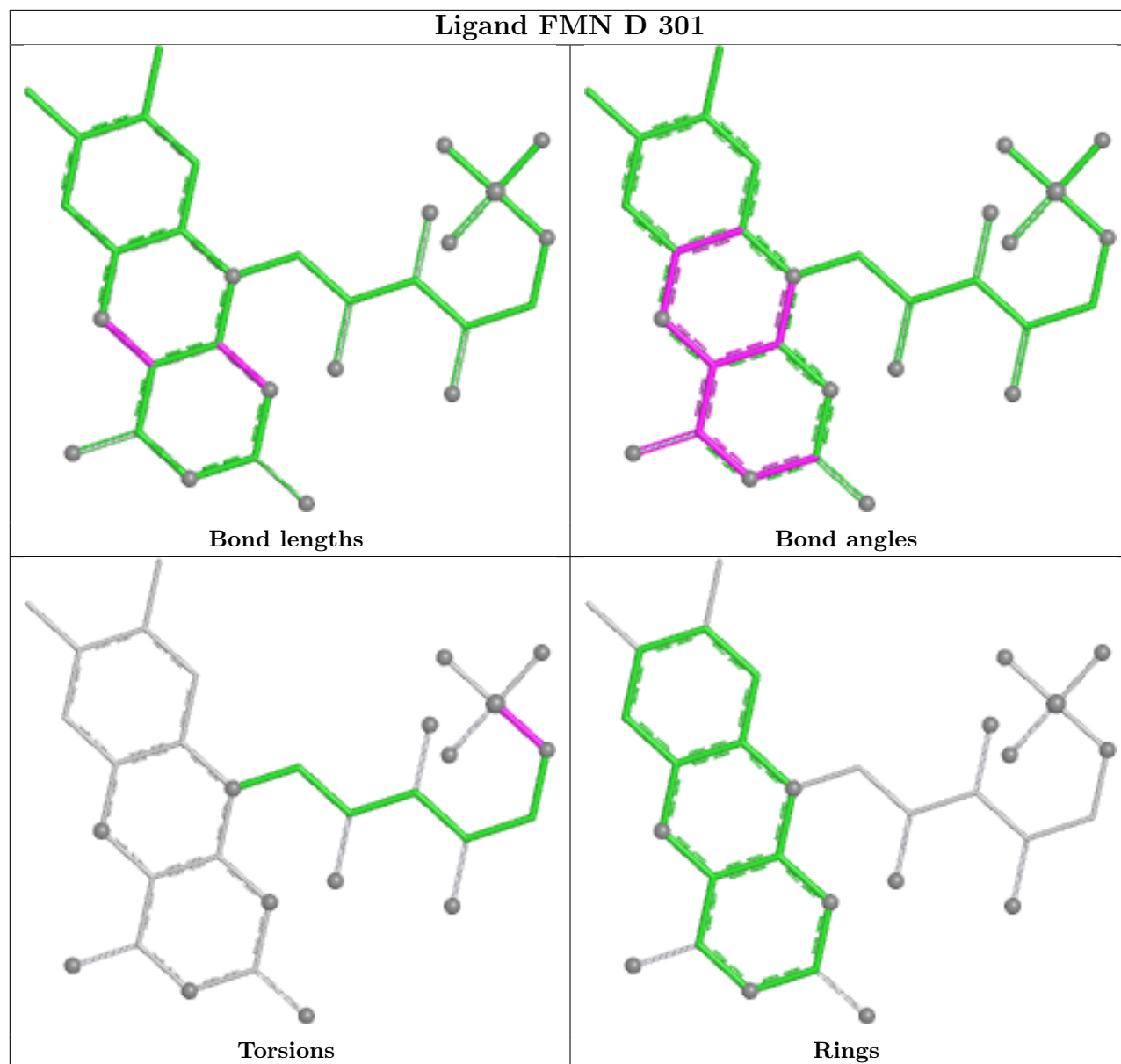


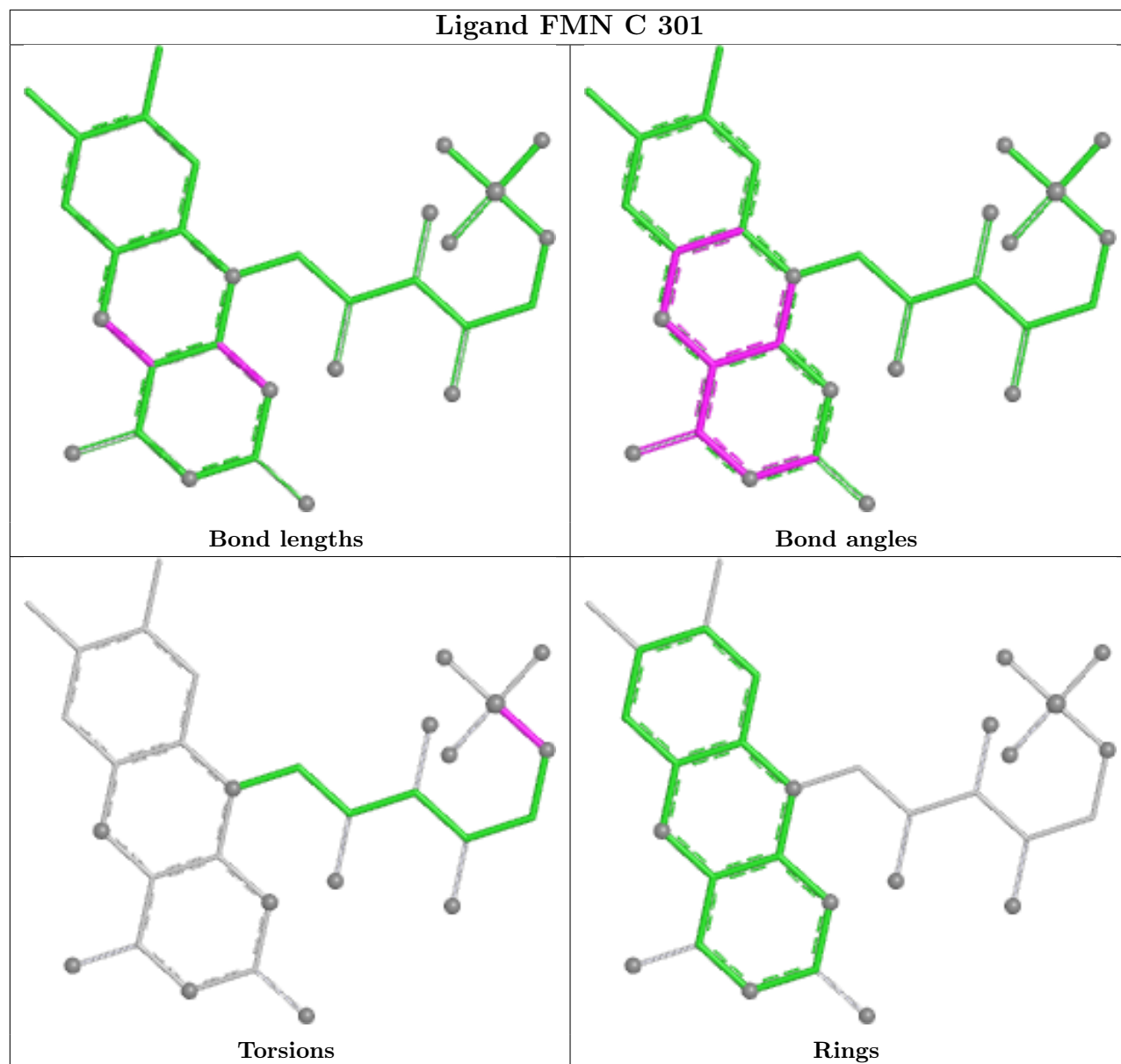


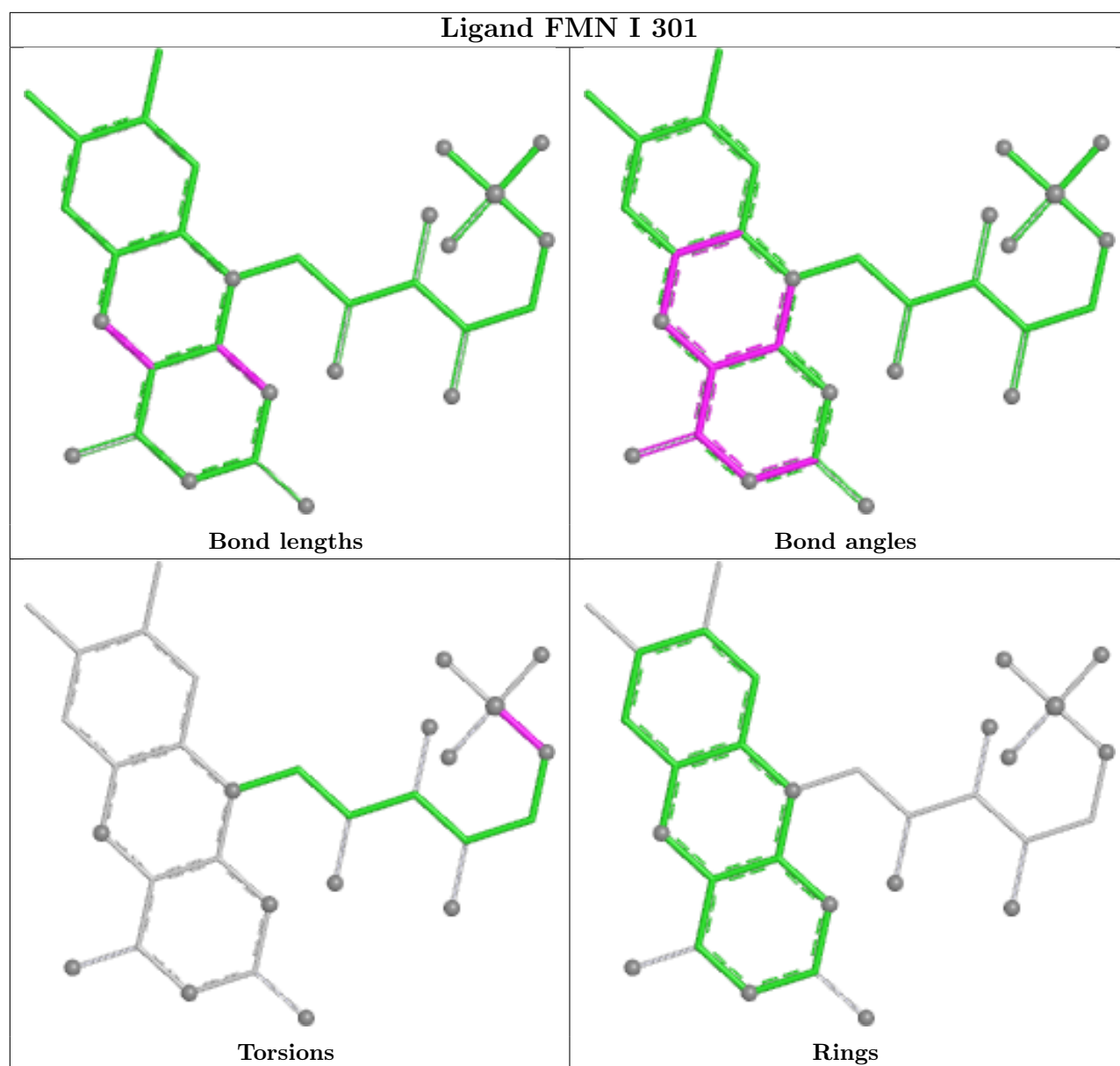


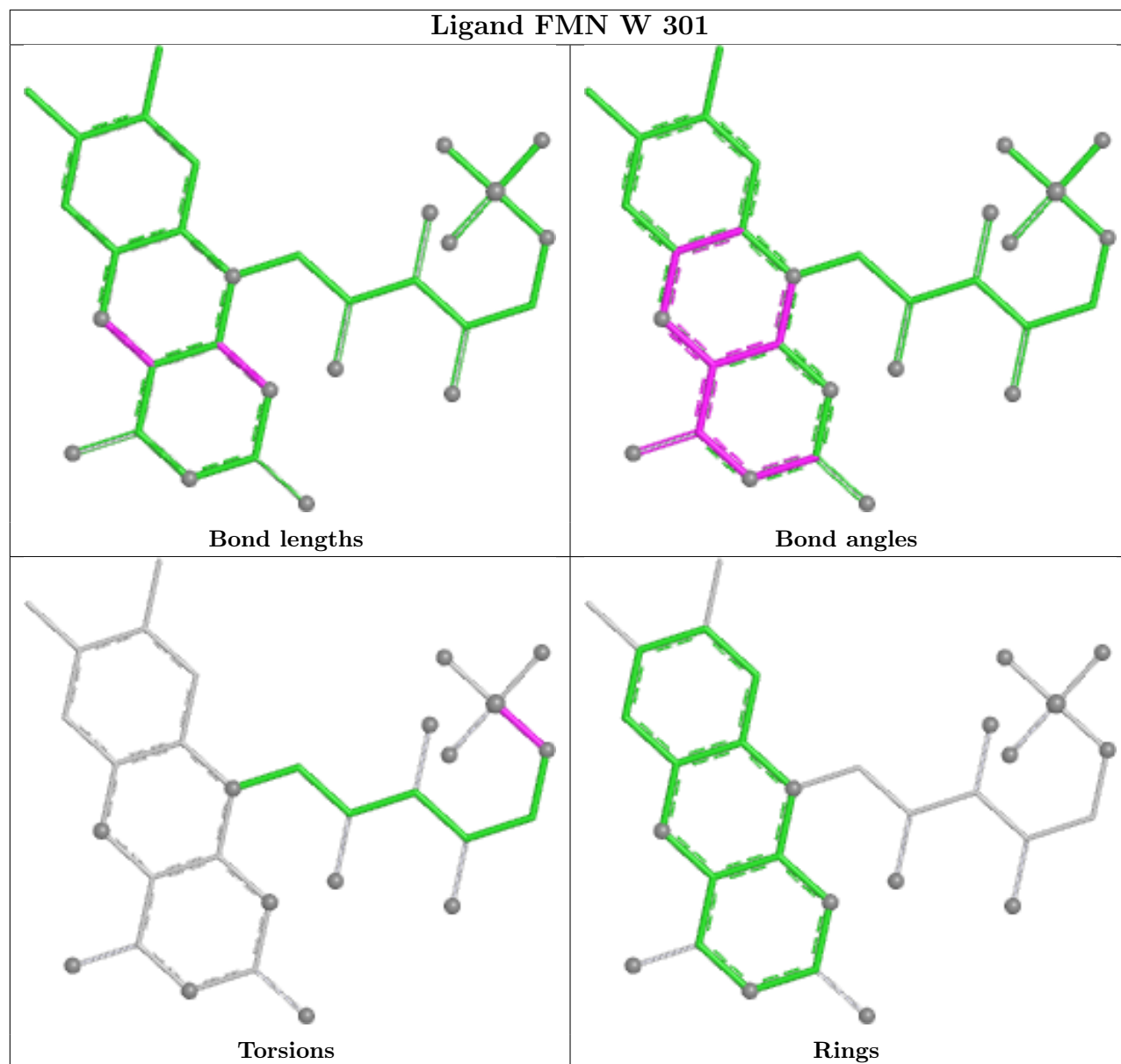


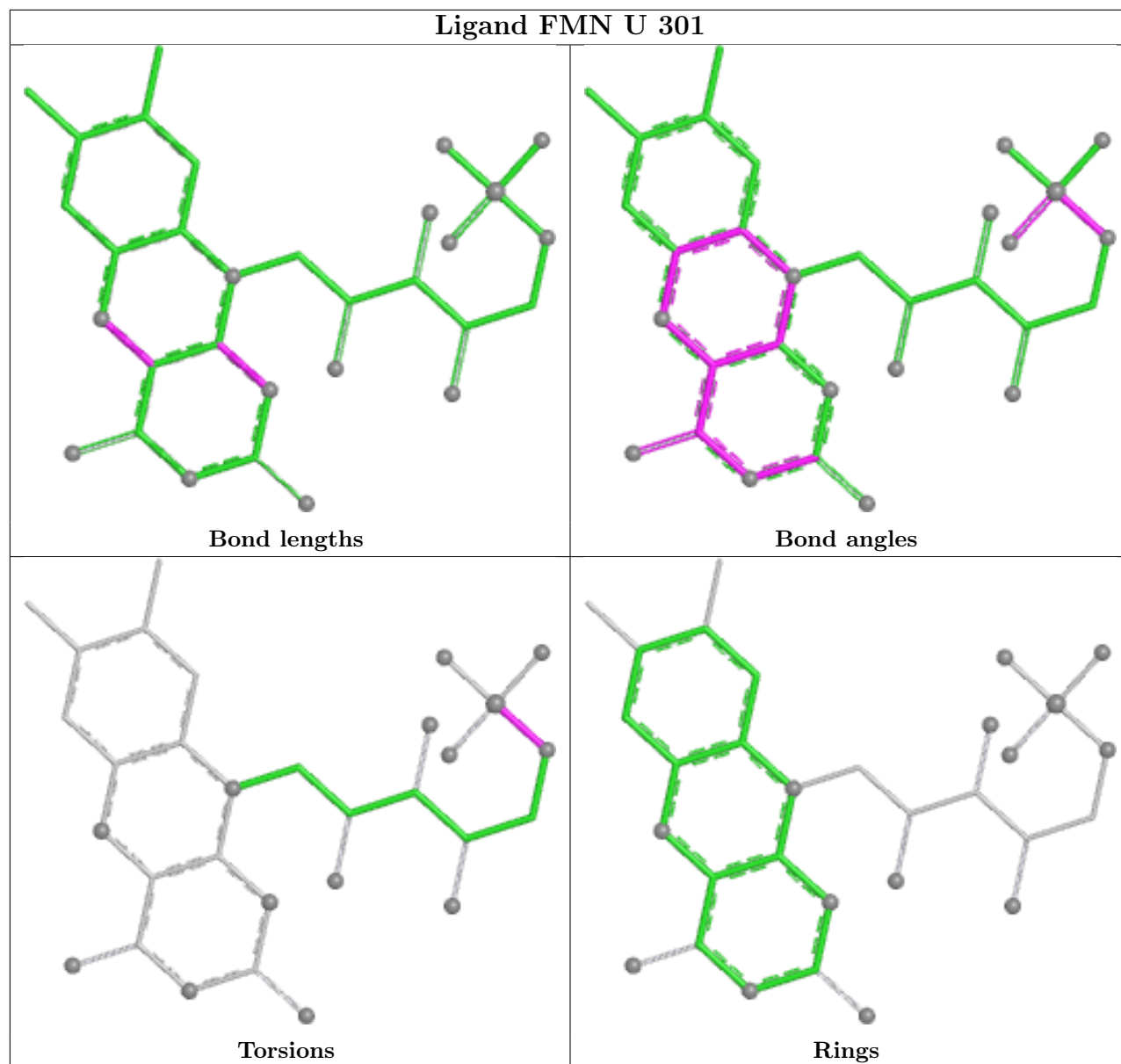


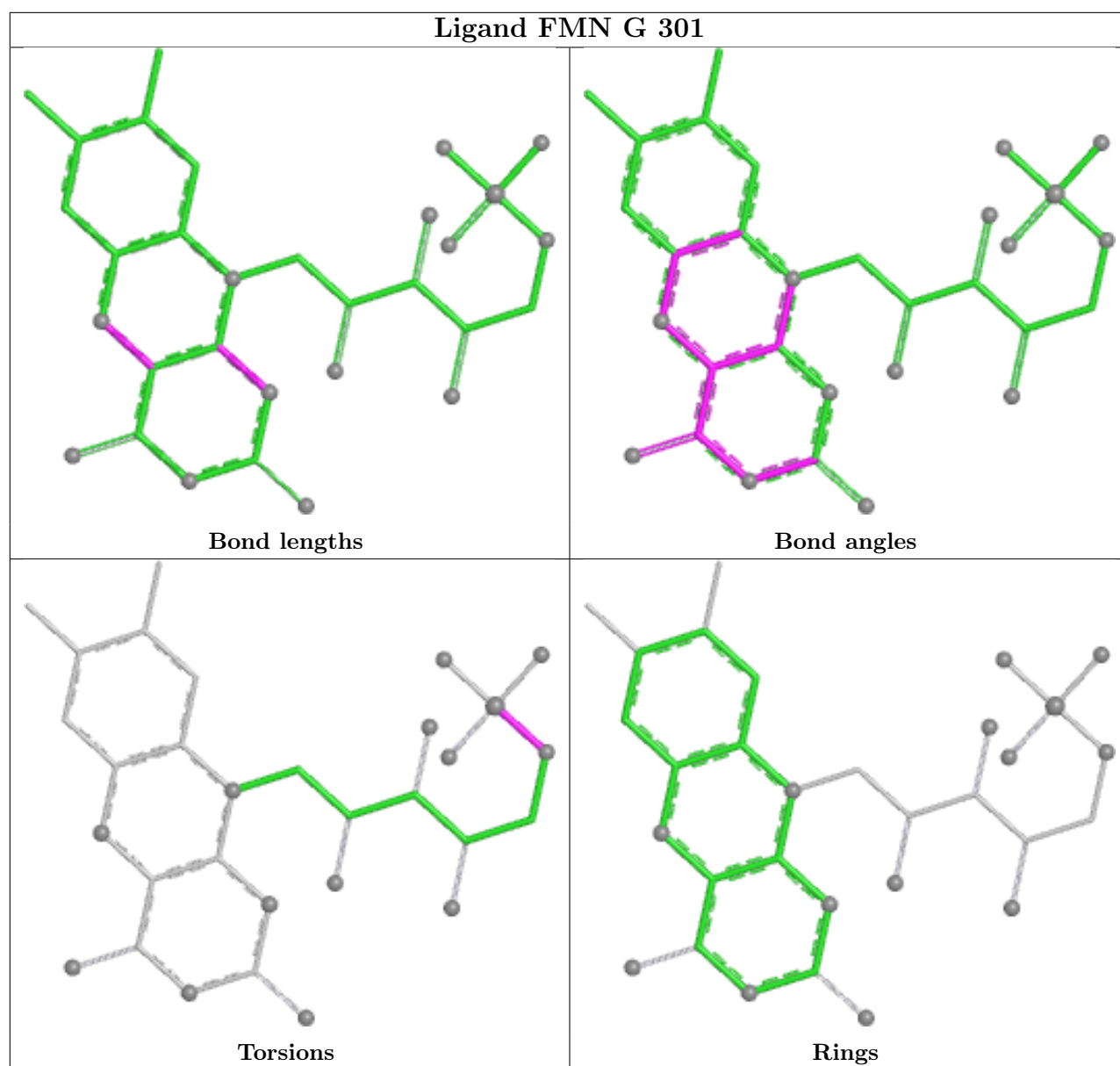


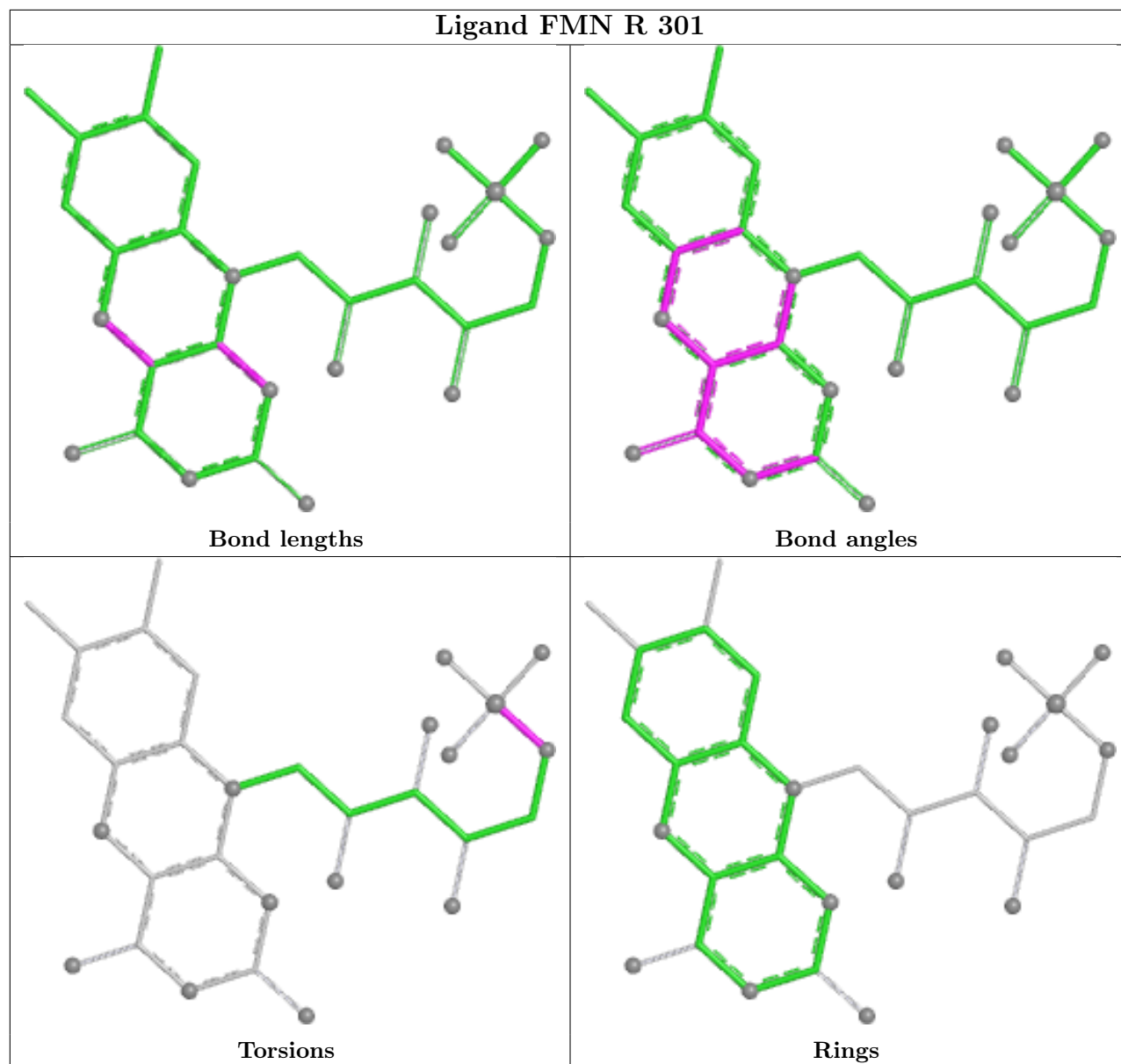


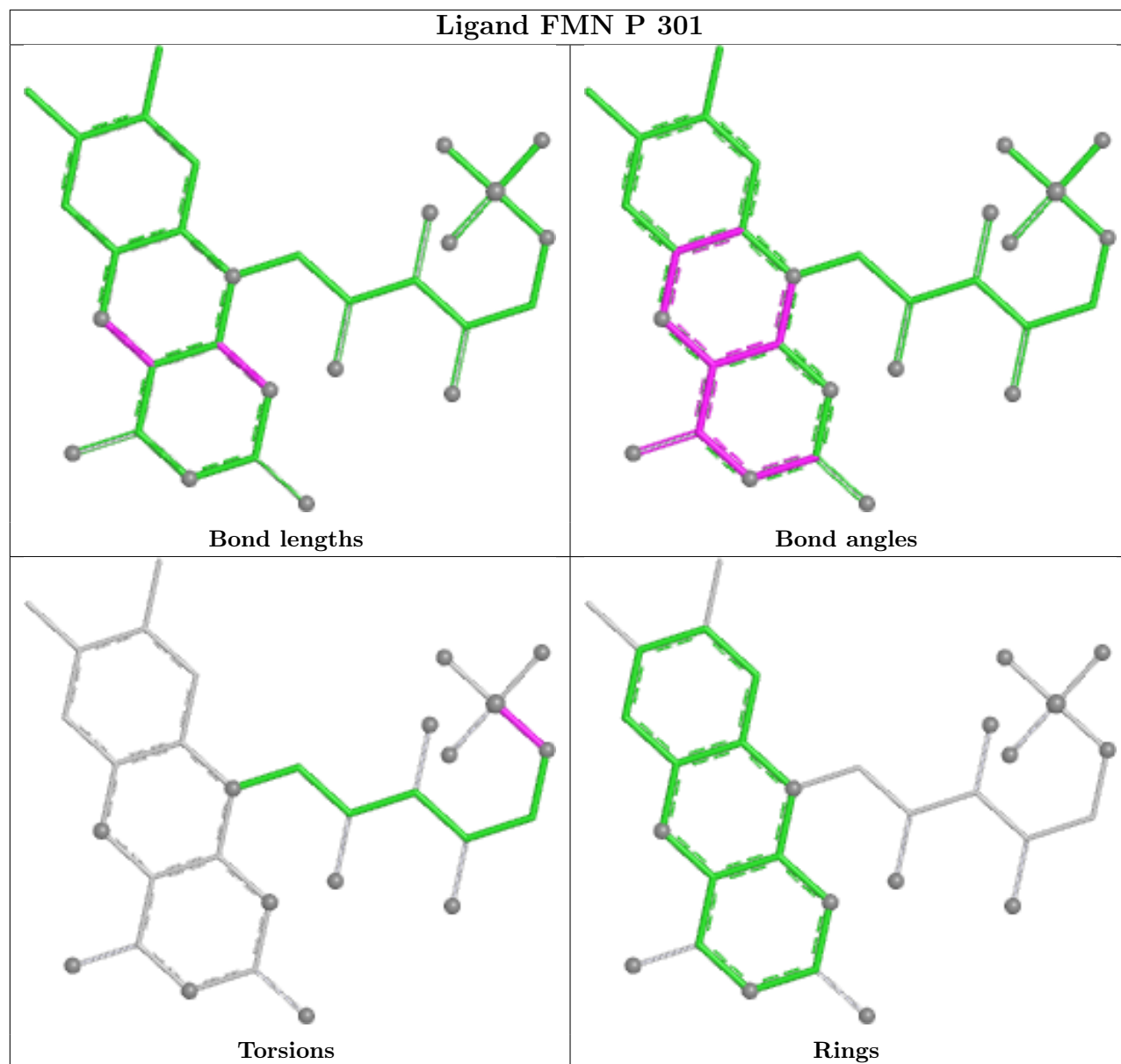


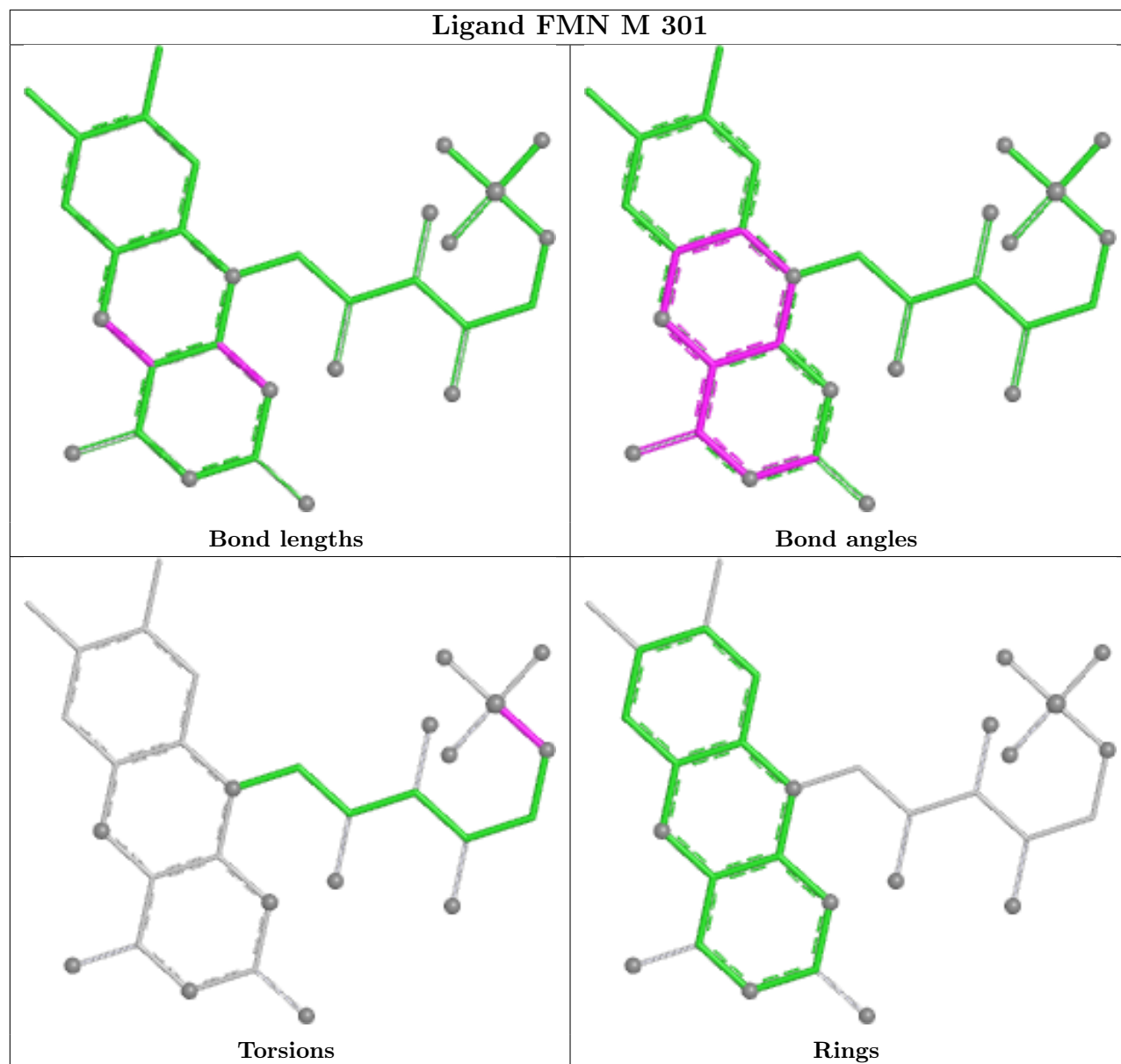


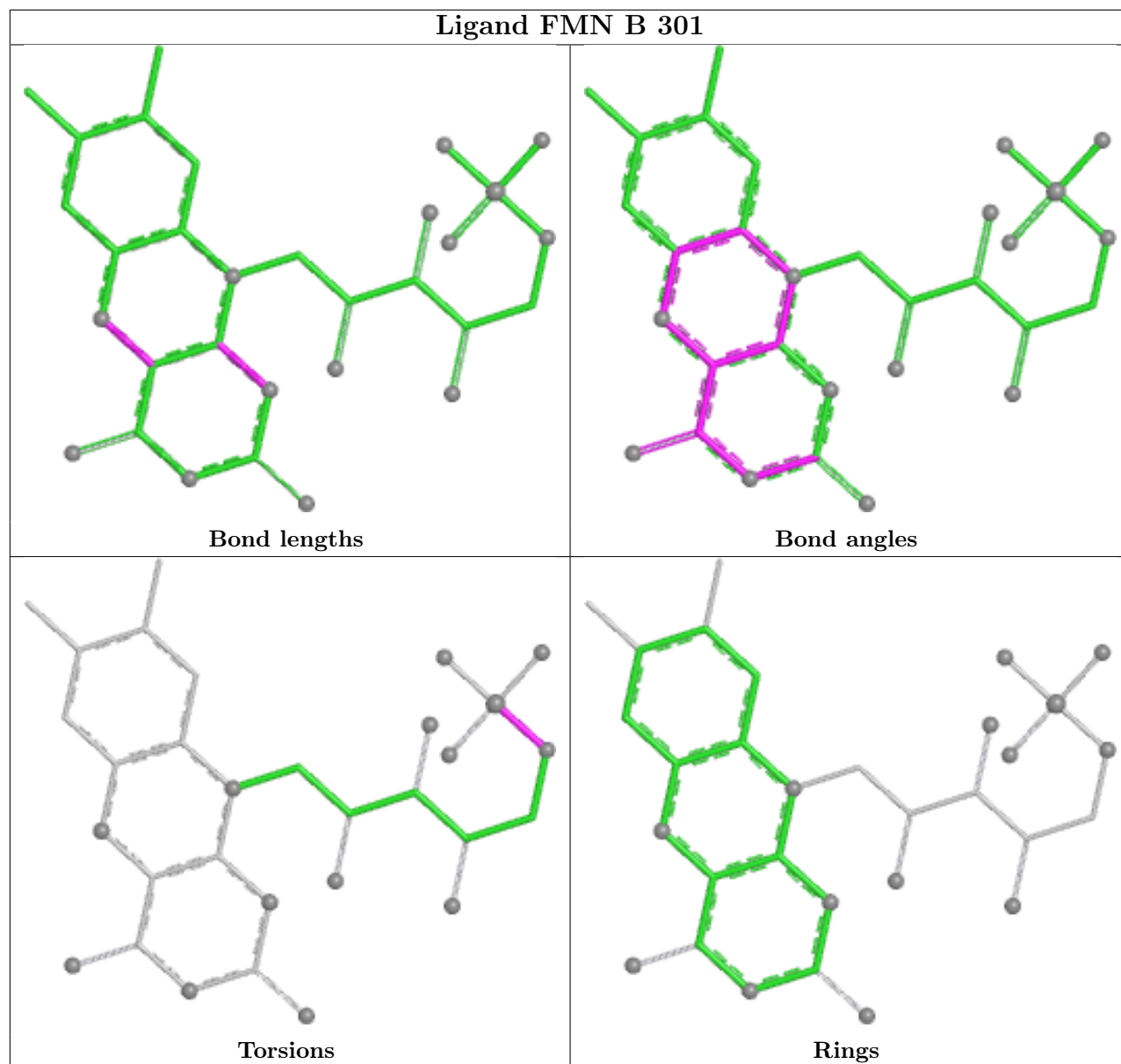


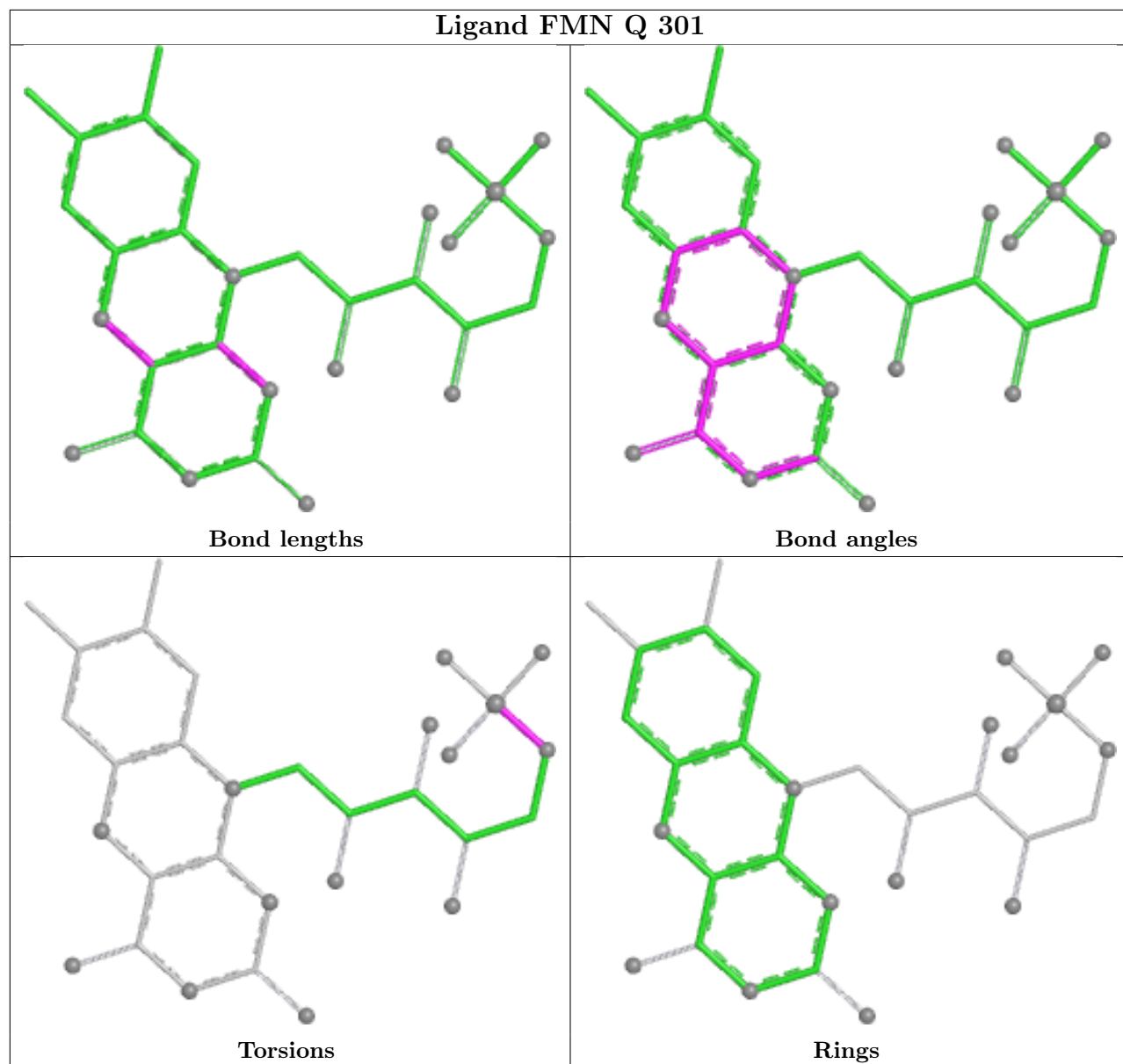


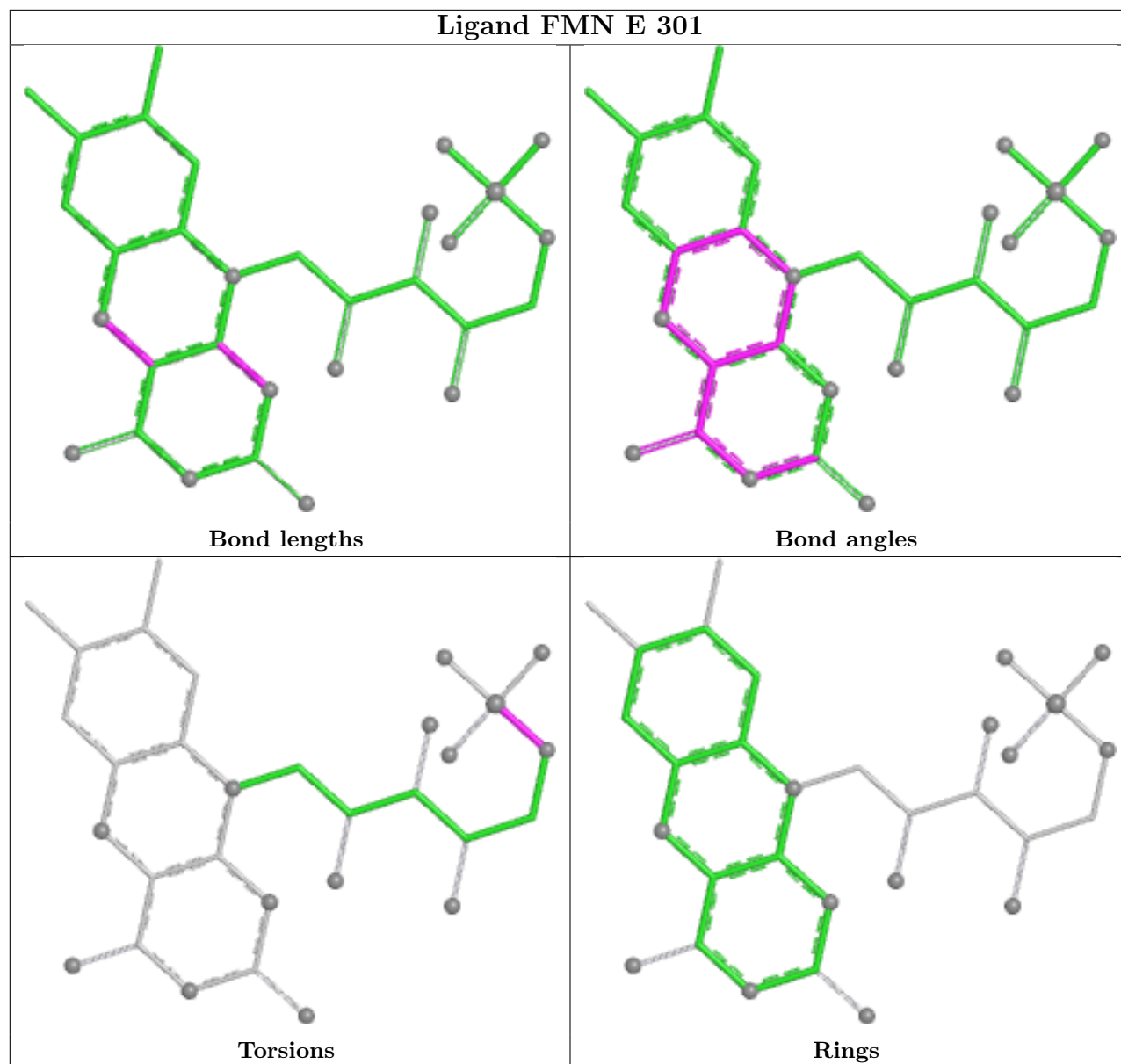


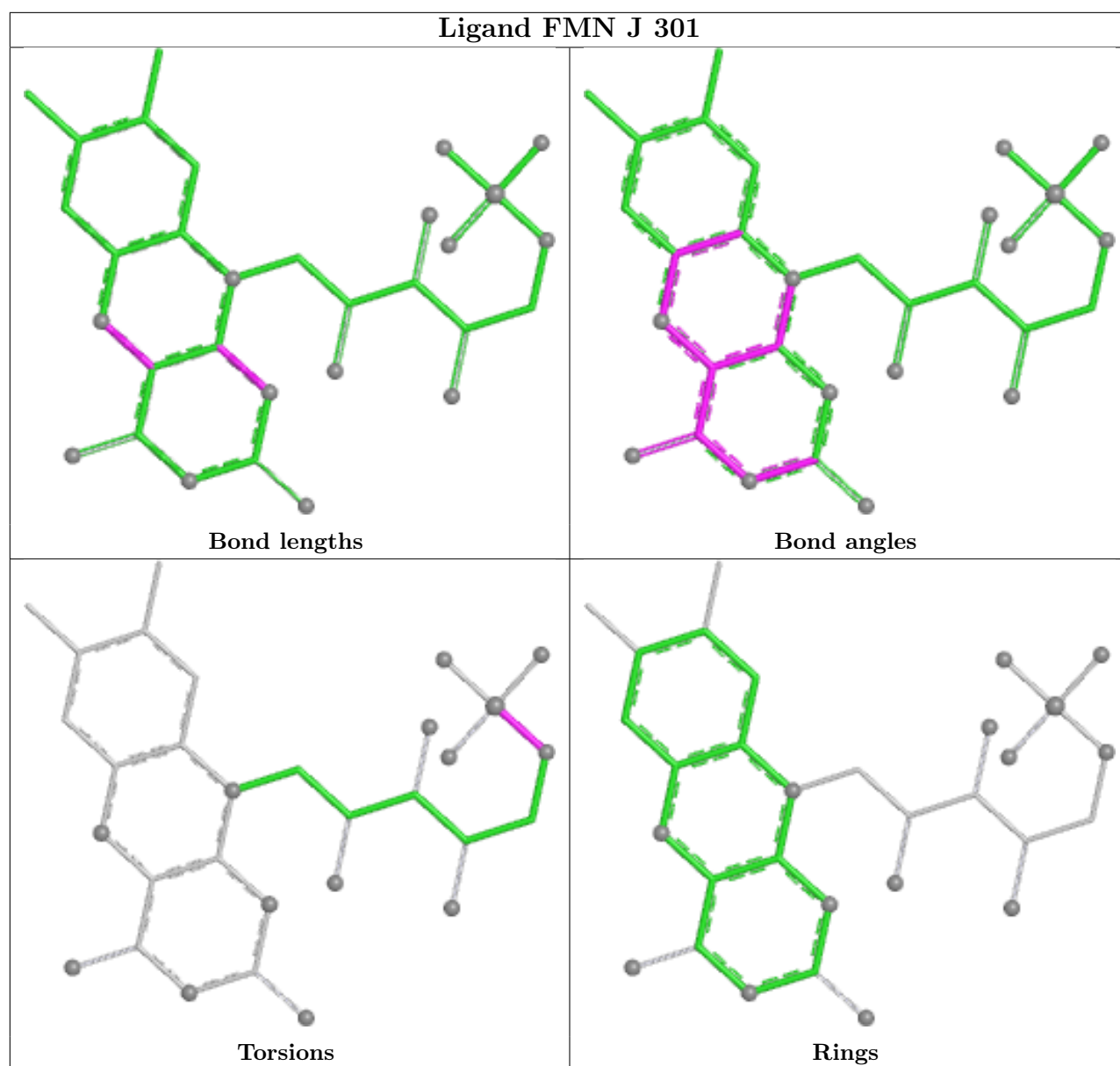


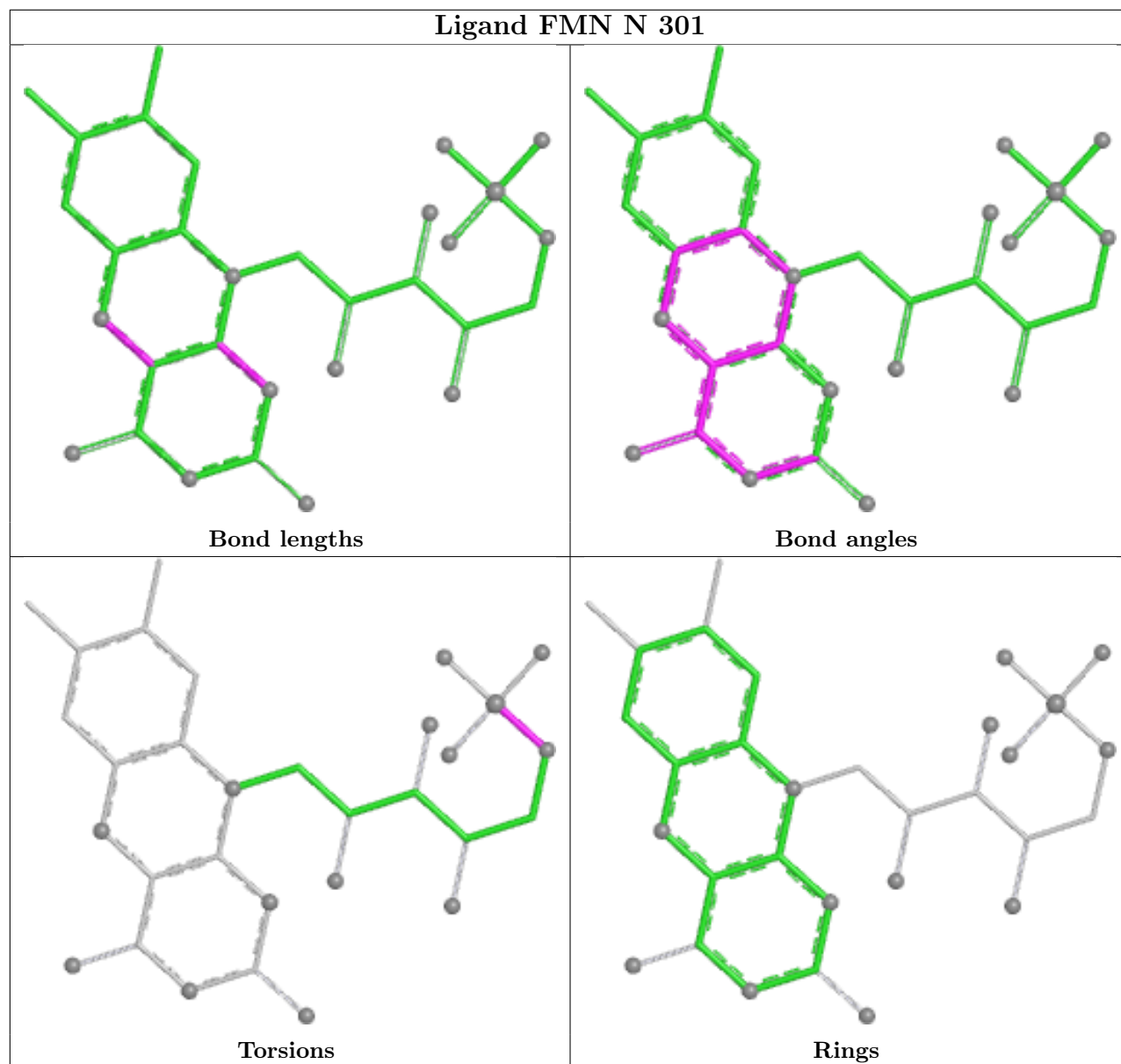


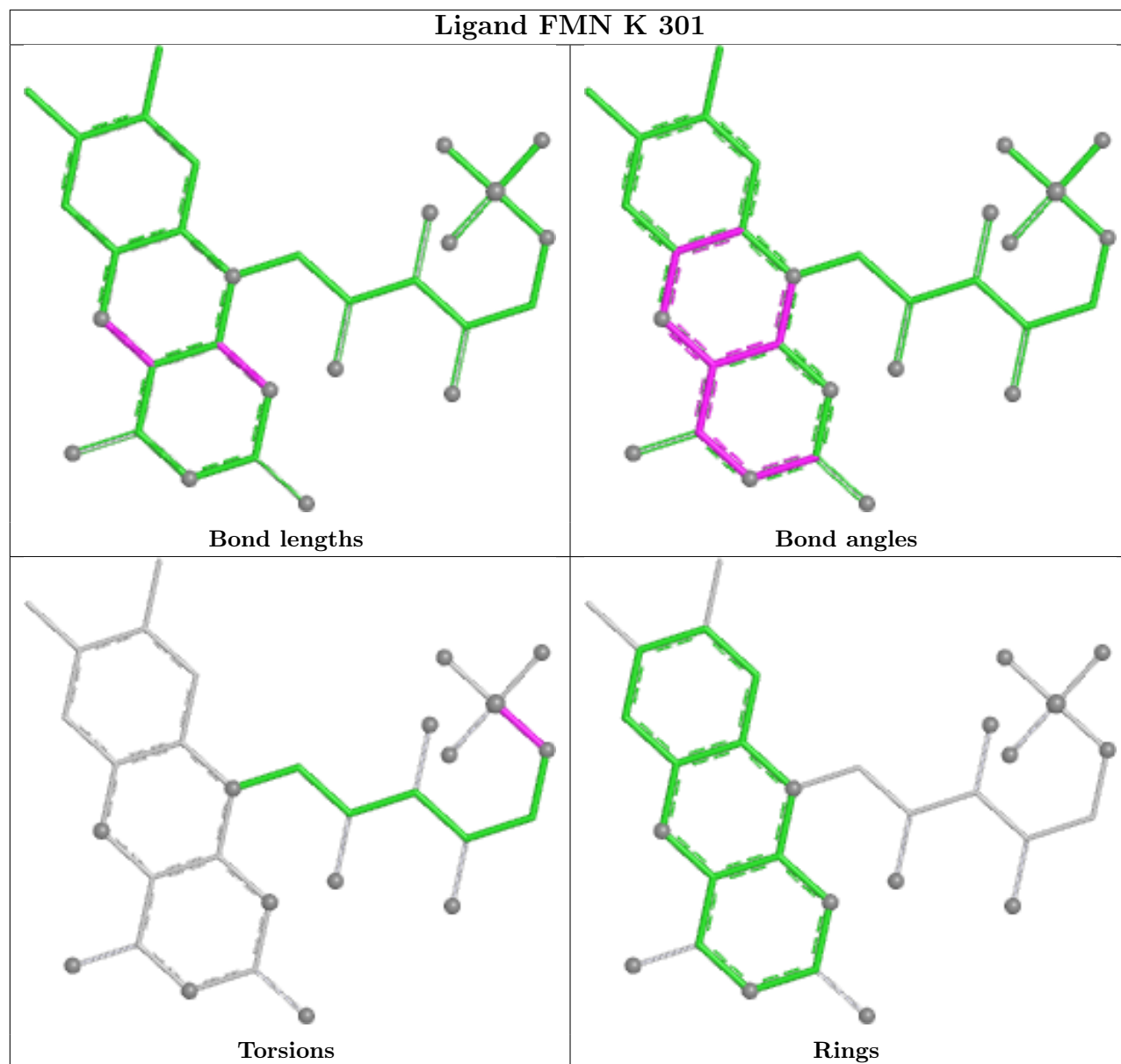


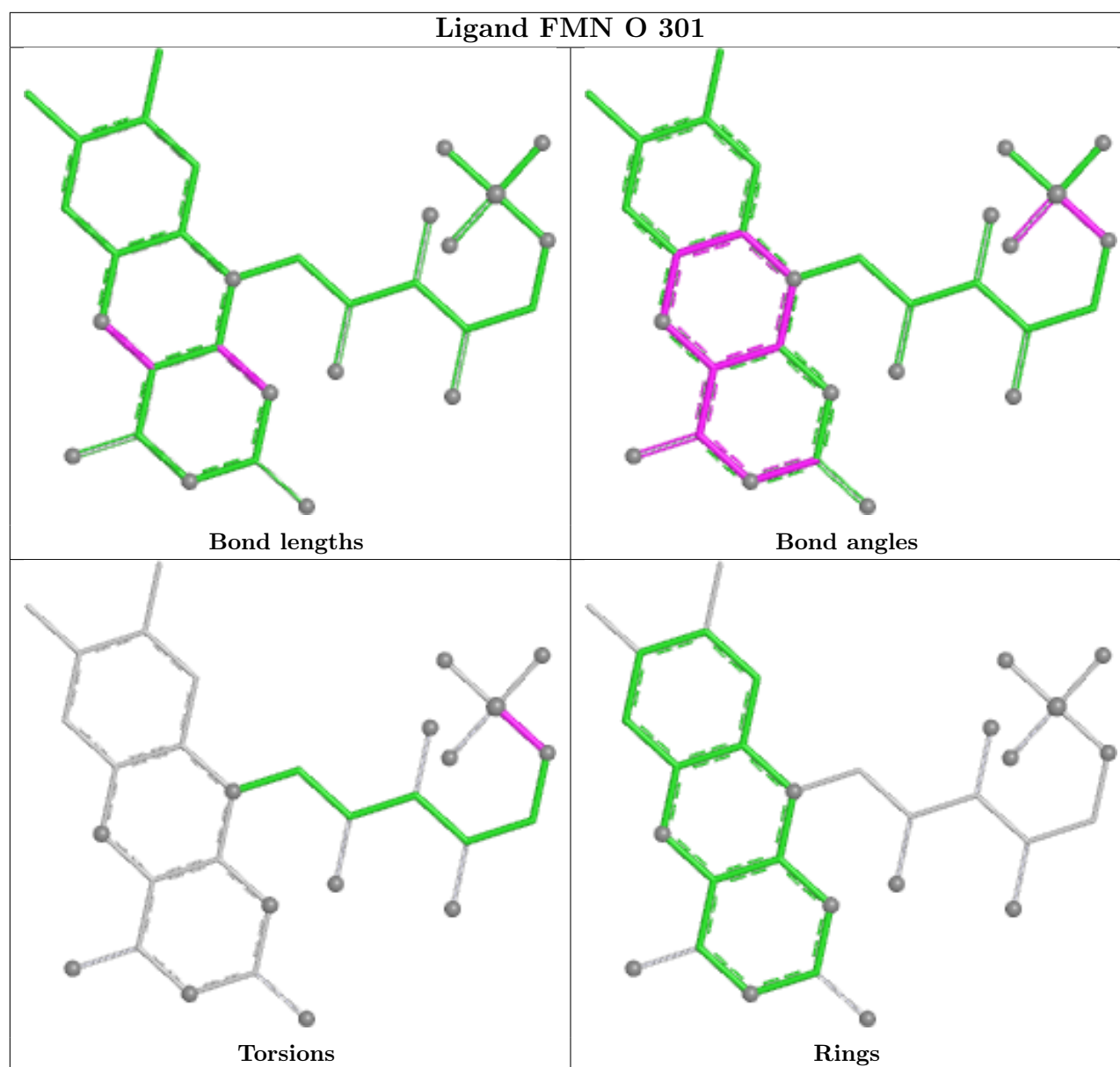


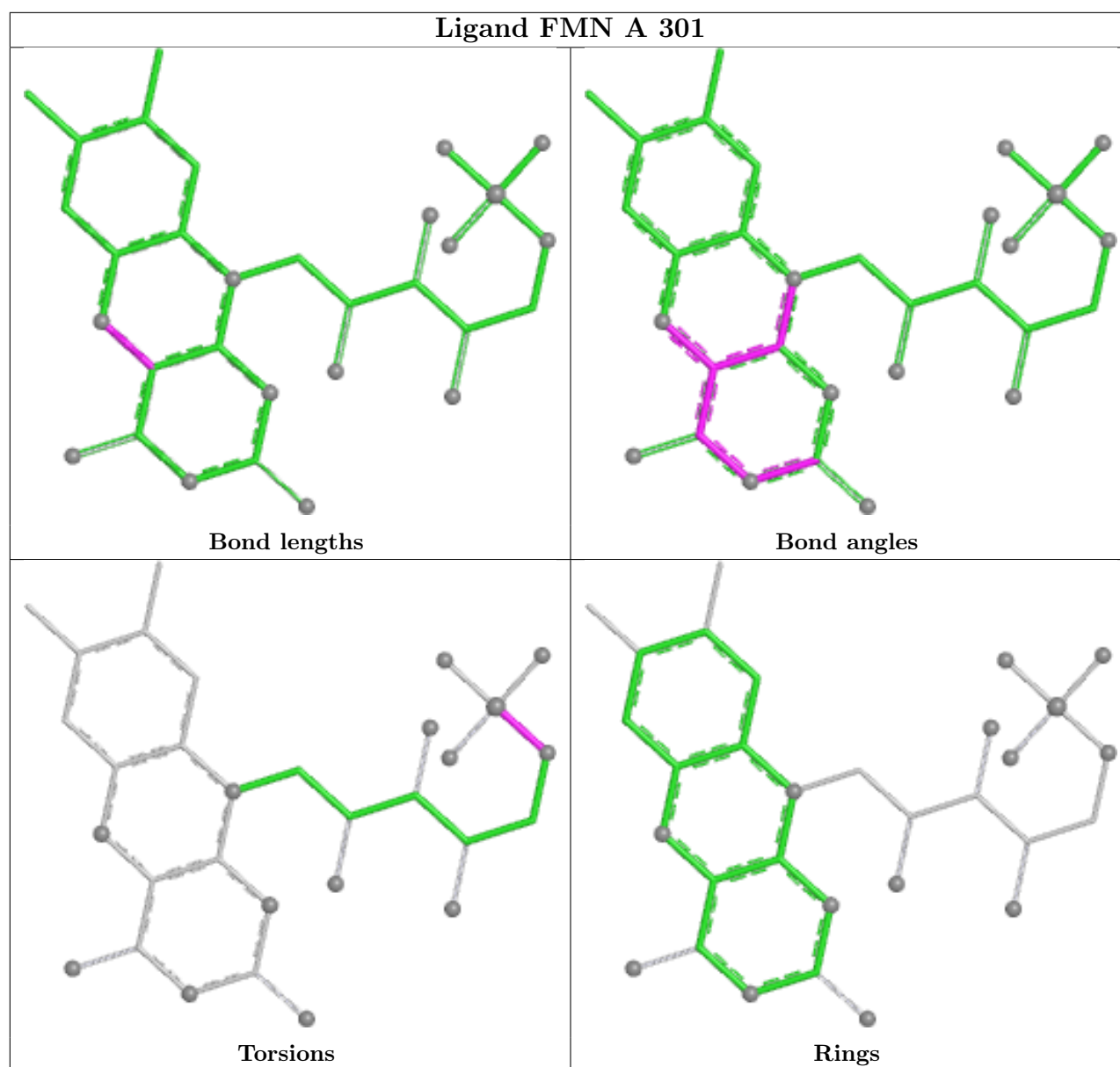












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	175/208 (84%)	0.81	19 (10%) 10 12	27, 42, 72, 107	0
1	B	175/208 (84%)	0.75	26 (14%) 5 6	26, 42, 73, 105	0
1	C	175/208 (84%)	0.88	26 (14%) 5 6	27, 43, 73, 115	0
1	D	175/208 (84%)	0.70	28 (16%) 5 5	25, 39, 69, 102	0
1	E	175/208 (84%)	0.72	27 (15%) 5 5	26, 41, 71, 113	0
1	F	175/208 (84%)	0.69	26 (14%) 5 6	26, 41, 72, 113	0
1	G	175/208 (84%)	0.68	23 (13%) 7 8	26, 40, 73, 104	0
1	H	175/208 (84%)	0.49	15 (8%) 16 17	25, 40, 68, 105	0
1	I	175/208 (84%)	0.77	22 (12%) 8 8	28, 43, 69, 112	0
1	J	175/208 (84%)	0.84	28 (16%) 5 5	28, 43, 75, 113	0
1	K	175/208 (84%)	0.80	26 (14%) 5 6	27, 43, 73, 117	0
1	L	175/208 (84%)	0.98	27 (15%) 5 5	28, 45, 70, 106	0
1	M	175/208 (84%)	0.83	33 (18%) 3 4	29, 44, 76, 107	0
1	N	175/208 (84%)	1.02	30 (17%) 4 5	28, 46, 78, 109	0
1	O	175/208 (84%)	0.85	27 (15%) 5 5	26, 43, 80, 110	0
1	P	175/208 (84%)	0.66	22 (12%) 8 8	25, 41, 75, 111	0
1	Q	175/208 (84%)	0.82	26 (14%) 5 6	27, 42, 74, 107	0
1	R	175/208 (84%)	0.80	25 (14%) 6 7	25, 41, 75, 108	0
1	S	175/208 (84%)	0.92	26 (14%) 5 6	29, 43, 66, 103	0
1	T	175/208 (84%)	0.86	26 (14%) 5 6	29, 44, 76, 103	0
1	U	175/208 (84%)	0.82	24 (13%) 6 7	29, 45, 73, 108	0
1	V	175/208 (84%)	0.92	30 (17%) 4 5	27, 42, 68, 110	0
1	W	175/208 (84%)	0.58	15 (8%) 16 17	27, 40, 65, 107	0
1	X	175/208 (84%)	0.62	18 (10%) 12 13	27, 41, 70, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4200/4992 (84%)	0.78	595 (14%) 6 7	25, 42, 73, 117	0

All (595) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	89	GLY	11.3
1	G	172	ILE	10.3
1	A	89	GLY	10.2
1	A	172	ILE	10.0
1	J	172	ILE	9.7
1	W	172	ILE	9.5
1	N	172	ILE	9.4
1	V	172	ILE	9.2
1	V	18	ALA	8.9
1	P	172	ILE	8.8
1	R	172	ILE	8.8
1	K	172	ILE	8.6
1	E	172	ILE	8.5
1	F	172	ILE	8.5
1	Q	89	GLY	8.4
1	T	172	ILE	8.3
1	R	72	ALA	8.3
1	O	172	ILE	8.3
1	L	172	ILE	8.2
1	I	172	ILE	8.1
1	A	88	GLY	8.0
1	C	172	ILE	8.0
1	O	181	PRO	7.9
1	G	72	ALA	7.9
1	H	172	ILE	7.9
1	S	172	ILE	7.8
1	U	172	ILE	7.7
1	D	172	ILE	7.6
1	S	88	GLY	7.5
1	O	19	LEU	7.3
1	V	67	PRO	7.3
1	M	172	ILE	7.2
1	T	171	GLY	7.1
1	Q	172	ILE	7.0
1	C	181	PRO	6.9
1	X	181	PRO	6.9
1	A	87	GLY	6.8

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Mol	Chain	Res	Type	RSRZ
1	D	181	PRO	6.8
1	X	172	ILE	6.8
1	U	18	ALA	6.7
1	P	181	PRO	6.6
1	I	18	ALA	6.6
1	K	181	PRO	6.6
1	I	181	PRO	6.5
1	J	171	GLY	6.5
1	R	171	GLY	6.4
1	X	89	GLY	6.4
1	P	89	GLY	6.4
1	K	171	GLY	6.4
1	E	181	PRO	6.3
1	B	172	ILE	6.3
1	R	73	VAL	6.2
1	O	171	GLY	6.2
1	B	69	MET	6.1
1	Q	87	GLY	6.1
1	N	181	PRO	6.0
1	F	18	ALA	5.8
1	D	171	GLY	5.8
1	S	171	GLY	5.8
1	E	89	GLY	5.8
1	V	89	GLY	5.8
1	W	171	GLY	5.7
1	D	21	GLN	5.7
1	C	171	GLY	5.7
1	D	18	ALA	5.7
1	T	181	PRO	5.7
1	S	87	GLY	5.6
1	Q	88	GLY	5.6
1	A	18	ALA	5.6
1	L	200	ALA	5.6
1	O	200	ALA	5.5
1	W	181	PRO	5.5
1	S	181	PRO	5.5
1	F	181	PRO	5.5
1	A	171	GLY	5.4
1	H	181	PRO	5.4
1	M	200	ALA	5.4
1	V	73	VAL	5.4
1	G	66	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	U	181	PRO	5.4
1	Q	200	ALA	5.4
1	R	67	PRO	5.3
1	F	89	GLY	5.3
1	J	200	ALA	5.3
1	X	88	GLY	5.3
1	V	72	ALA	5.2
1	N	171	GLY	5.2
1	Q	181	PRO	5.1
1	B	181	PRO	5.1
1	X	170	GLU	5.1
1	V	181	PRO	5.1
1	N	72	ALA	5.0
1	J	181	PRO	5.0
1	N	47	THR	5.0
1	B	73	VAL	5.0
1	B	171	GLY	5.0
1	N	18	ALA	5.0
1	O	199	ALA	5.0
1	T	76	HIS	5.0
1	A	181	PRO	4.9
1	X	171	GLY	4.9
1	I	200	ALA	4.9
1	L	181	PRO	4.9
1	P	88	GLY	4.9
1	G	73	VAL	4.9
1	G	171	GLY	4.8
1	T	69	MET	4.8
1	T	200	ALA	4.8
1	W	200	ALA	4.8
1	P	19	LEU	4.8
1	G	18	ALA	4.7
1	P	171	GLY	4.7
1	O	18	ALA	4.7
1	Q	86	LYS	4.7
1	R	69	MET	4.7
1	D	200	ALA	4.6
1	A	19	LEU	4.6
1	E	88	GLY	4.6
1	V	69	MET	4.6
1	B	200	ALA	4.6
1	T	67	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	P	170	GLU	4.6
1	L	171	GLY	4.6
1	R	75	GLY	4.6
1	T	75	GLY	4.5
1	F	68	ARG	4.5
1	P	85	HIS	4.5
1	E	171	GLY	4.5
1	B	75	GLY	4.5
1	X	18	ALA	4.5
1	M	171	GLY	4.5
1	R	18	ALA	4.4
1	H	171	GLY	4.4
1	T	72	ALA	4.4
1	R	181	PRO	4.3
1	S	18	ALA	4.3
1	C	18	ALA	4.3
1	N	73	VAL	4.3
1	I	171	GLY	4.3
1	G	69	MET	4.3
1	M	181	PRO	4.3
1	N	200	ALA	4.3
1	B	67	PRO	4.3
1	H	200	ALA	4.3
1	X	85	HIS	4.3
1	V	171	GLY	4.3
1	K	18	ALA	4.2
1	H	18	ALA	4.2
1	E	200	ALA	4.2
1	L	169	LYS	4.2
1	C	19	LEU	4.2
1	U	49	GLY	4.1
1	B	72	ALA	4.1
1	F	67	PRO	4.1
1	G	68	ARG	4.1
1	B	66	GLY	4.1
1	T	73	VAL	4.1
1	S	86	LYS	4.1
1	N	43	TRP	4.1
1	K	72	ALA	4.1
1	E	85	HIS	4.1
1	D	89	GLY	4.0
1	K	200	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	X	86	LYS	4.0
1	C	200	ALA	4.0
1	G	200	ALA	4.0
1	R	200	ALA	4.0
1	Q	18	ALA	3.9
1	F	73	VAL	3.9
1	A	86	LYS	3.9
1	W	65	MET	3.9
1	T	66	GLY	3.9
1	D	19	LEU	3.9
1	L	19	LEU	3.9
1	G	67	PRO	3.9
1	G	181	PRO	3.9
1	B	76	HIS	3.9
1	K	47	THR	3.9
1	Q	85	HIS	3.8
1	Q	171	GLY	3.8
1	U	171	GLY	3.8
1	P	18	ALA	3.8
1	C	65	MET	3.8
1	K	170	GLU	3.8
1	O	170	GLU	3.8
1	J	89	GLY	3.8
1	R	68	ARG	3.8
1	J	199	ALA	3.7
1	V	200	ALA	3.7
1	C	46	GLY	3.7
1	U	66	GLY	3.7
1	P	200	ALA	3.7
1	V	75	GLY	3.7
1	D	170	GLU	3.7
1	X	66	GLY	3.7
1	N	66	GLY	3.6
1	P	86	LYS	3.6
1	T	18	ALA	3.6
1	N	170	GLU	3.6
1	F	69	MET	3.6
1	R	76	HIS	3.6
1	O	51	GLN	3.6
1	R	71	GLU	3.6
1	J	18	ALA	3.5
1	M	21	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	W	18	ALA	3.5
1	X	200	ALA	3.5
1	A	200	ALA	3.5
1	D	20	ALA	3.5
1	E	18	ALA	3.5
1	C	66	GLY	3.5
1	T	19	LEU	3.5
1	C	45	ARG	3.5
1	T	52	GLU	3.5
1	E	86	LYS	3.5
1	V	86	LYS	3.5
1	P	21	GLN	3.5
1	B	18	ALA	3.4
1	Q	46	GLY	3.4
1	N	69	MET	3.4
1	F	46	GLY	3.4
1	E	199	ALA	3.4
1	Q	199	ALA	3.4
1	S	85	HIS	3.4
1	A	47	THR	3.4
1	I	45	ARG	3.4
1	N	189	SER	3.4
1	U	45	ARG	3.4
1	O	198	ALA	3.4
1	I	170	GLU	3.4
1	O	169	LYS	3.4
1	K	48	VAL	3.3
1	R	66	GLY	3.3
1	F	19	LEU	3.3
1	F	52	GLU	3.3
1	C	47	THR	3.3
1	F	171	GLY	3.3
1	C	89	GLY	3.3
1	N	48	VAL	3.3
1	M	18	ALA	3.3
1	V	68	ARG	3.3
1	I	189	SER	3.3
1	J	46	GLY	3.3
1	K	73	VAL	3.3
1	A	170	GLU	3.3
1	T	170	GLU	3.3
1	K	65	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	W	170	GLU	3.2
1	U	196	ILE	3.2
1	N	65	MET	3.2
1	U	46	GLY	3.2
1	E	170	GLU	3.2
1	I	169	LYS	3.2
1	U	19	LEU	3.2
1	V	19	LEU	3.2
1	R	74	THR	3.2
1	F	170	GLU	3.2
1	W	197	GLN	3.2
1	G	189	SER	3.2
1	Q	170	GLU	3.2
1	R	189	SER	3.2
1	H	65	MET	3.2
1	K	20	ALA	3.1
1	L	18	ALA	3.1
1	C	64	LEU	3.1
1	V	85	HIS	3.1
1	O	46	GLY	3.1
1	C	48	VAL	3.1
1	C	196	ILE	3.1
1	S	47	THR	3.1
1	I	46	GLY	3.1
1	K	49	GLY	3.1
1	K	66	GLY	3.1
1	S	109	ALA	3.1
1	G	170	GLU	3.1
1	J	52	GLU	3.1
1	C	50	VAL	3.1
1	U	86	LYS	3.1
1	K	19	LEU	3.1
1	M	49	GLY	3.0
1	S	68	ARG	3.0
1	S	170	GLU	3.0
1	U	48	VAL	3.0
1	O	45	ARG	3.0
1	U	182	GLY	3.0
1	K	43	TRP	3.0
1	A	85	HIS	3.0
1	P	65	MET	3.0
1	D	65	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	O	65	MET	3.0
1	J	21	GLN	3.0
1	U	200	ALA	3.0
1	A	68	ARG	3.0
1	C	49	GLY	3.0
1	M	46	GLY	3.0
1	R	170	GLU	3.0
1	L	43	TRP	3.0
1	E	21	GLN	3.0
1	M	194	ALA	3.0
1	T	68	ARG	3.0
1	P	66	GLY	3.0
1	V	46	GLY	3.0
1	G	65	MET	3.0
1	R	45	ARG	2.9
1	J	170	GLU	2.9
1	U	67	PRO	2.9
1	U	65	MET	2.9
1	N	19	LEU	2.9
1	H	66	GLY	2.9
1	B	89	GLY	2.9
1	E	66	GLY	2.9
1	D	22	VAL	2.9
1	T	196	ILE	2.9
1	X	65	MET	2.9
1	F	86	LYS	2.9
1	F	75	GLY	2.9
1	L	48	VAL	2.9
1	C	21	GLN	2.9
1	H	170	GLU	2.9
1	F	66	GLY	2.9
1	G	75	GLY	2.9
1	W	66	GLY	2.9
1	B	19	LEU	2.8
1	Q	21	GLN	2.8
1	N	67	PRO	2.8
1	M	86	LYS	2.8
1	H	21	GLN	2.8
1	X	21	GLN	2.8
1	F	72	ALA	2.8
1	P	20	ALA	2.8
1	E	87	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	72	ALA	2.8
1	E	19	LEU	2.8
1	S	21	GLN	2.8
1	I	21	GLN	2.8
1	U	21	GLN	2.8
1	A	49	GLY	2.8
1	D	66	GLY	2.8
1	M	89	GLY	2.8
1	N	46	GLY	2.8
1	V	88	GLY	2.8
1	M	19	LEU	2.8
1	U	47	THR	2.8
1	V	74	THR	2.8
1	I	134	PRO	2.8
1	V	170	GLU	2.8
1	I	89	GLY	2.8
1	D	199	ALA	2.8
1	G	47	THR	2.8
1	W	21	GLN	2.7
1	S	65	MET	2.7
1	G	76	HIS	2.7
1	P	83	GLU	2.7
1	S	46	GLY	2.7
1	V	66	GLY	2.7
1	Q	19	LEU	2.7
1	W	19	LEU	2.7
1	L	76	HIS	2.7
1	L	170	GLU	2.7
1	M	189	SER	2.7
1	N	169	LYS	2.7
1	Q	194	ALA	2.7
1	H	19	LEU	2.7
1	M	47	THR	2.7
1	X	19	LEU	2.7
1	W	52	GLU	2.7
1	D	196	ILE	2.7
1	F	200	ALA	2.7
1	M	20	ALA	2.7
1	M	198	ALA	2.7
1	C	170	GLU	2.7
1	Q	83	GLU	2.7
1	M	101	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	V	189	SER	2.7
1	G	70	ILE	2.7
1	Q	84	ASP	2.7
1	L	49	GLY	2.7
1	D	51	GLN	2.6
1	F	85	HIS	2.6
1	J	86	LYS	2.6
1	F	76	HIS	2.6
1	N	76	HIS	2.6
1	B	86	LYS	2.6
1	N	45	ARG	2.6
1	B	70	ILE	2.6
1	D	46	GLY	2.6
1	R	21	GLN	2.6
1	L	160	GLU	2.6
1	E	65	MET	2.6
1	I	47	THR	2.6
1	L	47	THR	2.6
1	O	164	ARG	2.6
1	C	51	GLN	2.6
1	M	196	ILE	2.6
1	N	21	GLN	2.6
1	O	21	GLN	2.6
1	K	52	GLU	2.6
1	P	87	GLY	2.6
1	E	46	GLY	2.6
1	O	20	ALA	2.6
1	R	19	LEU	2.6
1	Q	50	VAL	2.5
1	U	50	VAL	2.5
1	A	46	GLY	2.5
1	J	49	GLY	2.5
1	L	75	GLY	2.5
1	T	49	GLY	2.5
1	S	169	LYS	2.5
1	M	199	ALA	2.5
1	R	77	ALA	2.5
1	V	47	THR	2.5
1	K	38	PRO	2.5
1	D	197	GLN	2.5
1	Q	197	GLN	2.5
1	M	83	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	S	48	VAL	2.5
1	D	49	GLY	2.5
1	L	66	GLY	2.5
1	N	49	GLY	2.5
1	N	87	GLY	2.5
1	S	126	ALA	2.5
1	G	77	ALA	2.5
1	J	83	GLU	2.5
1	L	189	SER	2.5
1	Q	160	GLU	2.5
1	F	39	HIS	2.5
1	S	66	GLY	2.5
1	J	66	GLY	2.5
1	Q	66	GLY	2.5
1	V	76	HIS	2.5
1	J	68	ARG	2.5
1	L	73	VAL	2.5
1	M	22	VAL	2.5
1	P	84	ASP	2.5
1	N	186	ASP	2.5
1	S	200	ALA	2.5
1	C	134	PRO	2.5
1	O	42	ALA	2.5
1	U	64	LEU	2.5
1	J	65	MET	2.5
1	H	169	LYS	2.5
1	S	49	GLY	2.5
1	M	88	GLY	2.5
1	O	196	ILE	2.5
1	P	29	CYS	2.4
1	F	47	THR	2.4
1	J	47	THR	2.4
1	K	69	MET	2.4
1	D	85	HIS	2.4
1	A	66	GLY	2.4
1	I	49	GLY	2.4
1	F	21	GLN	2.4
1	U	52	GLU	2.4
1	I	48	VAL	2.4
1	O	194	ALA	2.4
1	J	19	LEU	2.4
1	M	39	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	R	39	HIS	2.4
1	H	49	GLY	2.4
1	P	49	GLY	2.4
1	K	39	HIS	2.4
1	L	39	HIS	2.4
1	H	197	GLN	2.4
1	I	188	GLN	2.4
1	L	89	GLY	2.4
1	V	21	GLN	2.4
1	X	87	GLY	2.4
1	C	52	GLU	2.3
1	R	20	ALA	2.3
1	Q	49	GLY	2.3
1	T	70	ILE	2.3
1	S	166	VAL	2.3
1	J	50	VAL	2.3
1	H	39	HIS	2.3
1	G	38	PRO	2.3
1	M	170	GLU	2.3
1	N	160	GLU	2.3
1	N	51	GLN	2.3
1	O	64	LEU	2.3
1	W	64	LEU	2.3
1	B	65	MET	2.3
1	D	86	LYS	2.3
1	A	48	VAL	2.3
1	E	83	GLU	2.3
1	P	47	THR	2.3
1	B	21	GLN	2.3
1	O	197	GLN	2.3
1	L	194	ALA	2.3
1	N	194	ALA	2.3
1	B	49	GLY	2.3
1	M	66	GLY	2.3
1	L	65	MET	2.3
1	J	39	HIS	2.3
1	J	196	ILE	2.3
1	M	197	GLN	2.3
1	N	188	GLN	2.3
1	V	169	LYS	2.3
1	V	39	HIS	2.2
1	D	192	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	51	GLN	2.2
1	J	51	GLN	2.2
1	K	51	GLN	2.2
1	U	197	GLN	2.2
1	B	196	ILE	2.2
1	L	134	PRO	2.2
1	O	166	VAL	2.2
1	V	48	VAL	2.2
1	B	170	GLU	2.2
1	C	132	GLU	2.2
1	F	189	SER	2.2
1	Q	189	SER	2.2
1	D	169	LYS	2.2
1	D	193	THR	2.2
1	M	53	ILE	2.2
1	L	166	VAL	2.2
1	T	86	LYS	2.2
1	O	49	GLY	2.2
1	O	66	GLY	2.2
1	B	160	GLU	2.2
1	E	198	ALA	2.2
1	J	197	GLN	2.2
1	K	76	HIS	2.2
1	K	23	ARG	2.2
1	K	67	PRO	2.2
1	M	50	VAL	2.2
1	X	50	VAL	2.2
1	D	88	GLY	2.2
1	E	52	GLU	2.2
1	M	87	GLY	2.2
1	V	87	GLY	2.2
1	B	39	HIS	2.2
1	D	188	GLN	2.2
1	Q	198	ALA	2.2
1	D	189	SER	2.2
1	I	86	LYS	2.2
1	V	71	GLU	2.1
1	I	50	VAL	2.1
1	E	197	GLN	2.1
1	W	199	ALA	2.1
1	G	19	LEU	2.1
1	C	86	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	86	LYS	2.1
1	M	65	MET	2.1
1	K	160	GLU	2.1
1	X	134	PRO	2.1
1	I	43	TRP	2.1
1	B	188	GLN	2.1
1	J	73	VAL	2.1
1	O	22	VAL	2.1
1	B	68	ARG	2.1
1	B	194	ALA	2.1
1	M	42	ALA	2.1
1	T	199	ALA	2.1
1	F	169	LYS	2.1
1	D	64	LEU	2.1
1	E	189	SER	2.1
1	K	189	SER	2.1
1	I	52	GLU	2.1
1	R	47	THR	2.1
1	T	21	GLN	2.1
1	S	39	HIS	2.1
1	H	89	GLY	2.1
1	P	46	GLY	2.1
1	V	49	GLY	2.1
1	O	195	LEU	2.1
1	J	160	GLU	2.1
1	I	186	ASP	2.1
1	L	186	ASP	2.1
1	J	164	ARG	2.1
1	E	49	GLY	2.1
1	S	50	VAL	2.1
1	E	22	VAL	2.1
1	N	22	VAL	2.1
1	S	199	ALA	2.1
1	U	72	ALA	2.1
1	M	195	LEU	2.0
1	C	188	GLN	2.0
1	T	188	GLN	2.0
1	U	186	ASP	2.0
1	G	74	THR	2.0
1	Q	67	PRO	2.0
1	J	87	GLY	2.0
1	R	46	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	T	89	GLY	2.0
1	T	22	VAL	2.0
1	W	73	VAL	2.0
1	A	20	ALA	2.0
1	C	20	ALA	2.0
1	M	190	ALA	2.0
1	T	77	ALA	2.0
1	F	186	ASP	2.0
1	E	84	ASP	2.0
1	X	84	ASP	2.0
1	E	39	HIS	2.0
1	L	46	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

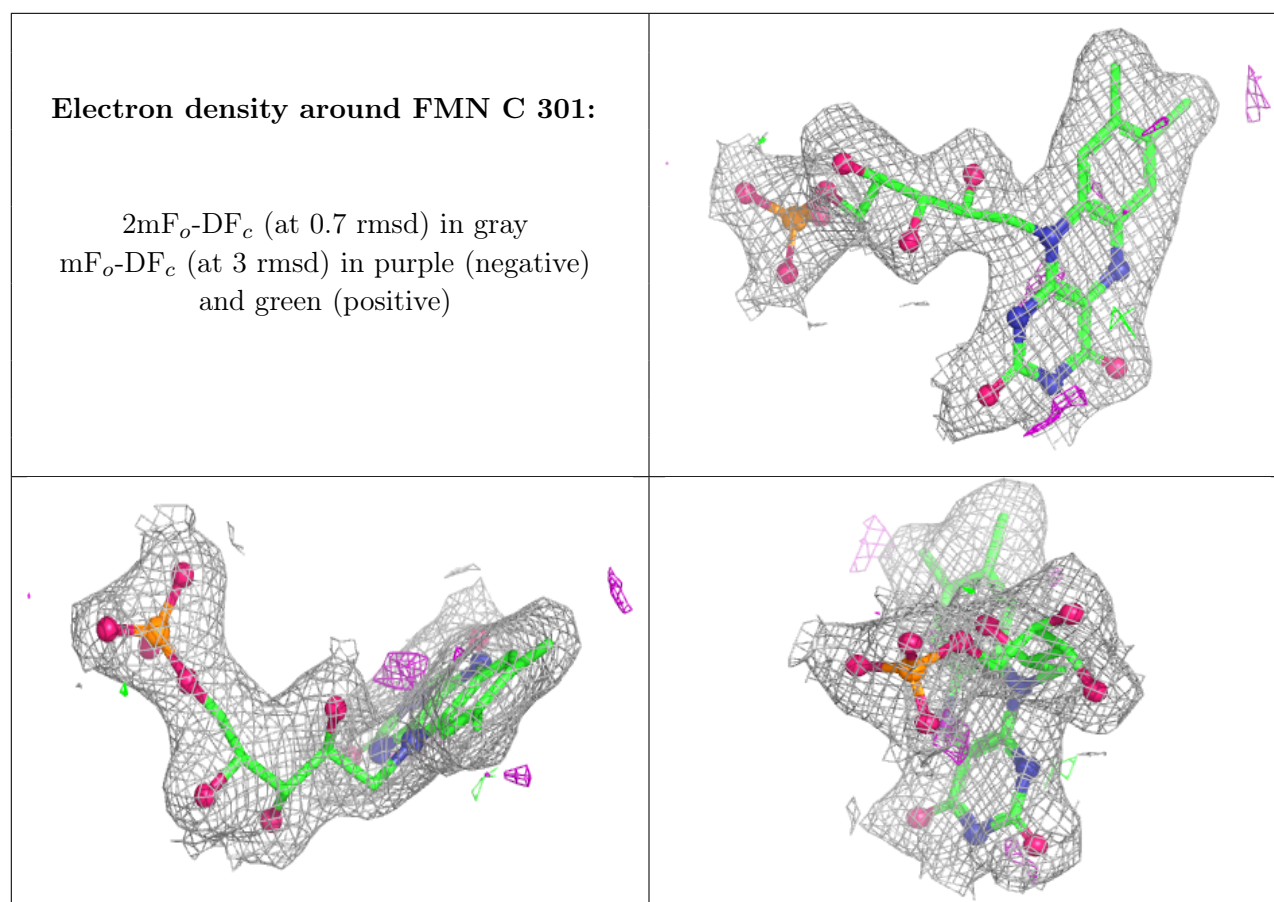
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ARG	S	301	11/12	0.70	0.25	60,69,77,80	0
2	FMN	C	301	31/31	0.96	0.08	28,33,39,39	0
2	FMN	E	301	31/31	0.96	0.07	26,31,36,40	0
2	FMN	Q	301	31/31	0.96	0.08	28,32,37,38	0
2	FMN	U	301	31/31	0.96	0.07	28,33,37,39	0
2	FMN	W	301	31/31	0.96	0.07	28,32,38,40	0
2	FMN	S	302	31/31	0.96	0.08	28,32,37,42	0
2	FMN	D	301	31/31	0.97	0.07	26,31,37,38	0
2	FMN	H	301	31/31	0.97	0.07	25,30,35,36	0
2	FMN	I	301	31/31	0.97	0.07	27,32,35,39	0
2	FMN	J	301	31/31	0.97	0.07	26,33,38,40	0

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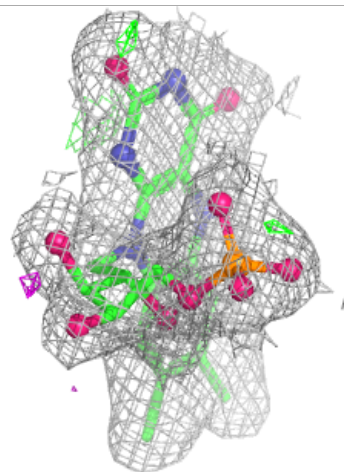
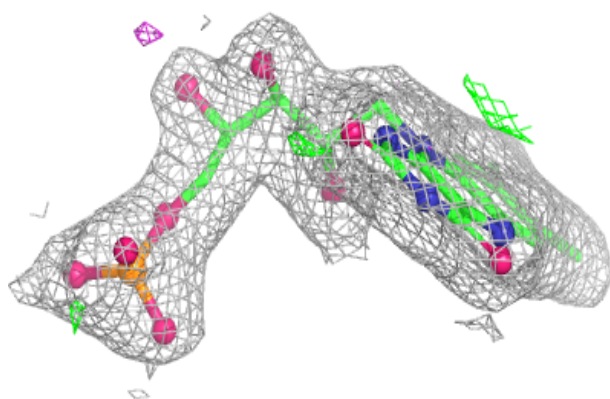
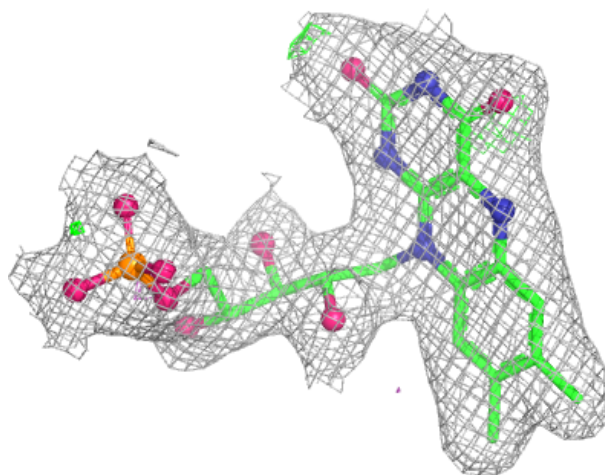
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMN	K	301	31/31	0.97	0.06	23,30,34,38	0
2	FMN	L	301	31/31	0.97	0.07	27,31,37,37	0
2	FMN	M	301	31/31	0.97	0.07	26,34,38,40	0
2	FMN	N	301	31/31	0.97	0.07	29,32,36,37	0
2	FMN	O	301	31/31	0.97	0.06	25,31,34,34	0
2	FMN	P	301	31/31	0.97	0.07	25,31,35,36	0
2	FMN	T	301	31/31	0.97	0.07	27,32,36,38	0
2	FMN	A	301	31/31	0.97	0.07	24,30,35,38	0
2	FMN	V	301	31/31	0.97	0.07	25,30,32,37	0
2	FMN	B	301	31/31	0.97	0.07	23,32,36,39	0
2	FMN	X	301	31/31	0.97	0.06	25,29,33,38	0
2	FMN	F	301	31/31	0.97	0.06	25,29,33,34	0
2	FMN	G	301	31/31	0.98	0.05	24,29,35,37	0
2	FMN	R	301	31/31	0.98	0.06	25,30,34,35	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.



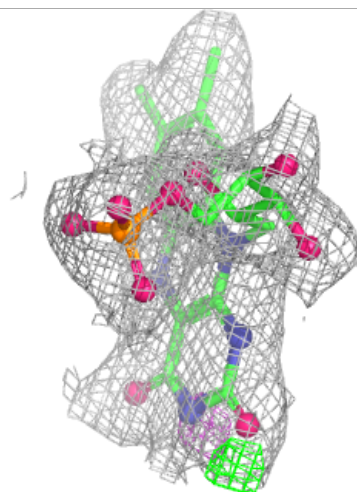
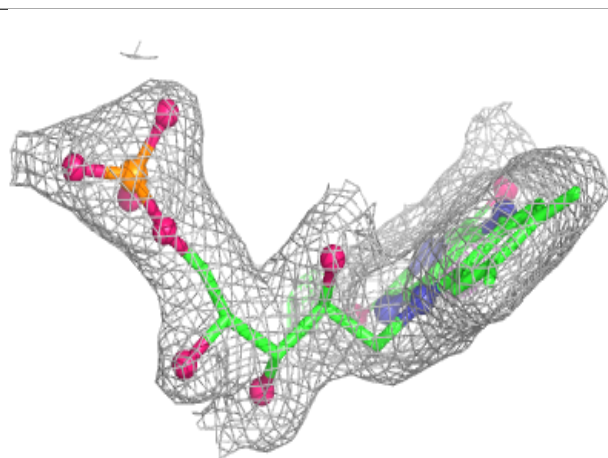
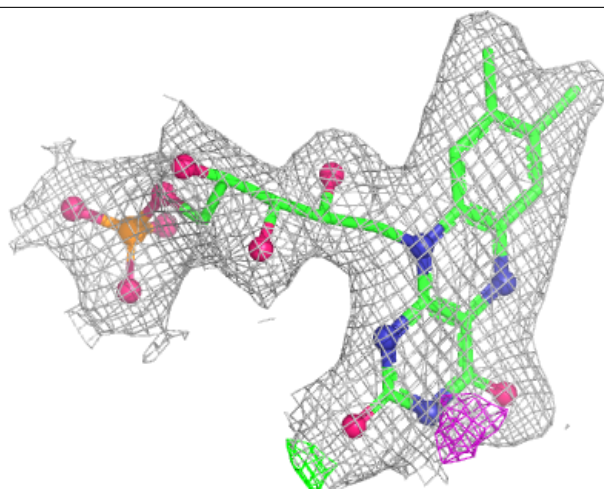
Electron density around FMN E 301:

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



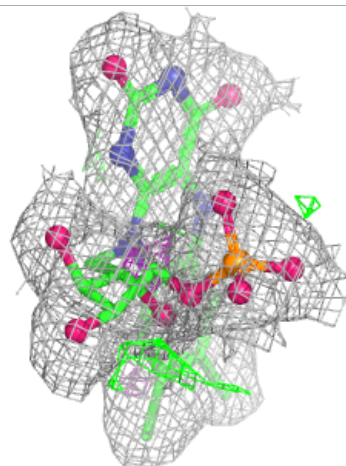
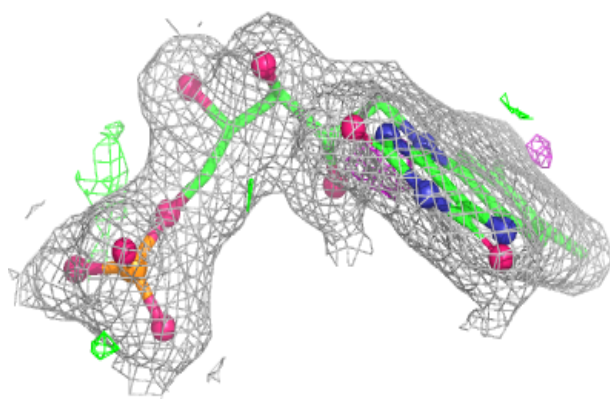
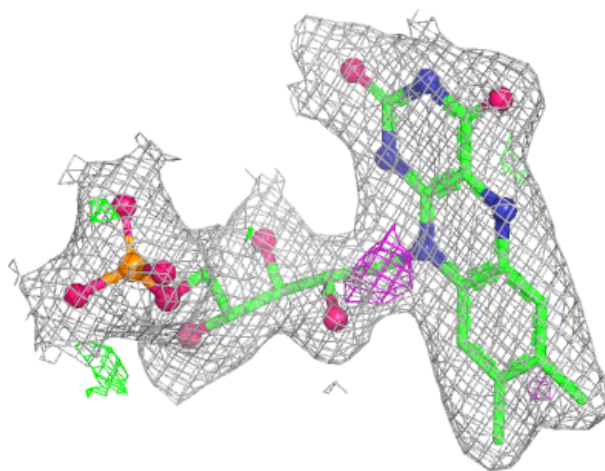
Electron density around FMN Q 301:

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



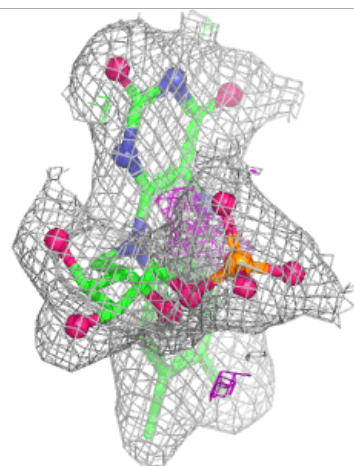
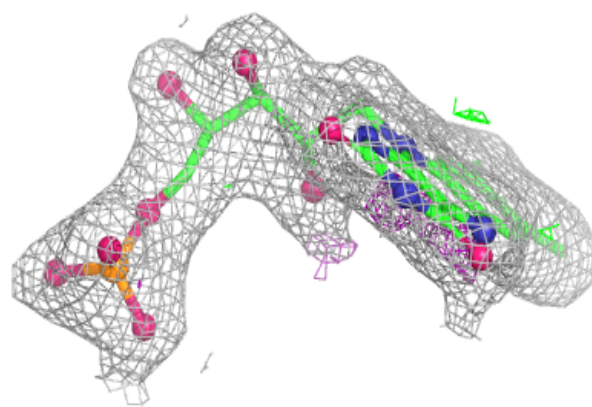
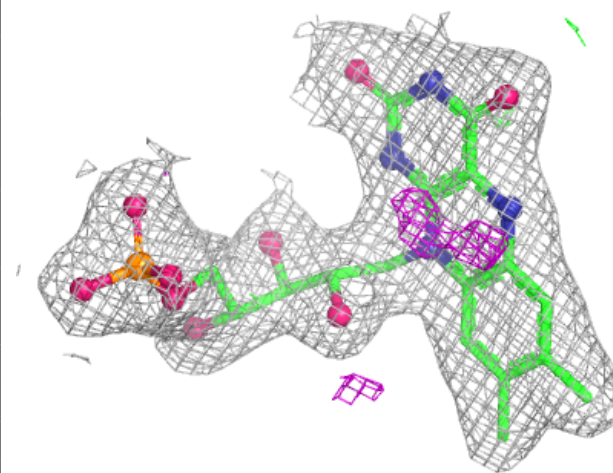
Electron density around FMN U 301:

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



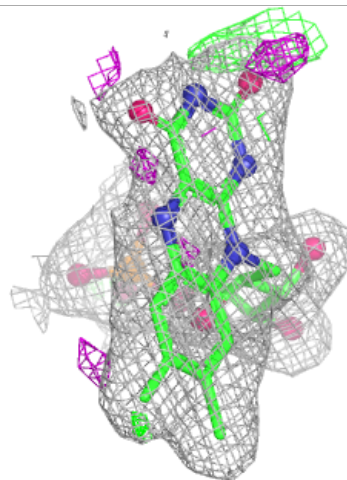
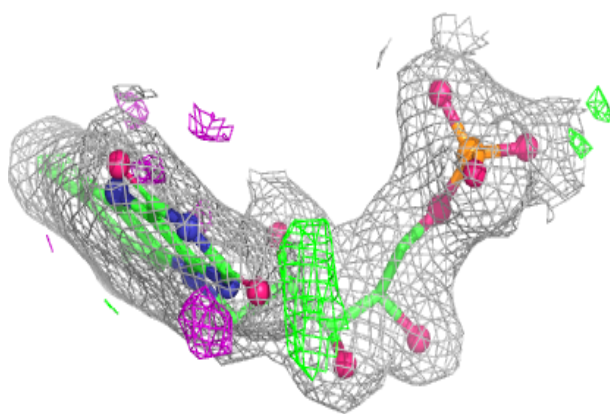
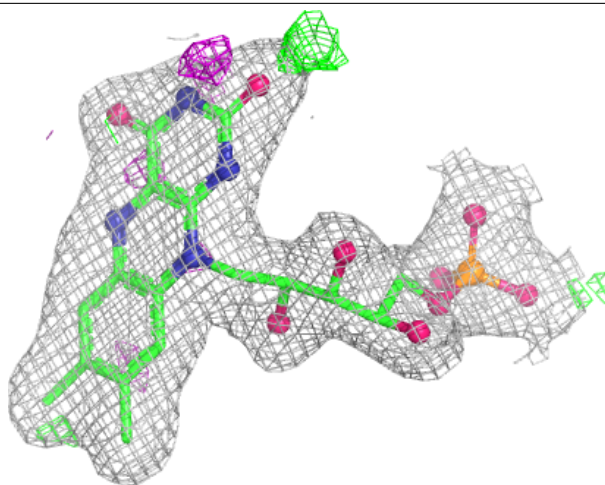
Electron density around FMN W 301:

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



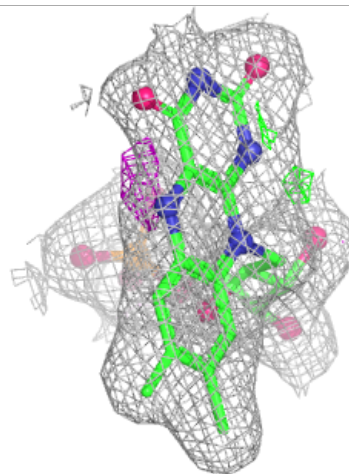
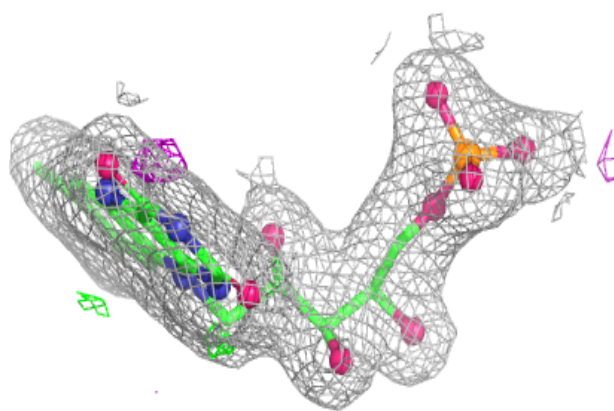
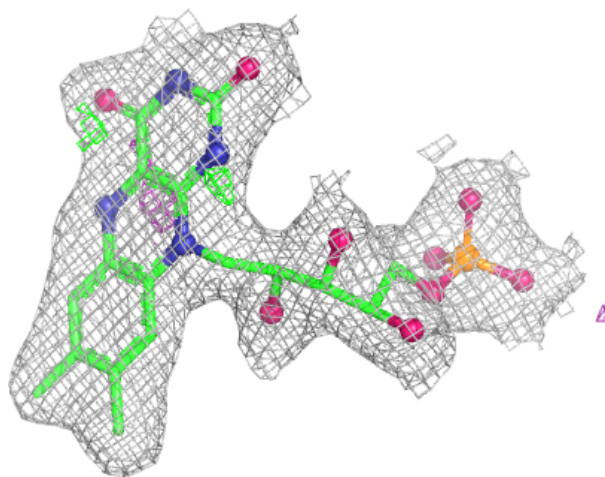
Electron density around FMN S 302:

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



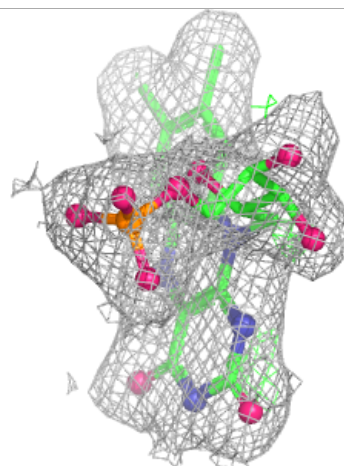
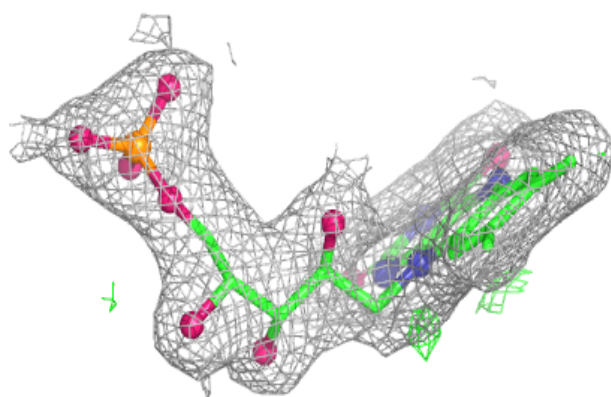
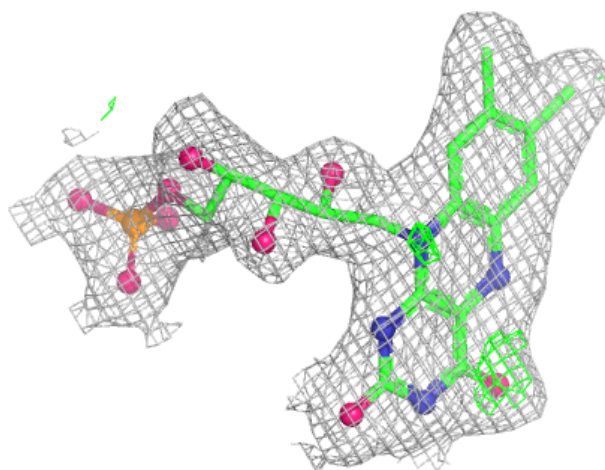
Electron density around FMN D 301:

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



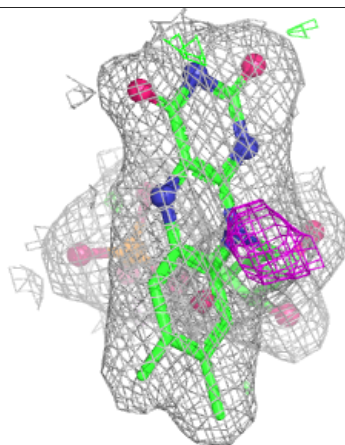
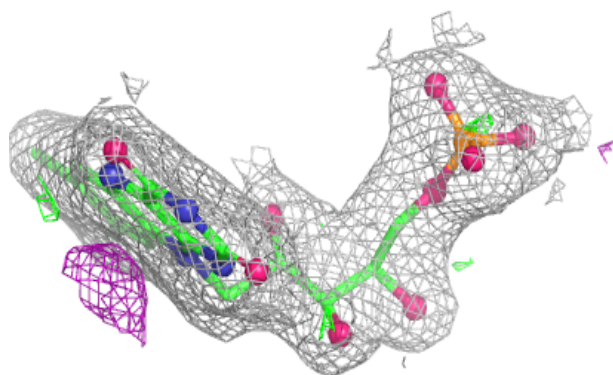
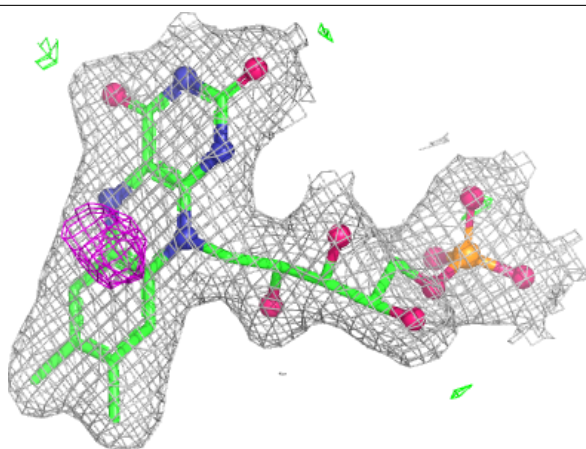
Electron density around FMN H 301:

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



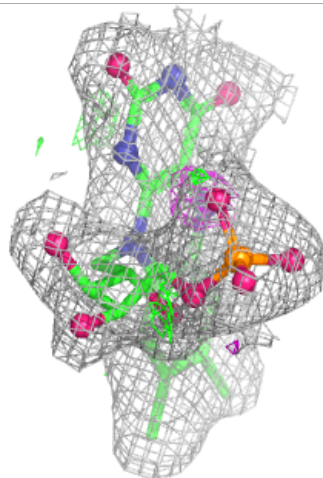
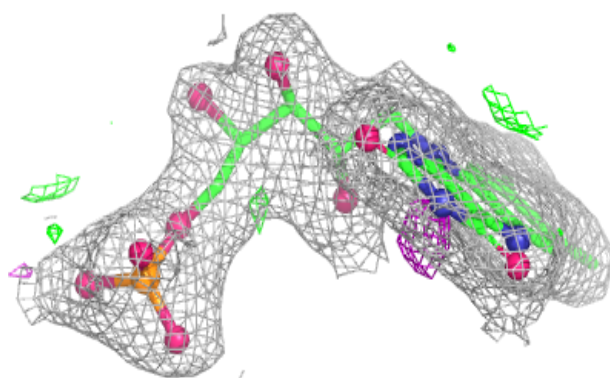
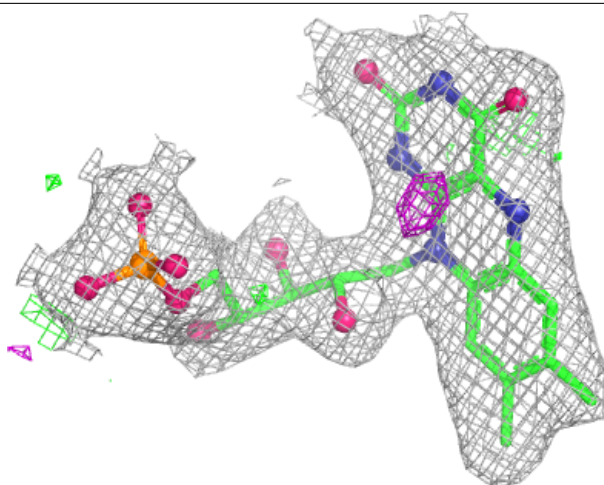
Electron density around FMN I 301:

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



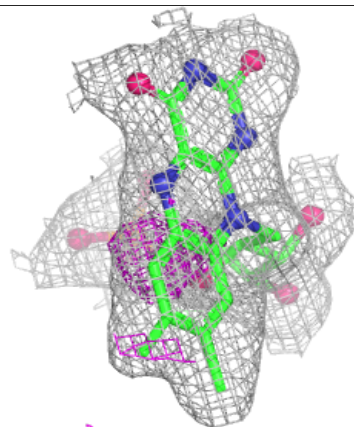
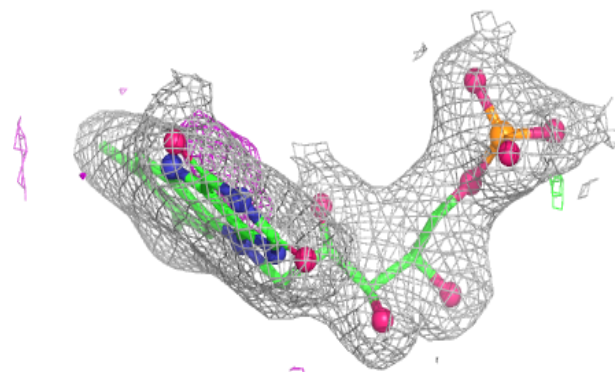
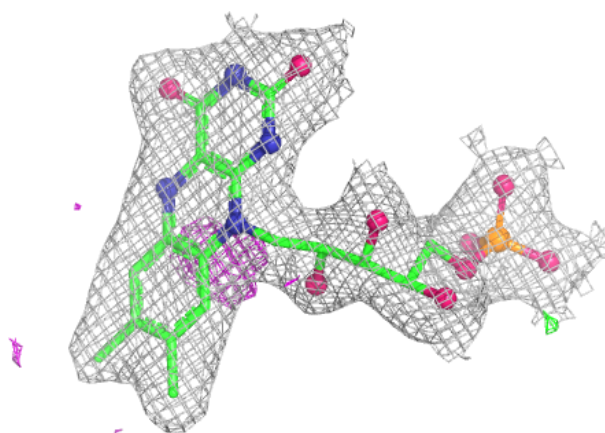
Electron density around FMN J 301:

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



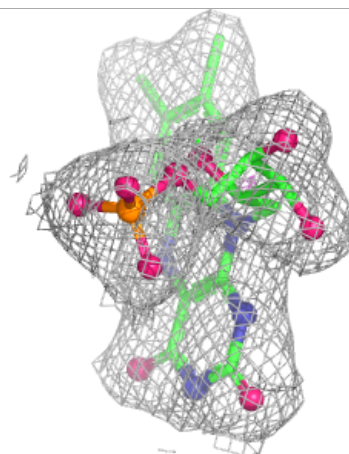
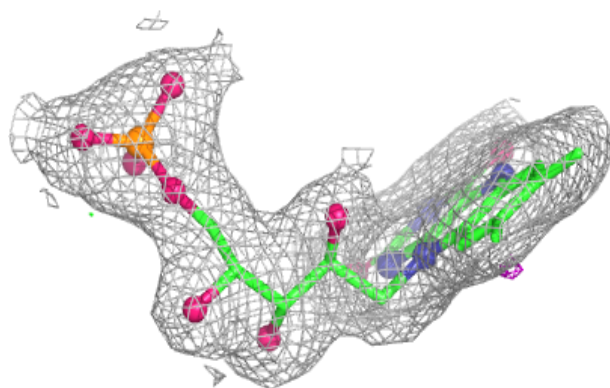
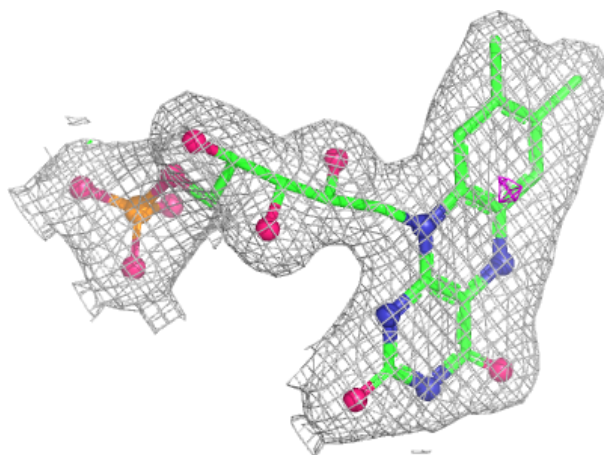
Electron density around FMN K 301:

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



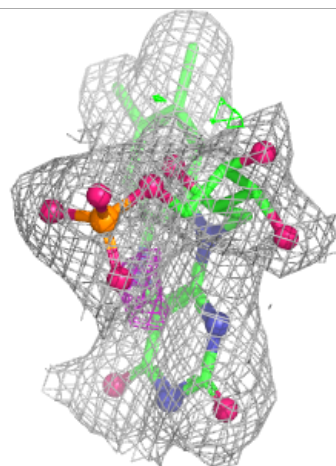
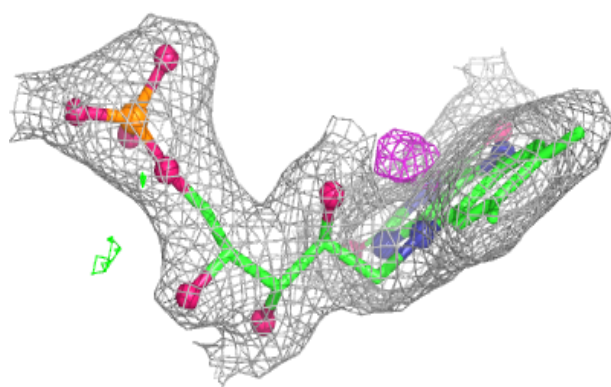
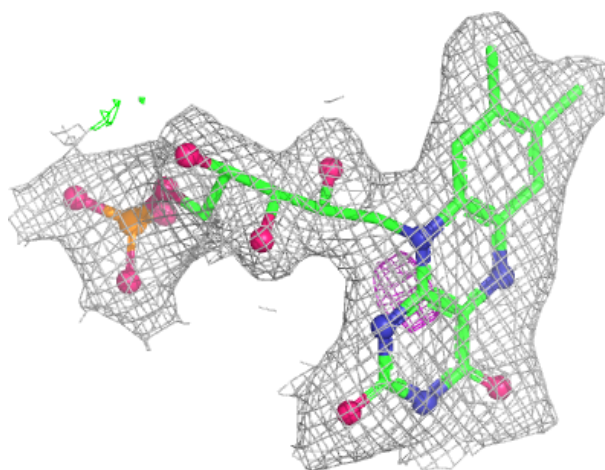
Electron density around FMN L 301:

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



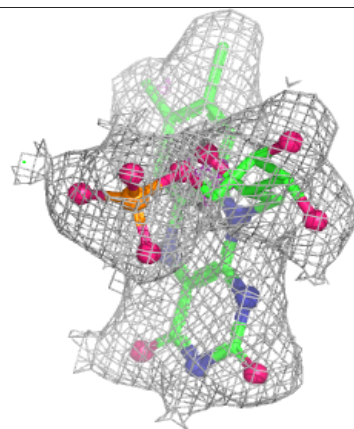
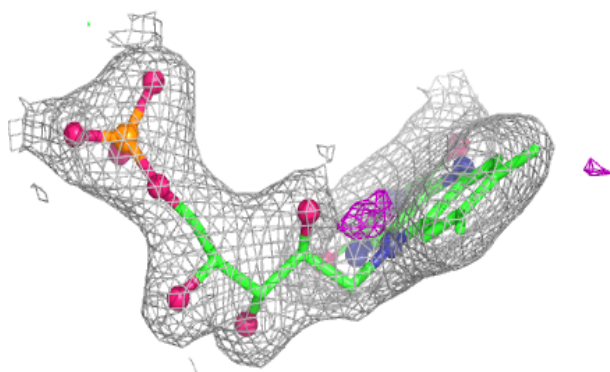
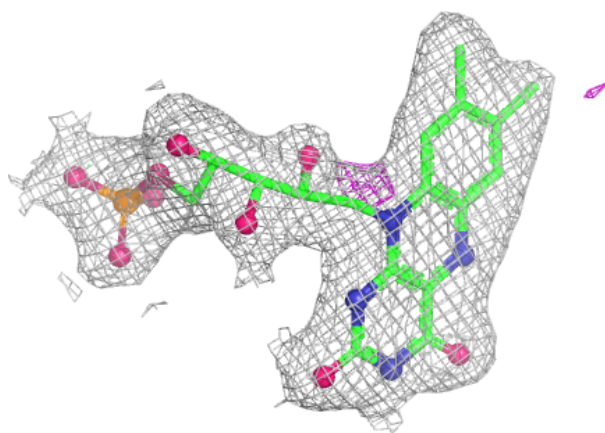
Electron density around FMN M 301:

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



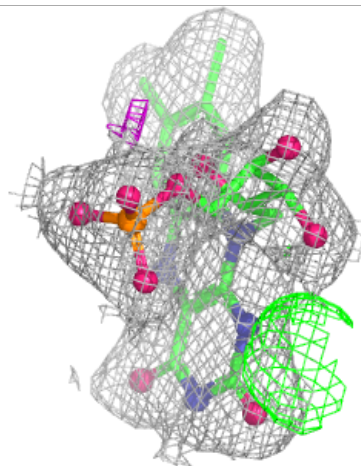
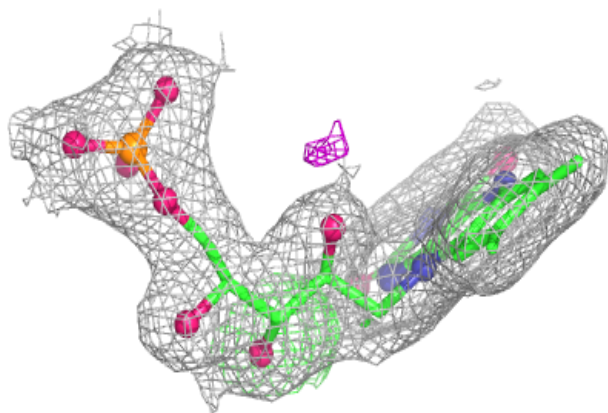
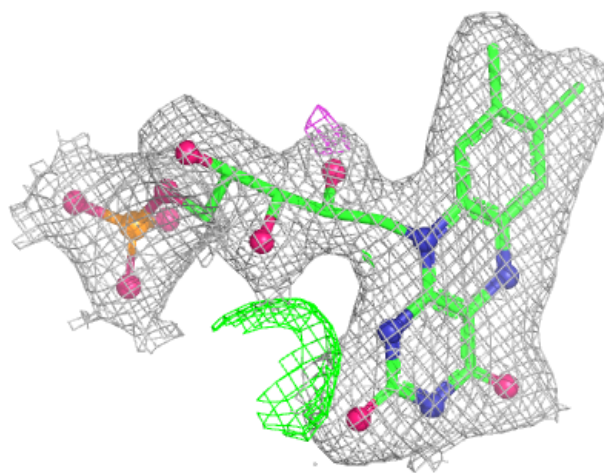
Electron density around FMN N 301:

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



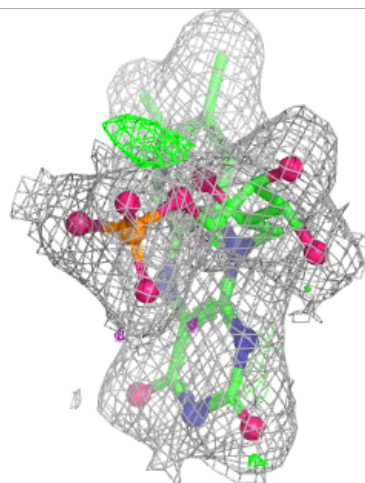
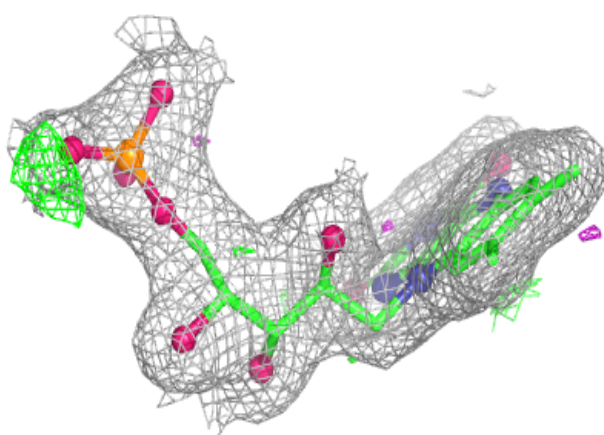
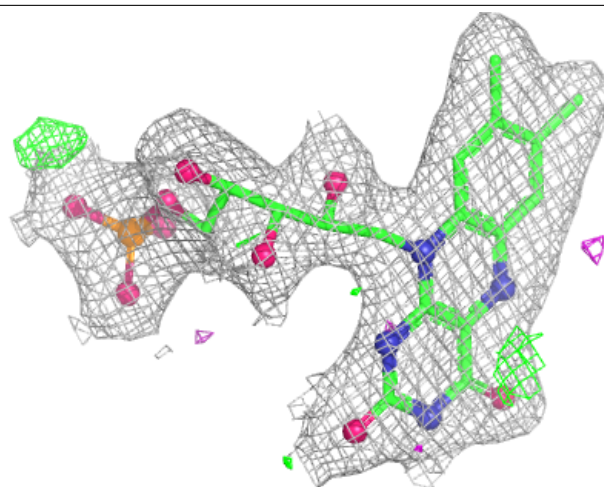
Electron density around FMN O 301:

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



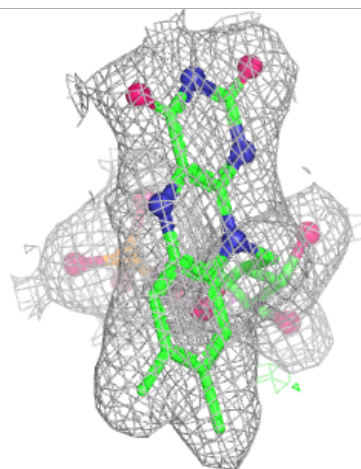
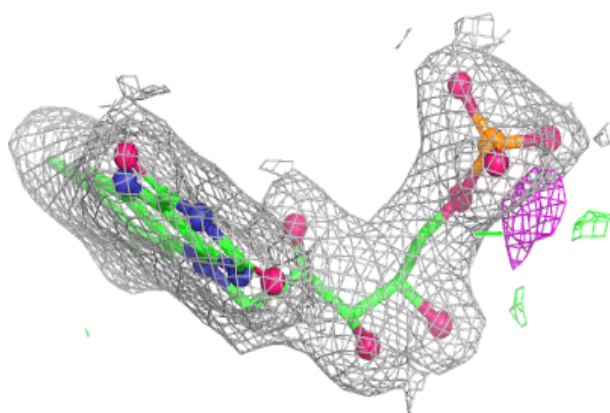
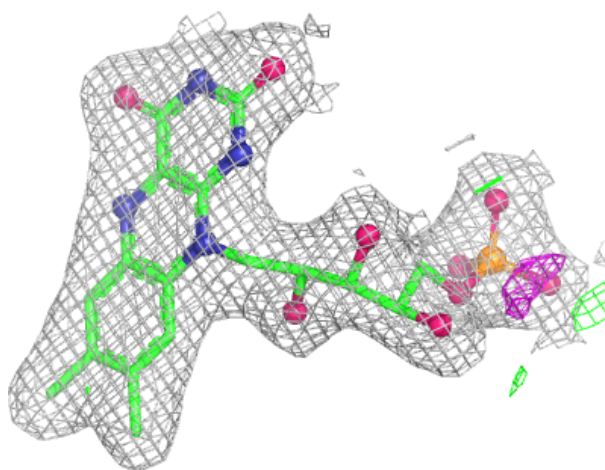
Electron density around FMN P 301:

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



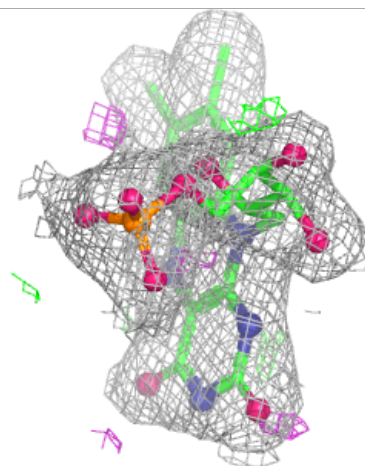
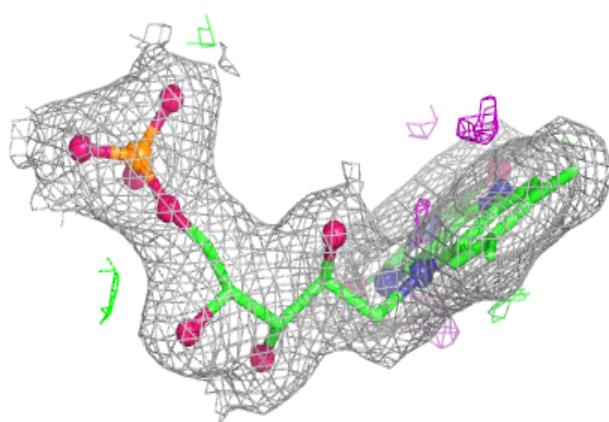
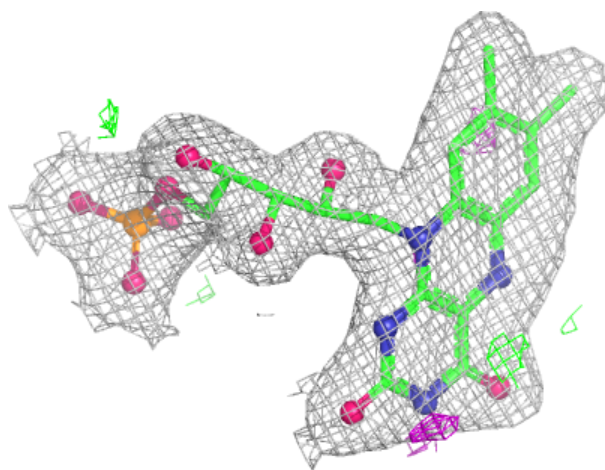
Electron density around FMN T 301:

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



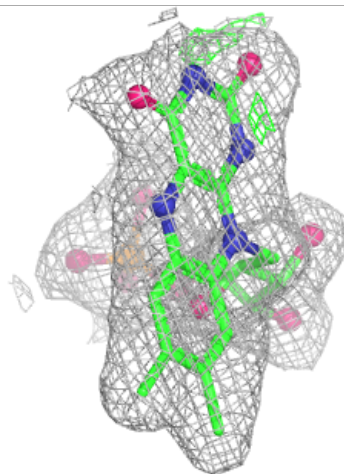
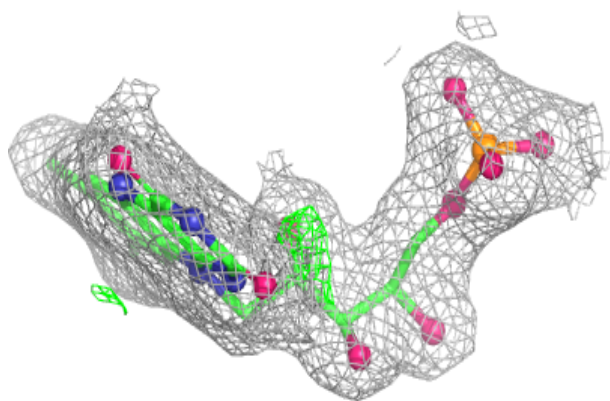
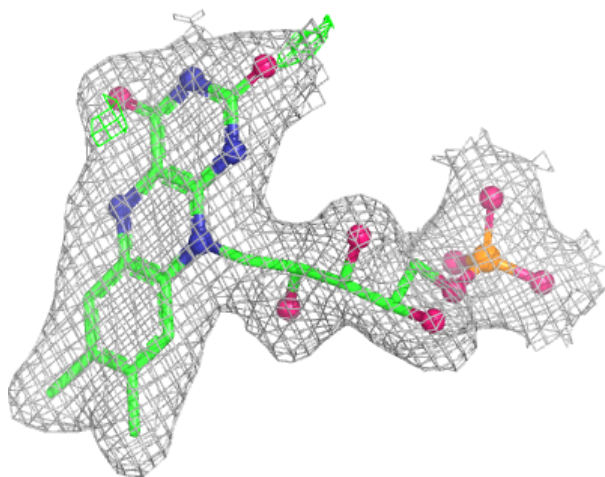
Electron density around FMN A 301:

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



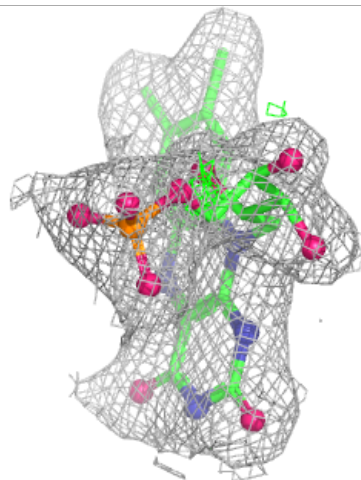
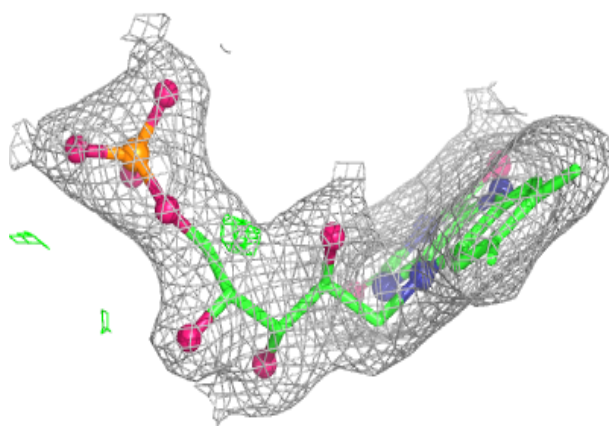
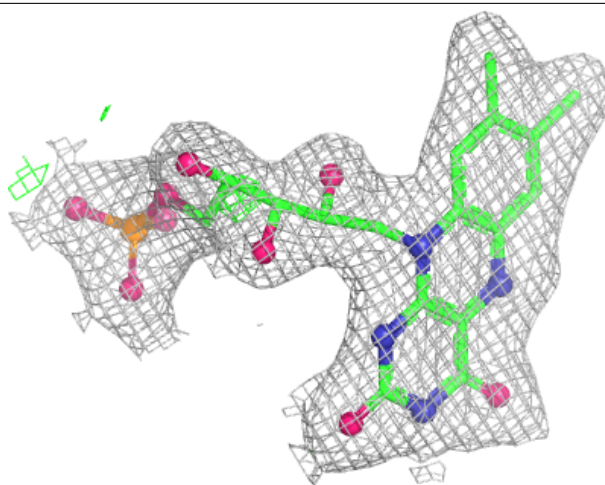
Electron density around FMN V 301:

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



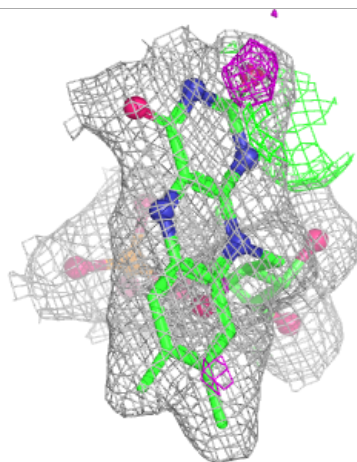
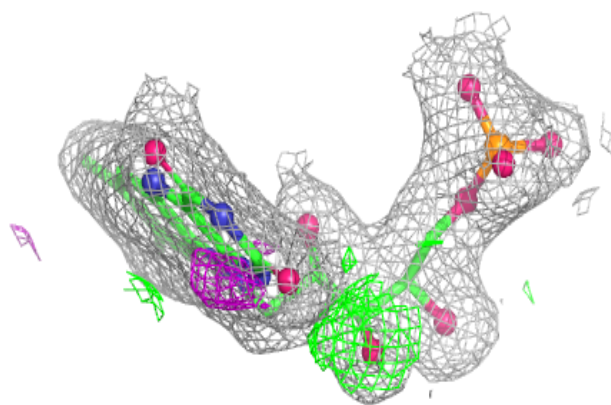
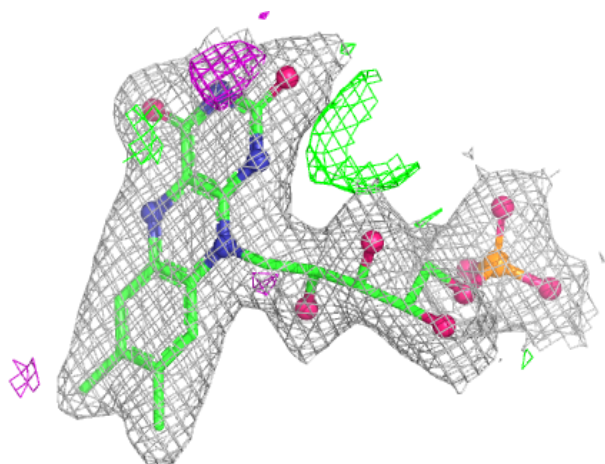
Electron density around FMN B 301:

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



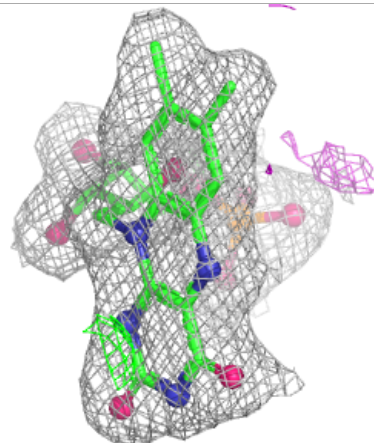
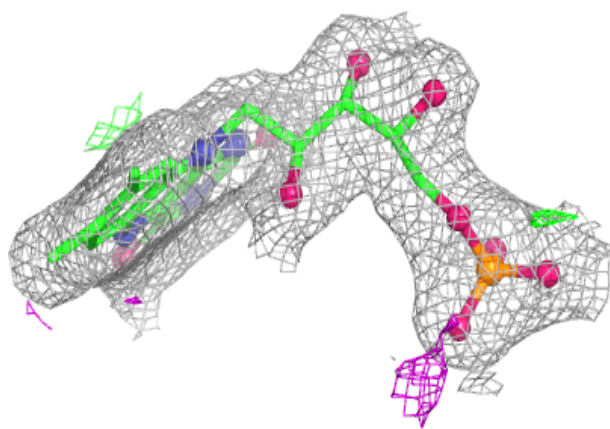
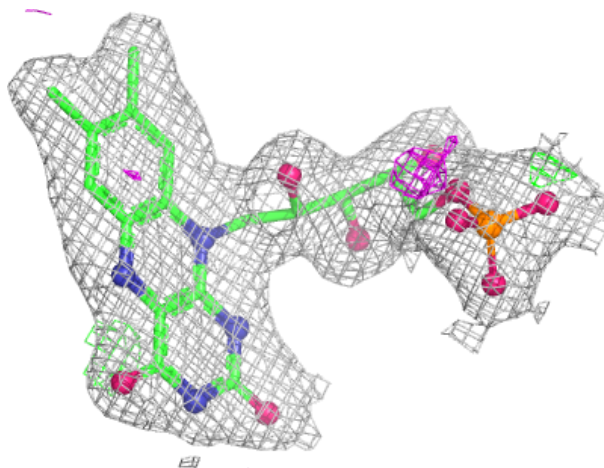
Electron density around FMN X 301:

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



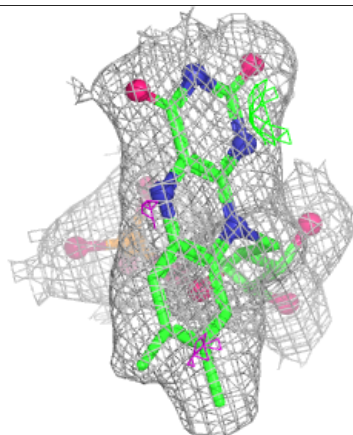
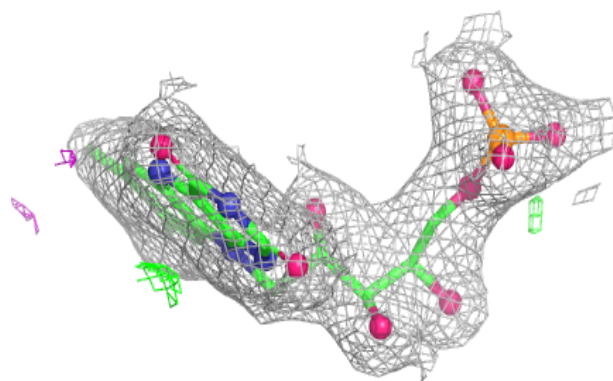
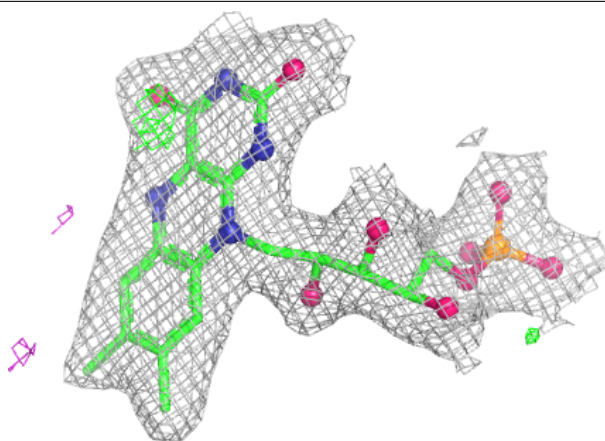
Electron density around FMN F 301:

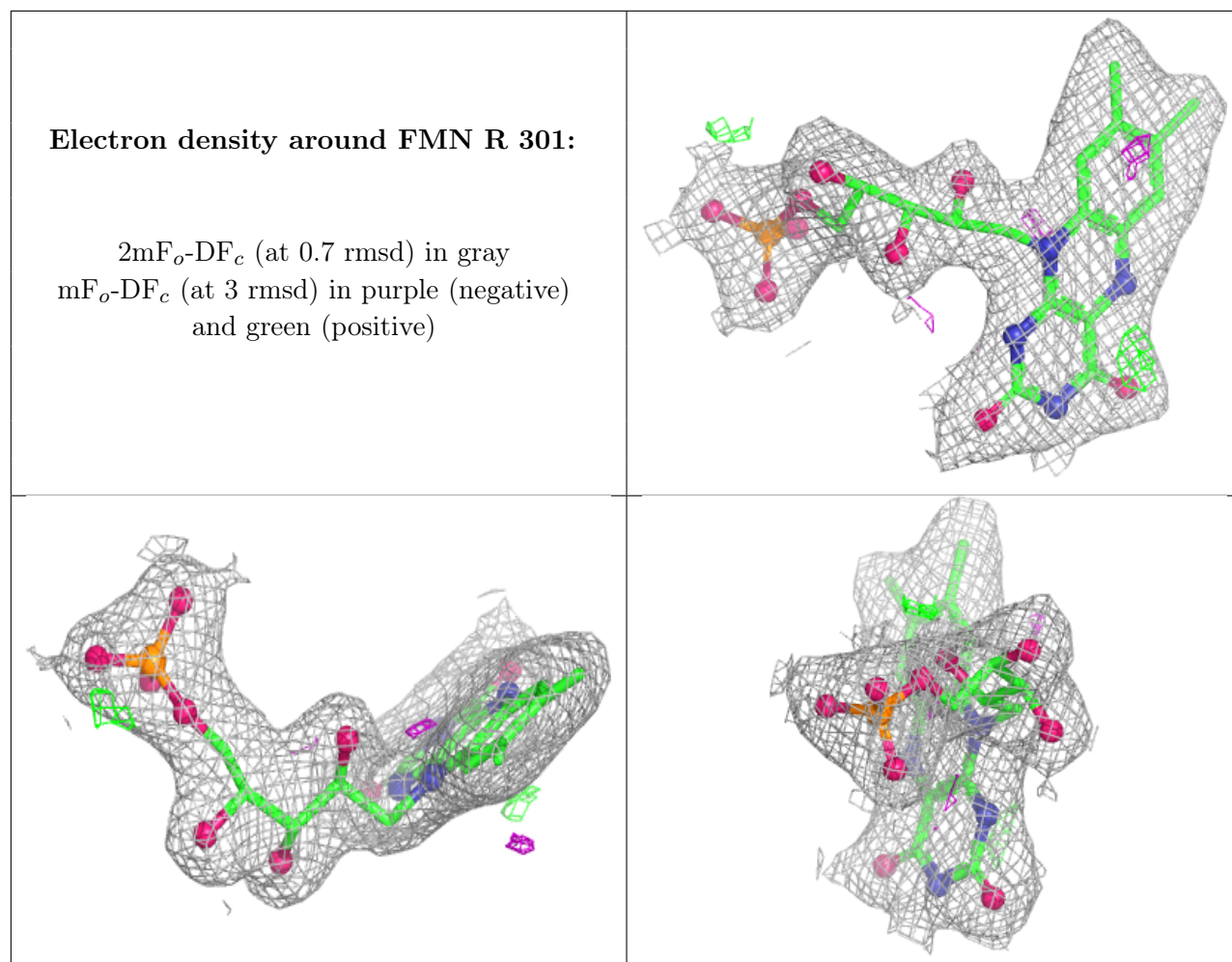
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.