



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 07:38 AM UTC

PDB ID : 8I98 / pdb_00008i98
Title : Crystal structure of TePixD Y8F
Authors : Hu, R.; Lin, L.; Lu, Q.
Deposited on : 2023-02-06
Resolution : 2.54 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

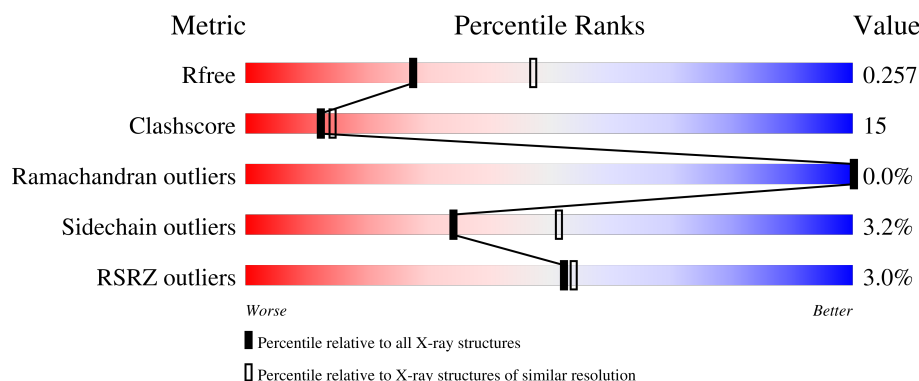
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	163	3% 64% 21% 14%
1	B	163	2% 66% 20% 13%
1	C	163	60% 25% 14%
1	D	163	2% 71% 15% 13%
1	E	163	0% 64% 23% 13%

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Mol	Chain	Length	Quality of chain
1	F	163	
1	G	163	
1	H	163	
1	I	163	
1	J	163	
1	K	163	
1	L	163	
1	M	163	
1	N	163	
1	O	163	
1	P	163	
1	Q	163	
1	R	163	
1	S	163	
1	T	163	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMN	T	9201	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23005 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 Tll0078 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1113	703	189	210	11			
1	B	141	Total	C	N	O	S	0	0	0
			1136	715	199	211	11			
1	C	140	Total	C	N	O	S	0	0	0
			1119	706	192	210	11			
1	D	141	Total	C	N	O	S	0	0	0
			1128	710	196	211	11			
1	E	142	Total	C	N	O	S	0	0	0
			1154	724	206	213	11			
1	F	143	Total	C	N	O	S	0	0	0
			1148	721	202	214	11			
1	G	140	Total	C	N	O	S	0	0	0
			1119	703	196	209	11			
1	H	141	Total	C	N	O	S	0	0	0
			1128	710	197	210	11			
1	I	141	Total	C	N	O	S	0	0	0
			1116	704	193	208	11			
1	J	141	Total	C	N	O	S	0	0	0
			1130	711	199	209	11			
1	K	140	Total	C	N	O	S	0	0	0
			1097	690	188	209	10			
1	L	141	Total	C	N	O	S	0	0	0
			1119	705	194	209	11			
1	M	140	Total	C	N	O	S	0	0	0
			1113	702	192	208	11			
1	N	140	Total	C	N	O	S	0	0	0
			1104	697	189	208	10			
1	O	140	Total	C	N	O	S	0	0	0
			1108	701	189	208	10			
1	P	141	Total	C	N	O	S	0	0	0
			1078	680	184	205	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	140	Total	C	N	O	S	0	0	0
			1125	708	198	208	11			
1	R	140	Total	C	N	O	S	0	0	0
			1113	703	195	205	10			
1	S	141	Total	C	N	O	S	0	0	0
			1118	704	192	211	11			
1	T	140	Total	C	N	O	S	0	0	0
			1119	704	194	210	11			

There are 420 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8DMN3
A	-18	GLY	-	expression tag	UNP Q8DMN3
A	-17	SER	-	expression tag	UNP Q8DMN3
A	-16	SER	-	expression tag	UNP Q8DMN3
A	-15	HIS	-	expression tag	UNP Q8DMN3
A	-14	HIS	-	expression tag	UNP Q8DMN3
A	-13	HIS	-	expression tag	UNP Q8DMN3
A	-12	HIS	-	expression tag	UNP Q8DMN3
A	-11	HIS	-	expression tag	UNP Q8DMN3
A	-10	HIS	-	expression tag	UNP Q8DMN3
A	-9	SER	-	expression tag	UNP Q8DMN3
A	-8	SER	-	expression tag	UNP Q8DMN3
A	-7	GLY	-	expression tag	UNP Q8DMN3
A	-6	LEU	-	expression tag	UNP Q8DMN3
A	-5	VAL	-	expression tag	UNP Q8DMN3
A	-4	PRO	-	expression tag	UNP Q8DMN3
A	-3	ARG	-	expression tag	UNP Q8DMN3
A	-2	GLY	-	expression tag	UNP Q8DMN3
A	-1	SER	-	expression tag	UNP Q8DMN3
A	0	HIS	-	expression tag	UNP Q8DMN3
A	8	PHE	TYR	conflict	UNP Q8DMN3
B	981	MET	-	initiating methionine	UNP Q8DMN3
B	982	GLY	-	expression tag	UNP Q8DMN3
B	983	SER	-	expression tag	UNP Q8DMN3
B	984	SER	-	expression tag	UNP Q8DMN3
B	985	HIS	-	expression tag	UNP Q8DMN3
B	986	HIS	-	expression tag	UNP Q8DMN3
B	987	HIS	-	expression tag	UNP Q8DMN3
B	988	HIS	-	expression tag	UNP Q8DMN3
B	989	HIS	-	expression tag	UNP Q8DMN3
B	990	HIS	-	expression tag	UNP Q8DMN3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	991	SER	-	expression tag	UNP Q8DMN3
B	992	SER	-	expression tag	UNP Q8DMN3
B	993	GLY	-	expression tag	UNP Q8DMN3
B	994	LEU	-	expression tag	UNP Q8DMN3
B	995	VAL	-	expression tag	UNP Q8DMN3
B	996	PRO	-	expression tag	UNP Q8DMN3
B	997	ARG	-	expression tag	UNP Q8DMN3
B	998	GLY	-	expression tag	UNP Q8DMN3
B	999	SER	-	expression tag	UNP Q8DMN3
B	1000	HIS	-	expression tag	UNP Q8DMN3
B	1008	PHE	TYR	conflict	UNP Q8DMN3
C	1981	MET	-	initiating methionine	UNP Q8DMN3
C	1982	GLY	-	expression tag	UNP Q8DMN3
C	1983	SER	-	expression tag	UNP Q8DMN3
C	1984	SER	-	expression tag	UNP Q8DMN3
C	1985	HIS	-	expression tag	UNP Q8DMN3
C	1986	HIS	-	expression tag	UNP Q8DMN3
C	1987	HIS	-	expression tag	UNP Q8DMN3
C	1988	HIS	-	expression tag	UNP Q8DMN3
C	1989	HIS	-	expression tag	UNP Q8DMN3
C	1990	HIS	-	expression tag	UNP Q8DMN3
C	1991	SER	-	expression tag	UNP Q8DMN3
C	1992	SER	-	expression tag	UNP Q8DMN3
C	1993	GLY	-	expression tag	UNP Q8DMN3
C	1994	LEU	-	expression tag	UNP Q8DMN3
C	1995	VAL	-	expression tag	UNP Q8DMN3
C	1996	PRO	-	expression tag	UNP Q8DMN3
C	1997	ARG	-	expression tag	UNP Q8DMN3
C	1998	GLY	-	expression tag	UNP Q8DMN3
C	1999	SER	-	expression tag	UNP Q8DMN3
C	2000	HIS	-	expression tag	UNP Q8DMN3
C	2008	PHE	TYR	conflict	UNP Q8DMN3
D	2981	MET	-	initiating methionine	UNP Q8DMN3
D	2982	GLY	-	expression tag	UNP Q8DMN3
D	2983	SER	-	expression tag	UNP Q8DMN3
D	2984	SER	-	expression tag	UNP Q8DMN3
D	2985	HIS	-	expression tag	UNP Q8DMN3
D	2986	HIS	-	expression tag	UNP Q8DMN3
D	2987	HIS	-	expression tag	UNP Q8DMN3
D	2988	HIS	-	expression tag	UNP Q8DMN3
D	2989	HIS	-	expression tag	UNP Q8DMN3
D	2990	HIS	-	expression tag	UNP Q8DMN3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2991	SER	-	expression tag	UNP Q8DMN3
D	2992	SER	-	expression tag	UNP Q8DMN3
D	2993	GLY	-	expression tag	UNP Q8DMN3
D	2994	LEU	-	expression tag	UNP Q8DMN3
D	2995	VAL	-	expression tag	UNP Q8DMN3
D	2996	PRO	-	expression tag	UNP Q8DMN3
D	2997	ARG	-	expression tag	UNP Q8DMN3
D	2998	GLY	-	expression tag	UNP Q8DMN3
D	2999	SER	-	expression tag	UNP Q8DMN3
D	3000	HIS	-	expression tag	UNP Q8DMN3
D	3008	PHE	TYR	conflict	UNP Q8DMN3
E	3981	MET	-	initiating methionine	UNP Q8DMN3
E	3982	GLY	-	expression tag	UNP Q8DMN3
E	3983	SER	-	expression tag	UNP Q8DMN3
E	3984	SER	-	expression tag	UNP Q8DMN3
E	3985	HIS	-	expression tag	UNP Q8DMN3
E	3986	HIS	-	expression tag	UNP Q8DMN3
E	3987	HIS	-	expression tag	UNP Q8DMN3
E	3988	HIS	-	expression tag	UNP Q8DMN3
E	3989	HIS	-	expression tag	UNP Q8DMN3
E	3990	HIS	-	expression tag	UNP Q8DMN3
E	3991	SER	-	expression tag	UNP Q8DMN3
E	3992	SER	-	expression tag	UNP Q8DMN3
E	3993	GLY	-	expression tag	UNP Q8DMN3
E	3994	LEU	-	expression tag	UNP Q8DMN3
E	3995	VAL	-	expression tag	UNP Q8DMN3
E	3996	PRO	-	expression tag	UNP Q8DMN3
E	3997	ARG	-	expression tag	UNP Q8DMN3
E	3998	GLY	-	expression tag	UNP Q8DMN3
E	3999	SER	-	expression tag	UNP Q8DMN3
E	4000	HIS	-	expression tag	UNP Q8DMN3
E	4008	PHE	TYR	conflict	UNP Q8DMN3
F	4981	MET	-	initiating methionine	UNP Q8DMN3
F	4982	GLY	-	expression tag	UNP Q8DMN3
F	4983	SER	-	expression tag	UNP Q8DMN3
F	4984	SER	-	expression tag	UNP Q8DMN3
F	4985	HIS	-	expression tag	UNP Q8DMN3
F	4986	HIS	-	expression tag	UNP Q8DMN3
F	4987	HIS	-	expression tag	UNP Q8DMN3
F	4988	HIS	-	expression tag	UNP Q8DMN3
F	4989	HIS	-	expression tag	UNP Q8DMN3
F	4990	HIS	-	expression tag	UNP Q8DMN3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	4991	SER	-	expression tag	UNP Q8DMN3
F	4992	SER	-	expression tag	UNP Q8DMN3
F	4993	GLY	-	expression tag	UNP Q8DMN3
F	4994	LEU	-	expression tag	UNP Q8DMN3
F	4995	VAL	-	expression tag	UNP Q8DMN3
F	4996	PRO	-	expression tag	UNP Q8DMN3
F	4997	ARG	-	expression tag	UNP Q8DMN3
F	4998	GLY	-	expression tag	UNP Q8DMN3
F	4999	SER	-	expression tag	UNP Q8DMN3
F	5000	HIS	-	expression tag	UNP Q8DMN3
F	5008	PHE	TYR	conflict	UNP Q8DMN3
G	5981	MET	-	initiating methionine	UNP Q8DMN3
G	5982	GLY	-	expression tag	UNP Q8DMN3
G	5983	SER	-	expression tag	UNP Q8DMN3
G	5984	SER	-	expression tag	UNP Q8DMN3
G	5985	HIS	-	expression tag	UNP Q8DMN3
G	5986	HIS	-	expression tag	UNP Q8DMN3
G	5987	HIS	-	expression tag	UNP Q8DMN3
G	5988	HIS	-	expression tag	UNP Q8DMN3
G	5989	HIS	-	expression tag	UNP Q8DMN3
G	5990	HIS	-	expression tag	UNP Q8DMN3
G	5991	SER	-	expression tag	UNP Q8DMN3
G	5992	SER	-	expression tag	UNP Q8DMN3
G	5993	GLY	-	expression tag	UNP Q8DMN3
G	5994	LEU	-	expression tag	UNP Q8DMN3
G	5995	VAL	-	expression tag	UNP Q8DMN3
G	5996	PRO	-	expression tag	UNP Q8DMN3
G	5997	ARG	-	expression tag	UNP Q8DMN3
G	5998	GLY	-	expression tag	UNP Q8DMN3
G	5999	SER	-	expression tag	UNP Q8DMN3
G	6000	HIS	-	expression tag	UNP Q8DMN3
G	6008	PHE	TYR	conflict	UNP Q8DMN3
H	6981	MET	-	initiating methionine	UNP Q8DMN3
H	6982	GLY	-	expression tag	UNP Q8DMN3
H	6983	SER	-	expression tag	UNP Q8DMN3
H	6984	SER	-	expression tag	UNP Q8DMN3
H	6985	HIS	-	expression tag	UNP Q8DMN3
H	6986	HIS	-	expression tag	UNP Q8DMN3
H	6987	HIS	-	expression tag	UNP Q8DMN3
H	6988	HIS	-	expression tag	UNP Q8DMN3
H	6989	HIS	-	expression tag	UNP Q8DMN3
H	6990	HIS	-	expression tag	UNP Q8DMN3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	6991	SER	-	expression tag	UNP Q8DMN3
H	6992	SER	-	expression tag	UNP Q8DMN3
H	6993	GLY	-	expression tag	UNP Q8DMN3
H	6994	LEU	-	expression tag	UNP Q8DMN3
H	6995	VAL	-	expression tag	UNP Q8DMN3
H	6996	PRO	-	expression tag	UNP Q8DMN3
H	6997	ARG	-	expression tag	UNP Q8DMN3
H	6998	GLY	-	expression tag	UNP Q8DMN3
H	6999	SER	-	expression tag	UNP Q8DMN3
H	7000	HIS	-	expression tag	UNP Q8DMN3
H	7008	PHE	TYR	conflict	UNP Q8DMN3
I	7981	MET	-	initiating methionine	UNP Q8DMN3
I	7982	GLY	-	expression tag	UNP Q8DMN3
I	7983	SER	-	expression tag	UNP Q8DMN3
I	7984	SER	-	expression tag	UNP Q8DMN3
I	7985	HIS	-	expression tag	UNP Q8DMN3
I	7986	HIS	-	expression tag	UNP Q8DMN3
I	7987	HIS	-	expression tag	UNP Q8DMN3
I	7988	HIS	-	expression tag	UNP Q8DMN3
I	7989	HIS	-	expression tag	UNP Q8DMN3
I	7990	HIS	-	expression tag	UNP Q8DMN3
I	7991	SER	-	expression tag	UNP Q8DMN3
I	7992	SER	-	expression tag	UNP Q8DMN3
I	7993	GLY	-	expression tag	UNP Q8DMN3
I	7994	LEU	-	expression tag	UNP Q8DMN3
I	7995	VAL	-	expression tag	UNP Q8DMN3
I	7996	PRO	-	expression tag	UNP Q8DMN3
I	7997	ARG	-	expression tag	UNP Q8DMN3
I	7998	GLY	-	expression tag	UNP Q8DMN3
I	7999	SER	-	expression tag	UNP Q8DMN3
I	8000	HIS	-	expression tag	UNP Q8DMN3
I	8008	PHE	TYR	conflict	UNP Q8DMN3
J	8981	MET	-	initiating methionine	UNP Q8DMN3
J	8982	GLY	-	expression tag	UNP Q8DMN3
J	8983	SER	-	expression tag	UNP Q8DMN3
J	8984	SER	-	expression tag	UNP Q8DMN3
J	8985	HIS	-	expression tag	UNP Q8DMN3
J	8986	HIS	-	expression tag	UNP Q8DMN3
J	8987	HIS	-	expression tag	UNP Q8DMN3
J	8988	HIS	-	expression tag	UNP Q8DMN3
J	8989	HIS	-	expression tag	UNP Q8DMN3
J	8990	HIS	-	expression tag	UNP Q8DMN3

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Chain	Residue	Modelled	Actual	Comment	Reference
J	8991	SER	-	expression tag	UNP Q8DMN3
J	8992	SER	-	expression tag	UNP Q8DMN3
J	8993	GLY	-	expression tag	UNP Q8DMN3
J	8994	LEU	-	expression tag	UNP Q8DMN3
J	8995	VAL	-	expression tag	UNP Q8DMN3
J	8996	PRO	-	expression tag	UNP Q8DMN3
J	8997	ARG	-	expression tag	UNP Q8DMN3
J	8998	GLY	-	expression tag	UNP Q8DMN3
J	8999	SER	-	expression tag	UNP Q8DMN3
J	9000	HIS	-	expression tag	UNP Q8DMN3
J	9008	PHE	TYR	conflict	UNP Q8DMN3
K	81	MET	-	initiating methionine	UNP Q8DMN3
K	82	GLY	-	expression tag	UNP Q8DMN3
K	83	SER	-	expression tag	UNP Q8DMN3
K	84	SER	-	expression tag	UNP Q8DMN3
K	85	HIS	-	expression tag	UNP Q8DMN3
K	86	HIS	-	expression tag	UNP Q8DMN3
K	87	HIS	-	expression tag	UNP Q8DMN3
K	88	HIS	-	expression tag	UNP Q8DMN3
K	89	HIS	-	expression tag	UNP Q8DMN3
K	90	HIS	-	expression tag	UNP Q8DMN3
K	91	SER	-	expression tag	UNP Q8DMN3
K	92	SER	-	expression tag	UNP Q8DMN3
K	93	GLY	-	expression tag	UNP Q8DMN3
K	94	LEU	-	expression tag	UNP Q8DMN3
K	95	VAL	-	expression tag	UNP Q8DMN3
K	96	PRO	-	expression tag	UNP Q8DMN3
K	97	ARG	-	expression tag	UNP Q8DMN3
K	98	GLY	-	expression tag	UNP Q8DMN3
K	99	SER	-	expression tag	UNP Q8DMN3
K	100	HIS	-	expression tag	UNP Q8DMN3
K	108	PHE	TYR	conflict	UNP Q8DMN3
L	981	MET	-	initiating methionine	UNP Q8DMN3
L	982	GLY	-	expression tag	UNP Q8DMN3
L	983	SER	-	expression tag	UNP Q8DMN3
L	984	SER	-	expression tag	UNP Q8DMN3
L	985	HIS	-	expression tag	UNP Q8DMN3
L	986	HIS	-	expression tag	UNP Q8DMN3
L	987	HIS	-	expression tag	UNP Q8DMN3
L	988	HIS	-	expression tag	UNP Q8DMN3
L	989	HIS	-	expression tag	UNP Q8DMN3
L	990	HIS	-	expression tag	UNP Q8DMN3

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Chain	Residue	Modelled	Actual	Comment	Reference
L	991	SER	-	expression tag	UNP Q8DMN3
L	992	SER	-	expression tag	UNP Q8DMN3
L	993	GLY	-	expression tag	UNP Q8DMN3
L	994	LEU	-	expression tag	UNP Q8DMN3
L	995	VAL	-	expression tag	UNP Q8DMN3
L	996	PRO	-	expression tag	UNP Q8DMN3
L	997	ARG	-	expression tag	UNP Q8DMN3
L	998	GLY	-	expression tag	UNP Q8DMN3
L	999	SER	-	expression tag	UNP Q8DMN3
L	1000	HIS	-	expression tag	UNP Q8DMN3
L	1008	PHE	TYR	conflict	UNP Q8DMN3
M	1981	MET	-	initiating methionine	UNP Q8DMN3
M	1982	GLY	-	expression tag	UNP Q8DMN3
M	1983	SER	-	expression tag	UNP Q8DMN3
M	1984	SER	-	expression tag	UNP Q8DMN3
M	1985	HIS	-	expression tag	UNP Q8DMN3
M	1986	HIS	-	expression tag	UNP Q8DMN3
M	1987	HIS	-	expression tag	UNP Q8DMN3
M	1988	HIS	-	expression tag	UNP Q8DMN3
M	1989	HIS	-	expression tag	UNP Q8DMN3
M	1990	HIS	-	expression tag	UNP Q8DMN3
M	1991	SER	-	expression tag	UNP Q8DMN3
M	1992	SER	-	expression tag	UNP Q8DMN3
M	1993	GLY	-	expression tag	UNP Q8DMN3
M	1994	LEU	-	expression tag	UNP Q8DMN3
M	1995	VAL	-	expression tag	UNP Q8DMN3
M	1996	PRO	-	expression tag	UNP Q8DMN3
M	1997	ARG	-	expression tag	UNP Q8DMN3
M	1998	GLY	-	expression tag	UNP Q8DMN3
M	1999	SER	-	expression tag	UNP Q8DMN3
M	2000	HIS	-	expression tag	UNP Q8DMN3
M	2008	PHE	TYR	conflict	UNP Q8DMN3
N	2981	MET	-	initiating methionine	UNP Q8DMN3
N	2982	GLY	-	expression tag	UNP Q8DMN3
N	2983	SER	-	expression tag	UNP Q8DMN3
N	2984	SER	-	expression tag	UNP Q8DMN3
N	2985	HIS	-	expression tag	UNP Q8DMN3
N	2986	HIS	-	expression tag	UNP Q8DMN3
N	2987	HIS	-	expression tag	UNP Q8DMN3
N	2988	HIS	-	expression tag	UNP Q8DMN3
N	2989	HIS	-	expression tag	UNP Q8DMN3
N	2990	HIS	-	expression tag	UNP Q8DMN3

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Chain	Residue	Modelled	Actual	Comment	Reference
N	2991	SER	-	expression tag	UNP Q8DMN3
N	2992	SER	-	expression tag	UNP Q8DMN3
N	2993	GLY	-	expression tag	UNP Q8DMN3
N	2994	LEU	-	expression tag	UNP Q8DMN3
N	2995	VAL	-	expression tag	UNP Q8DMN3
N	2996	PRO	-	expression tag	UNP Q8DMN3
N	2997	ARG	-	expression tag	UNP Q8DMN3
N	2998	GLY	-	expression tag	UNP Q8DMN3
N	2999	SER	-	expression tag	UNP Q8DMN3
N	3000	HIS	-	expression tag	UNP Q8DMN3
N	3008	PHE	TYR	conflict	UNP Q8DMN3
O	3981	MET	-	initiating methionine	UNP Q8DMN3
O	3982	GLY	-	expression tag	UNP Q8DMN3
O	3983	SER	-	expression tag	UNP Q8DMN3
O	3984	SER	-	expression tag	UNP Q8DMN3
O	3985	HIS	-	expression tag	UNP Q8DMN3
O	3986	HIS	-	expression tag	UNP Q8DMN3
O	3987	HIS	-	expression tag	UNP Q8DMN3
O	3988	HIS	-	expression tag	UNP Q8DMN3
O	3989	HIS	-	expression tag	UNP Q8DMN3
O	3990	HIS	-	expression tag	UNP Q8DMN3
O	3991	SER	-	expression tag	UNP Q8DMN3
O	3992	SER	-	expression tag	UNP Q8DMN3
O	3993	GLY	-	expression tag	UNP Q8DMN3
O	3994	LEU	-	expression tag	UNP Q8DMN3
O	3995	VAL	-	expression tag	UNP Q8DMN3
O	3996	PRO	-	expression tag	UNP Q8DMN3
O	3997	ARG	-	expression tag	UNP Q8DMN3
O	3998	GLY	-	expression tag	UNP Q8DMN3
O	3999	SER	-	expression tag	UNP Q8DMN3
O	4000	HIS	-	expression tag	UNP Q8DMN3
O	4008	PHE	TYR	conflict	UNP Q8DMN3
P	4981	MET	-	initiating methionine	UNP Q8DMN3
P	4982	GLY	-	expression tag	UNP Q8DMN3
P	4983	SER	-	expression tag	UNP Q8DMN3
P	4984	SER	-	expression tag	UNP Q8DMN3
P	4985	HIS	-	expression tag	UNP Q8DMN3
P	4986	HIS	-	expression tag	UNP Q8DMN3
P	4987	HIS	-	expression tag	UNP Q8DMN3
P	4988	HIS	-	expression tag	UNP Q8DMN3
P	4989	HIS	-	expression tag	UNP Q8DMN3
P	4990	HIS	-	expression tag	UNP Q8DMN3

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Chain	Residue	Modelled	Actual	Comment	Reference
P	4991	SER	-	expression tag	UNP Q8DMN3
P	4992	SER	-	expression tag	UNP Q8DMN3
P	4993	GLY	-	expression tag	UNP Q8DMN3
P	4994	LEU	-	expression tag	UNP Q8DMN3
P	4995	VAL	-	expression tag	UNP Q8DMN3
P	4996	PRO	-	expression tag	UNP Q8DMN3
P	4997	ARG	-	expression tag	UNP Q8DMN3
P	4998	GLY	-	expression tag	UNP Q8DMN3
P	4999	SER	-	expression tag	UNP Q8DMN3
P	5000	HIS	-	expression tag	UNP Q8DMN3
P	5008	PHE	TYR	conflict	UNP Q8DMN3
Q	5981	MET	-	initiating methionine	UNP Q8DMN3
Q	5982	GLY	-	expression tag	UNP Q8DMN3
Q	5983	SER	-	expression tag	UNP Q8DMN3
Q	5984	SER	-	expression tag	UNP Q8DMN3
Q	5985	HIS	-	expression tag	UNP Q8DMN3
Q	5986	HIS	-	expression tag	UNP Q8DMN3
Q	5987	HIS	-	expression tag	UNP Q8DMN3
Q	5988	HIS	-	expression tag	UNP Q8DMN3
Q	5989	HIS	-	expression tag	UNP Q8DMN3
Q	5990	HIS	-	expression tag	UNP Q8DMN3
Q	5991	SER	-	expression tag	UNP Q8DMN3
Q	5992	SER	-	expression tag	UNP Q8DMN3
Q	5993	GLY	-	expression tag	UNP Q8DMN3
Q	5994	LEU	-	expression tag	UNP Q8DMN3
Q	5995	VAL	-	expression tag	UNP Q8DMN3
Q	5996	PRO	-	expression tag	UNP Q8DMN3
Q	5997	ARG	-	expression tag	UNP Q8DMN3
Q	5998	GLY	-	expression tag	UNP Q8DMN3
Q	5999	SER	-	expression tag	UNP Q8DMN3
Q	6000	HIS	-	expression tag	UNP Q8DMN3
Q	6008	PHE	TYR	conflict	UNP Q8DMN3
R	6981	MET	-	initiating methionine	UNP Q8DMN3
R	6982	GLY	-	expression tag	UNP Q8DMN3
R	6983	SER	-	expression tag	UNP Q8DMN3
R	6984	SER	-	expression tag	UNP Q8DMN3
R	6985	HIS	-	expression tag	UNP Q8DMN3
R	6986	HIS	-	expression tag	UNP Q8DMN3
R	6987	HIS	-	expression tag	UNP Q8DMN3
R	6988	HIS	-	expression tag	UNP Q8DMN3
R	6989	HIS	-	expression tag	UNP Q8DMN3
R	6990	HIS	-	expression tag	UNP Q8DMN3

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Chain	Residue	Modelled	Actual	Comment	Reference
R	6991	SER	-	expression tag	UNP Q8DMN3
R	6992	SER	-	expression tag	UNP Q8DMN3
R	6993	GLY	-	expression tag	UNP Q8DMN3
R	6994	LEU	-	expression tag	UNP Q8DMN3
R	6995	VAL	-	expression tag	UNP Q8DMN3
R	6996	PRO	-	expression tag	UNP Q8DMN3
R	6997	ARG	-	expression tag	UNP Q8DMN3
R	6998	GLY	-	expression tag	UNP Q8DMN3
R	6999	SER	-	expression tag	UNP Q8DMN3
R	7000	HIS	-	expression tag	UNP Q8DMN3
R	7008	PHE	TYR	conflict	UNP Q8DMN3
S	7981	MET	-	initiating methionine	UNP Q8DMN3
S	7982	GLY	-	expression tag	UNP Q8DMN3
S	7983	SER	-	expression tag	UNP Q8DMN3
S	7984	SER	-	expression tag	UNP Q8DMN3
S	7985	HIS	-	expression tag	UNP Q8DMN3
S	7986	HIS	-	expression tag	UNP Q8DMN3
S	7987	HIS	-	expression tag	UNP Q8DMN3
S	7988	HIS	-	expression tag	UNP Q8DMN3
S	7989	HIS	-	expression tag	UNP Q8DMN3
S	7990	HIS	-	expression tag	UNP Q8DMN3
S	7991	SER	-	expression tag	UNP Q8DMN3
S	7992	SER	-	expression tag	UNP Q8DMN3
S	7993	GLY	-	expression tag	UNP Q8DMN3
S	7994	LEU	-	expression tag	UNP Q8DMN3
S	7995	VAL	-	expression tag	UNP Q8DMN3
S	7996	PRO	-	expression tag	UNP Q8DMN3
S	7997	ARG	-	expression tag	UNP Q8DMN3
S	7998	GLY	-	expression tag	UNP Q8DMN3
S	7999	SER	-	expression tag	UNP Q8DMN3
S	8000	HIS	-	expression tag	UNP Q8DMN3
S	8008	PHE	TYR	conflict	UNP Q8DMN3
T	8981	MET	-	initiating methionine	UNP Q8DMN3
T	8982	GLY	-	expression tag	UNP Q8DMN3
T	8983	SER	-	expression tag	UNP Q8DMN3
T	8984	SER	-	expression tag	UNP Q8DMN3
T	8985	HIS	-	expression tag	UNP Q8DMN3
T	8986	HIS	-	expression tag	UNP Q8DMN3
T	8987	HIS	-	expression tag	UNP Q8DMN3
T	8988	HIS	-	expression tag	UNP Q8DMN3
T	8989	HIS	-	expression tag	UNP Q8DMN3
T	8990	HIS	-	expression tag	UNP Q8DMN3

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Chain	Residue	Modelled	Actual	Comment	Reference
T	8991	SER	-	expression tag	UNP Q8DMN3
T	8992	SER	-	expression tag	UNP Q8DMN3
T	8993	GLY	-	expression tag	UNP Q8DMN3
T	8994	LEU	-	expression tag	UNP Q8DMN3
T	8995	VAL	-	expression tag	UNP Q8DMN3
T	8996	PRO	-	expression tag	UNP Q8DMN3
T	8997	ARG	-	expression tag	UNP Q8DMN3
T	8998	GLY	-	expression tag	UNP Q8DMN3
T	8999	SER	-	expression tag	UNP Q8DMN3
T	9000	HIS	-	expression tag	UNP Q8DMN3
T	9008	PHE	TYR	conflict	UNP Q8DMN3

-
- The image displays the chemical structure of Flavin Mononucleotide (FMN). It features an isoalloxazine ring system, which is a tricyclic aromatic heterocycle consisting of a benzene ring fused to two pyrimidine rings. The atoms in the ring are labeled with standard chemical notation: carbons (C1-C10), nitrogens (N1-N5), and oxygens (O1-O4). The side chain is attached to the N10 position of the isoalloxazine ring. This side chain consists of a ribityl group (a three-carbon chain with hydroxyl groups at the 2' and 3' positions) linked to a phosphate group (C1P, O1P, O2P, O3P, P). The stereochemistry of the hydroxyl groups is indicated with wedges and dashes.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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



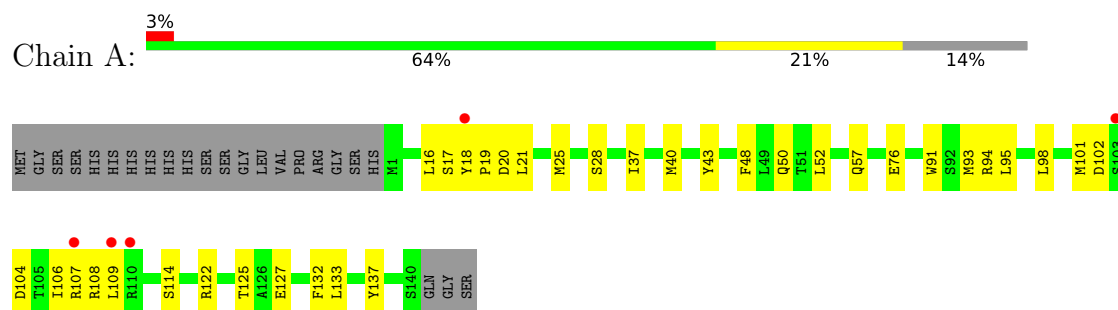
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	G	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	H	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	I	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	J	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	K	1	Total 31	C 17	N 4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

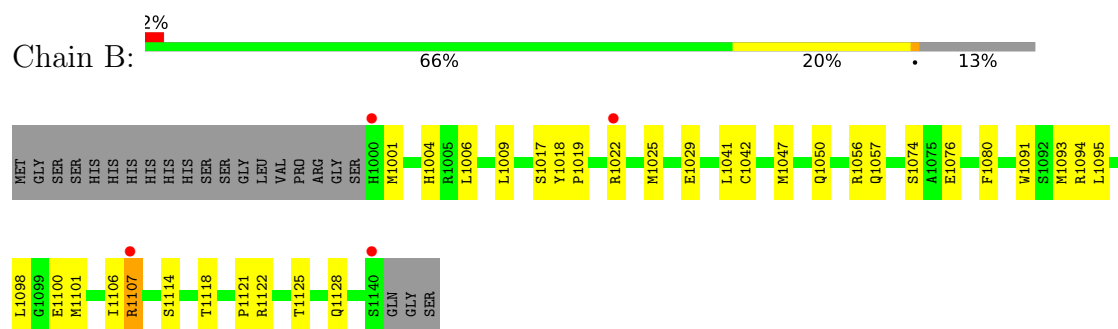
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

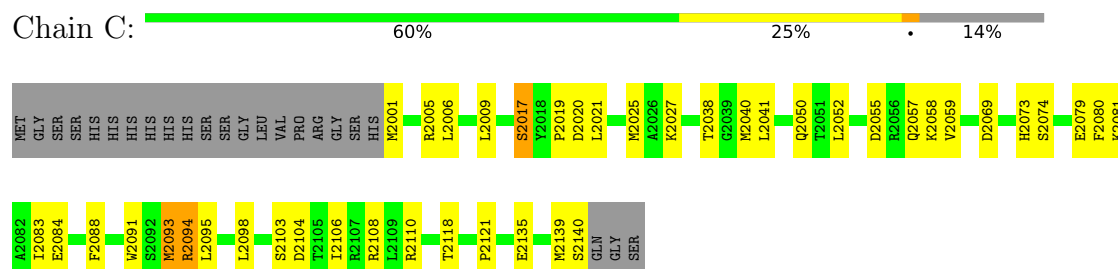
• Molecule 1: Tll0078 protein



• Molecule 1: Tll0078 protein

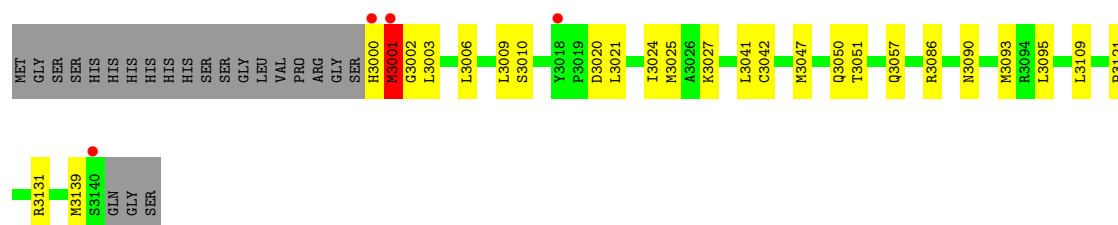


• Molecule 1: Tll0078 protein

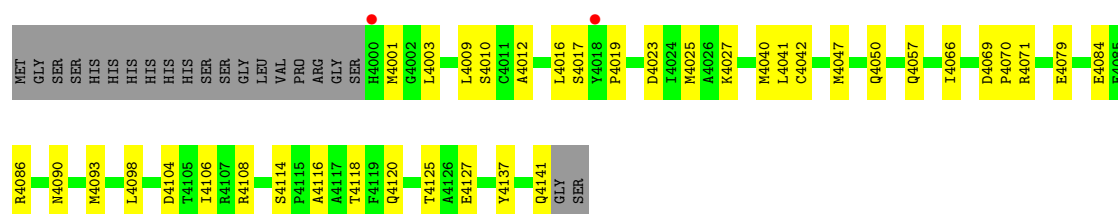


• Molecule 1: Tll0078 protein

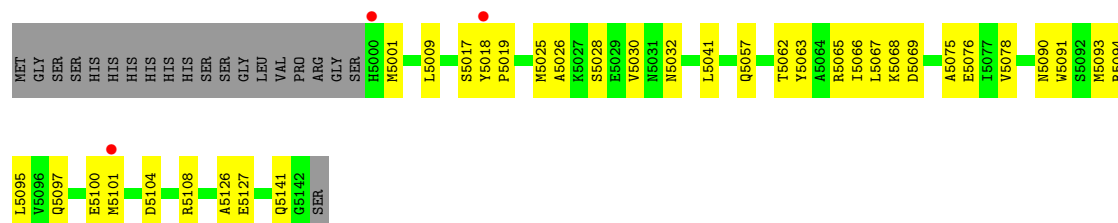




• Molecule 1: Tll0078 protein



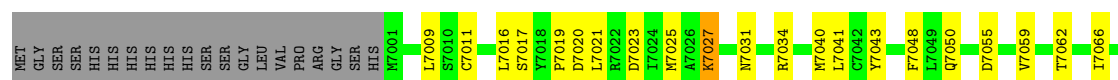
• Molecule 1: Tll0078 protein



• Molecule 1: Tll0078 protein

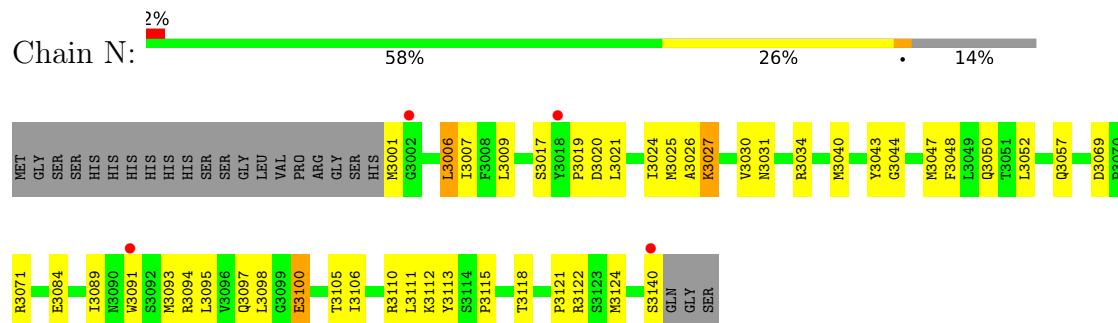


• Molecule 1: Tll0078 protein

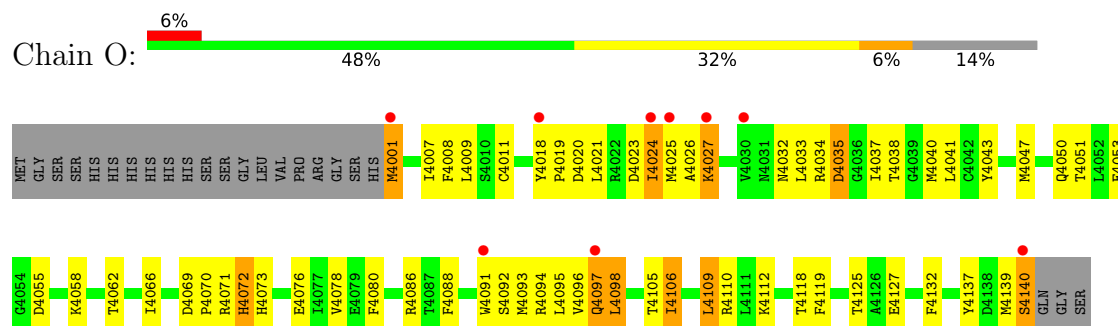




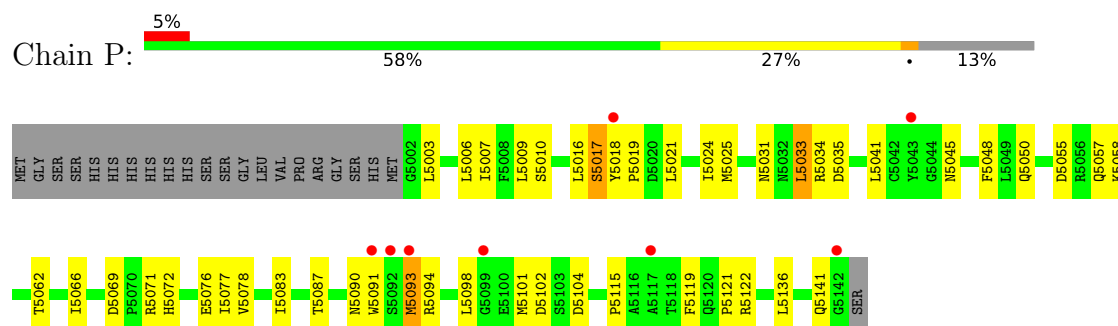
- Molecule 1: Tll0078 protein



- Molecule 1: Tll0078 protein



- Molecule 1: Tll0078 protein

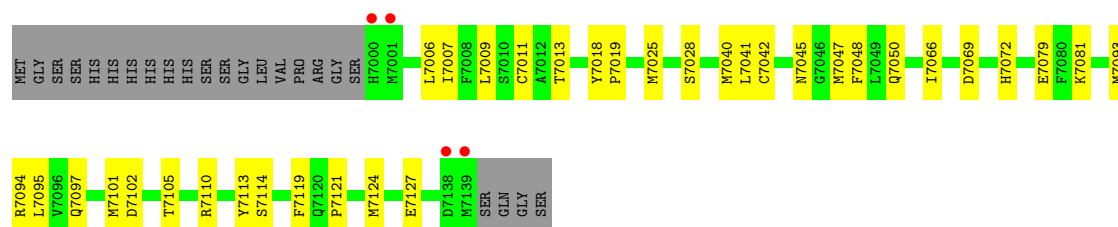


- Molecule 1: Tll0078 protein

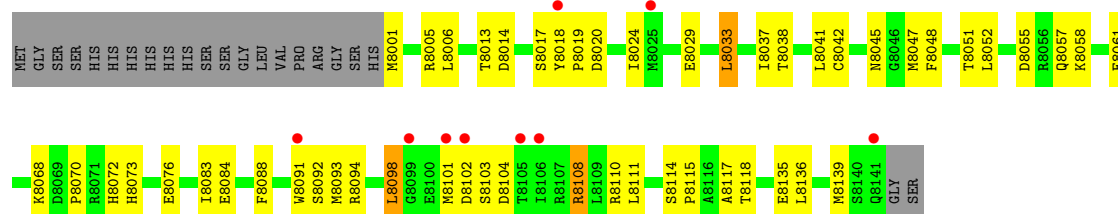




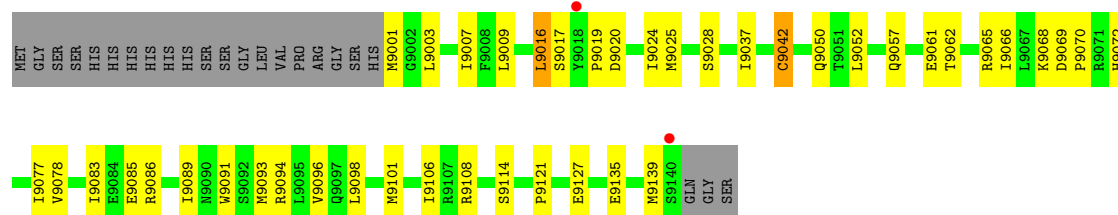
• Molecule 1: Tll0078 protein



• Molecule 1: Tll0078 protein



• Molecule 1: Tll0078 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.27Å 162.04Å 135.87Å 90.00° 92.60° 90.00°	Depositor
Resolution (Å)	35.88 – 2.54 35.88 – 2.54	Depositor EDS
% Data completeness (in resolution range)	98.4 (35.88-2.54) 98.4 (35.88-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.203 , 0.262 0.205 , 0.257	Depositor DCC
R_{free} test set	5753 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23005	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.62	0/1133	0.79	0/1524
1	B	0.63	0/1156	0.83	0/1552
1	C	0.57	0/1139	0.77	0/1531
1	D	0.60	0/1148	0.76	1/1543 (0.1%)
1	E	0.56	0/1175	0.69	0/1577
1	F	0.57	0/1168	0.75	0/1568
1	G	0.53	0/1138	0.73	0/1528
1	H	0.54	0/1148	0.75	0/1543
1	I	0.55	0/1136	0.71	0/1529
1	J	0.57	0/1150	0.75	0/1545
1	K	0.69	0/1116	0.99	0/1504
1	L	0.52	0/1140	0.81	0/1535
1	M	0.49	0/1133	0.68	0/1524
1	N	0.51	0/1124	0.74	0/1514
1	O	0.55	0/1128	0.85	0/1518
1	P	0.55	0/1097	0.80	1/1482 (0.1%)
1	Q	0.49	0/1145	0.70	0/1538
1	R	0.51	0/1133	0.70	0/1524
1	S	0.56	0/1138	0.73	0/1532
1	T	0.59	1/1139 (0.1%)	0.71	2/1532 (0.1%)
All	All	0.56	1/22784 (0.0%)	0.77	4/30643 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	9114	SER	C-N	-9.91	1.24	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	9108	ARG	CB-CG-CD	-5.49	98.67	111.30
1	D	3002	GLY	N-CA-C	5.48	118.71	111.70
1	P	5087	THR	N-CA-C	-5.46	107.17	113.88
1	T	9108	ARG	CA-CB-CG	5.04	124.19	114.10

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	1113	0	1093	35	0
1	B	1136	0	1125	22	0
1	C	1119	0	1101	36	0
1	D	1128	0	1110	19	0
1	E	1154	0	1145	26	0
1	F	1148	0	1134	30	0
1	G	1119	0	1107	24	0
1	H	1128	0	1112	30	0
1	I	1116	0	1090	26	0
1	J	1130	0	1117	32	0
1	K	1097	0	1061	27	0
1	L	1119	0	1089	48	0
1	M	1113	0	1093	55	0
1	N	1104	0	1075	46	0
1	O	1108	0	1083	75	0
1	P	1078	0	1029	40	0
1	Q	1125	0	1115	34	0
1	R	1113	0	1094	37	0
1	S	1118	0	1088	48	0
1	T	1119	0	1097	44	0
2	A	31	0	19	2	0
2	B	31	0	19	0	0
2	C	31	0	19	4	0
2	D	31	0	19	1	0
2	E	31	0	19	1	0
2	F	31	0	19	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	31	0	19	2	0
2	H	31	0	19	4	0
2	I	31	0	19	3	0
2	J	31	0	19	3	0
2	K	31	0	19	0	0
2	L	31	0	19	2	0
2	M	31	0	19	1	0
2	N	31	0	19	2	0
2	O	31	0	19	4	0
2	P	31	0	19	3	0
2	Q	31	0	19	1	0
2	R	31	0	19	1	0
2	S	31	0	19	0	0
2	T	31	0	19	10	0
All	All	23005	0	22338	697	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 15.

The worst 5 of 697 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:I:8093:MET:HA	1:I:8093:MET:HE2	1.26	1.12
1:B:1025:MET:HE1	1:B:1093:MET:HG3	1.34	1.09
1:T:9093:MET:HE2	1:T:9093:MET:HA	1.36	1.07
1:I:8025:MET:HE1	1:I:8093:MET:HG3	1.35	1.07
1:S:8001:MET:HE2	1:S:8001:MET:HA	1.39	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	138/163 (85%)	133 (96%)	5 (4%)	0	100	100
1	B	139/163 (85%)	136 (98%)	3 (2%)	0	100	100
1	C	138/163 (85%)	138 (100%)	0	0	100	100
1	D	139/163 (85%)	134 (96%)	4 (3%)	1 (1%)	18	25
1	E	140/163 (86%)	137 (98%)	3 (2%)	0	100	100
1	F	141/163 (86%)	140 (99%)	1 (1%)	0	100	100
1	G	138/163 (85%)	136 (99%)	2 (1%)	0	100	100
1	H	139/163 (85%)	135 (97%)	4 (3%)	0	100	100
1	I	139/163 (85%)	137 (99%)	2 (1%)	0	100	100
1	J	139/163 (85%)	136 (98%)	3 (2%)	0	100	100
1	K	138/163 (85%)	137 (99%)	1 (1%)	0	100	100
1	L	139/163 (85%)	133 (96%)	6 (4%)	0	100	100
1	M	138/163 (85%)	133 (96%)	5 (4%)	0	100	100
1	N	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
1	O	138/163 (85%)	131 (95%)	7 (5%)	0	100	100
1	P	139/163 (85%)	134 (96%)	5 (4%)	0	100	100
1	Q	138/163 (85%)	133 (96%)	5 (4%)	0	100	100
1	R	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
1	S	139/163 (85%)	134 (96%)	5 (4%)	0	100	100
1	T	138/163 (85%)	135 (98%)	3 (2%)	0	100	100
All	All	2773/3260 (85%)	2700 (97%)	72 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	3001	MET

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	120/143 (84%)	117 (98%)	3 (2%)	42	60
1	B	123/143 (86%)	118 (96%)	5 (4%)	27	41
1	C	121/143 (85%)	115 (95%)	6 (5%)	22	33
1	D	122/143 (85%)	121 (99%)	1 (1%)	73	84
1	E	126/143 (88%)	123 (98%)	3 (2%)	43	61
1	F	124/143 (87%)	123 (99%)	1 (1%)	73	84
1	G	121/143 (85%)	119 (98%)	2 (2%)	53	72
1	H	122/143 (85%)	118 (97%)	4 (3%)	33	50
1	I	119/143 (83%)	116 (98%)	3 (2%)	42	60
1	J	122/143 (85%)	121 (99%)	1 (1%)	73	84
1	K	117/143 (82%)	112 (96%)	5 (4%)	26	39
1	L	120/143 (84%)	114 (95%)	6 (5%)	22	33
1	M	120/143 (84%)	116 (97%)	4 (3%)	33	50
1	N	118/143 (82%)	115 (98%)	3 (2%)	42	60
1	O	118/143 (82%)	106 (90%)	12 (10%)	7	8
1	P	112/143 (78%)	106 (95%)	6 (5%)	20	30
1	Q	122/143 (85%)	122 (100%)	0	100	100
1	R	118/143 (82%)	117 (99%)	1 (1%)	73	84
1	S	120/143 (84%)	112 (93%)	8 (7%)	15	21
1	T	121/143 (85%)	118 (98%)	3 (2%)	42	60
All	All	2406/2860 (84%)	2329 (97%)	77 (3%)	34	51

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	4109	LEU
1	S	8101	MET
1	P	5017	SER
1	R	7013	THR
1	T	9042	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	9120	GLN

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Mol	Chain	Res	Type
1	T	9072	HIS
1	L	1050	GLN
1	Q	6128	GLN
1	K	173	HIS

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](#)

20 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	F	5201	-	33,33,33	1.10	2 (6%)	48,50,50	1.48	10 (20%)
2	FMN	C	2201	-	33,33,33	1.09	2 (6%)	48,50,50	1.41	7 (14%)
2	FMN	P	5201	-	33,33,33	1.05	2 (6%)	48,50,50	1.75	10 (20%)
2	FMN	Q	6201	-	33,33,33	1.11	2 (6%)	48,50,50	1.58	9 (18%)
2	FMN	L	1201	-	33,33,33	1.04	3 (9%)	48,50,50	1.54	12 (25%)
2	FMN	G	6201	-	33,33,33	1.14	3 (9%)	48,50,50	1.51	9 (18%)
2	FMN	D	3201	-	33,33,33	1.11	2 (6%)	48,50,50	1.53	9 (18%)
2	FMN	I	8201	-	33,33,33	1.13	2 (6%)	48,50,50	1.34	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	R	7201	-	33,33,33	1.11	2 (6%)	48,50,50	1.38	7 (14%)
2	FMN	S	8201	-	33,33,33	1.04	2 (6%)	48,50,50	1.91	13 (27%)
2	FMN	N	3201	-	33,33,33	1.12	3 (9%)	48,50,50	1.60	11 (22%)
2	FMN	K	301	-	33,33,33	1.02	2 (6%)	48,50,50	1.40	8 (16%)
2	FMN	H	7201	-	33,33,33	1.02	2 (6%)	48,50,50	1.68	11 (22%)
2	FMN	O	4201	-	33,33,33	1.06	2 (6%)	48,50,50	1.53	8 (16%)
2	FMN	B	1201	-	33,33,33	1.00	1 (3%)	48,50,50	1.69	10 (20%)
2	FMN	M	2201	-	33,33,33	1.07	2 (6%)	48,50,50	1.35	7 (14%)
2	FMN	T	9201	-	33,33,33	1.10	2 (6%)	48,50,50	1.38	8 (16%)
2	FMN	A	201	-	33,33,33	1.21	4 (12%)	48,50,50	1.37	7 (14%)
2	FMN	J	9201	-	33,33,33	1.19	3 (9%)	48,50,50	1.75	11 (22%)
2	FMN	E	4201	-	33,33,33	1.07	2 (6%)	48,50,50	1.59	11 (22%)

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	F	5201	-	-	6/18/18/18	0/3/3/3
2	FMN	C	2201	-	-	5/18/18/18	0/3/3/3
2	FMN	P	5201	-	-	4/18/18/18	0/3/3/3
2	FMN	Q	6201	-	-	2/18/18/18	0/3/3/3
2	FMN	L	1201	-	-	6/18/18/18	0/3/3/3
2	FMN	G	6201	-	-	2/18/18/18	0/3/3/3
2	FMN	D	3201	-	-	6/18/18/18	0/3/3/3
2	FMN	I	8201	-	-	2/18/18/18	0/3/3/3
2	FMN	R	7201	-	-	4/18/18/18	0/3/3/3
2	FMN	S	8201	-	-	5/18/18/18	0/3/3/3
2	FMN	N	3201	-	-	2/18/18/18	0/3/3/3
2	FMN	K	301	-	-	3/18/18/18	0/3/3/3
2	FMN	H	7201	-	-	6/18/18/18	0/3/3/3
2	FMN	O	4201	-	-	1/18/18/18	0/3/3/3
2	FMN	B	1201	-	-	4/18/18/18	0/3/3/3
2	FMN	M	2201	-	-	1/18/18/18	0/3/3/3
2	FMN	T	9201	-	-	3/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	A	201	-	-	0/18/18/18	0/3/3/3
2	FMN	J	9201	-	-	4/18/18/18	0/3/3/3
2	FMN	E	4201	-	-	4/18/18/18	0/3/3/3

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	6201	FMN	C4A-N5	3.78	1.38	1.30
2	D	3201	FMN	C4A-N5	3.69	1.38	1.30
2	B	1201	FMN	C4A-N5	3.66	1.38	1.30
2	C	2201	FMN	C4A-N5	3.58	1.38	1.30
2	N	3201	FMN	C4A-N5	3.52	1.38	1.30

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	8201	FMN	C5'-C4'-C3'	5.71	122.98	112.22
2	O	4201	FMN	C5'-C4'-C3'	-5.44	101.95	112.22
2	S	8201	FMN	C4'-C3'-C2'	-5.30	104.74	113.57
2	Q	6201	FMN	C5'-C4'-C3'	-5.11	102.58	112.22
2	P	5201	FMN	C4'-C3'-C2'	-4.90	105.42	113.57

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1201	FMN	C5'-O5'-P-O2P
2	B	1201	FMN	C5'-O5'-P-O3P
2	C	2201	FMN	O4'-C4'-C5'-O5'
2	C	2201	FMN	C5'-O5'-P-O1P
2	C	2201	FMN	C5'-O5'-P-O2P

There are no ring outliers.

17 monomers are involved in 46 short contacts:

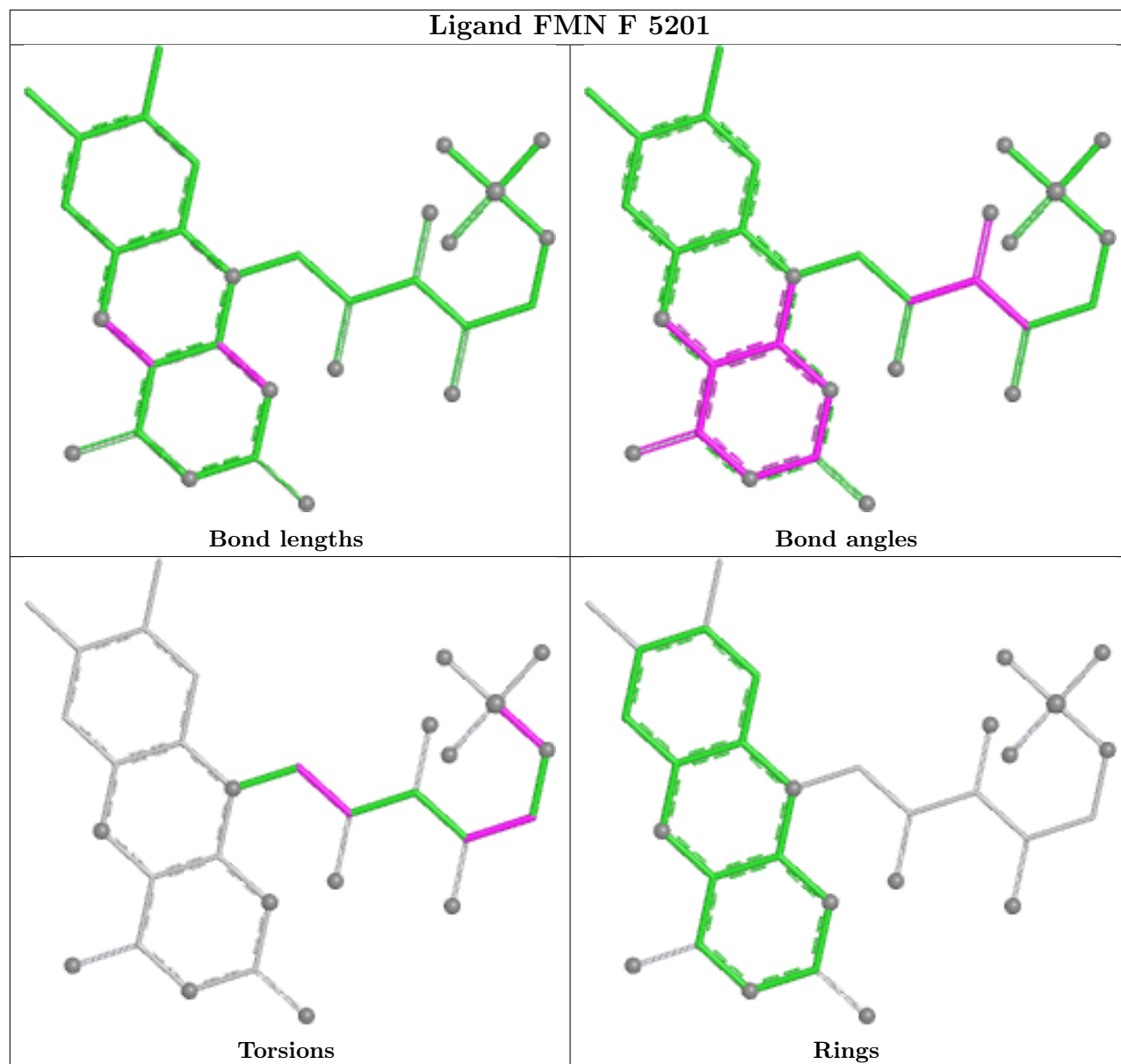
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	5201	FMN	2	0
2	C	2201	FMN	4	0
2	P	5201	FMN	3	0
2	Q	6201	FMN	1	0

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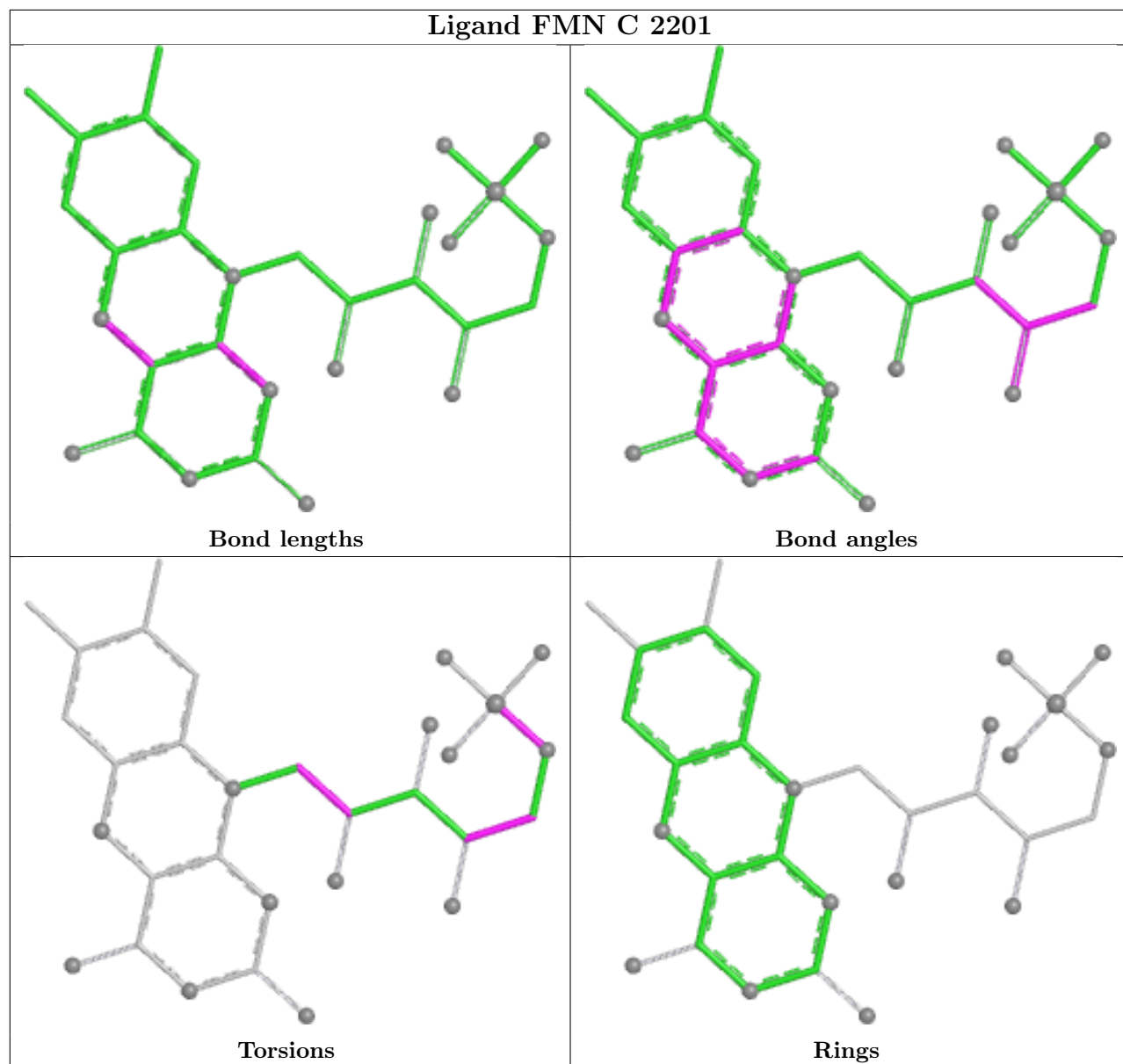
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1201	FMN	2	0
2	G	6201	FMN	2	0
2	D	3201	FMN	1	0
2	I	8201	FMN	3	0
2	R	7201	FMN	1	0
2	N	3201	FMN	2	0
2	H	7201	FMN	4	0
2	O	4201	FMN	4	0
2	M	2201	FMN	1	0
2	T	9201	FMN	10	0
2	A	201	FMN	2	0
2	J	9201	FMN	3	0
2	E	4201	FMN	1	0

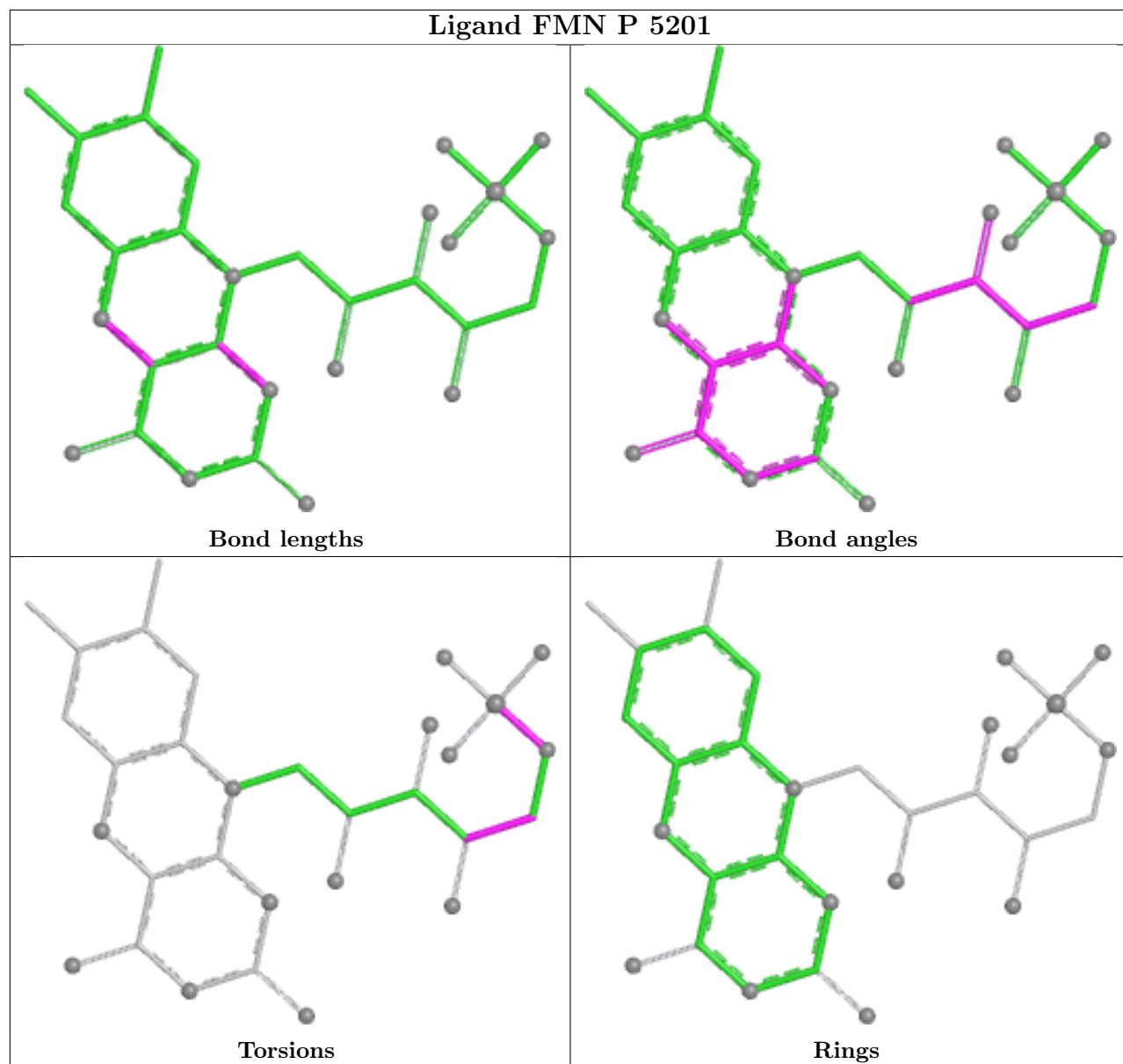
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



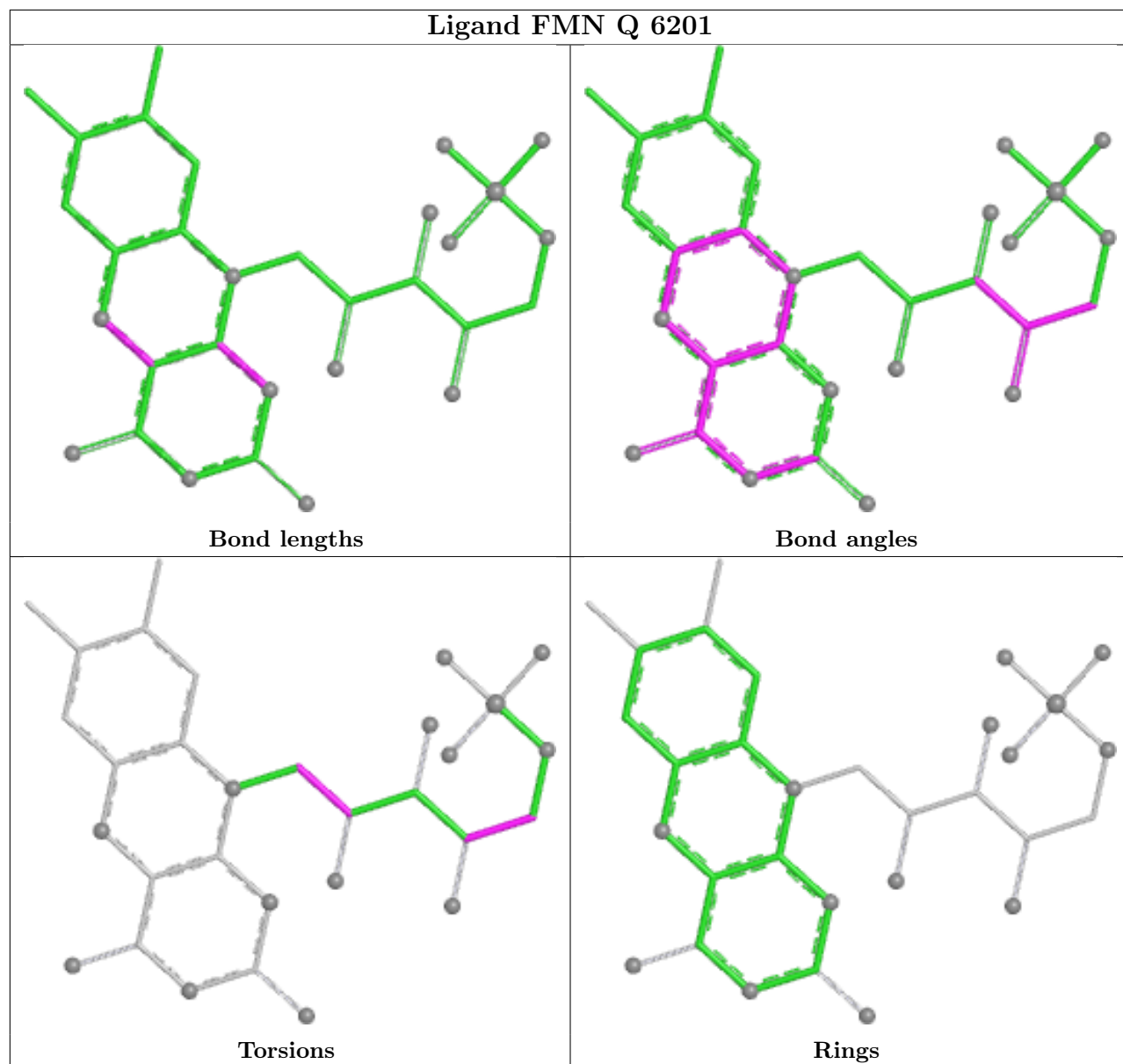
Ligand FMN C 2201



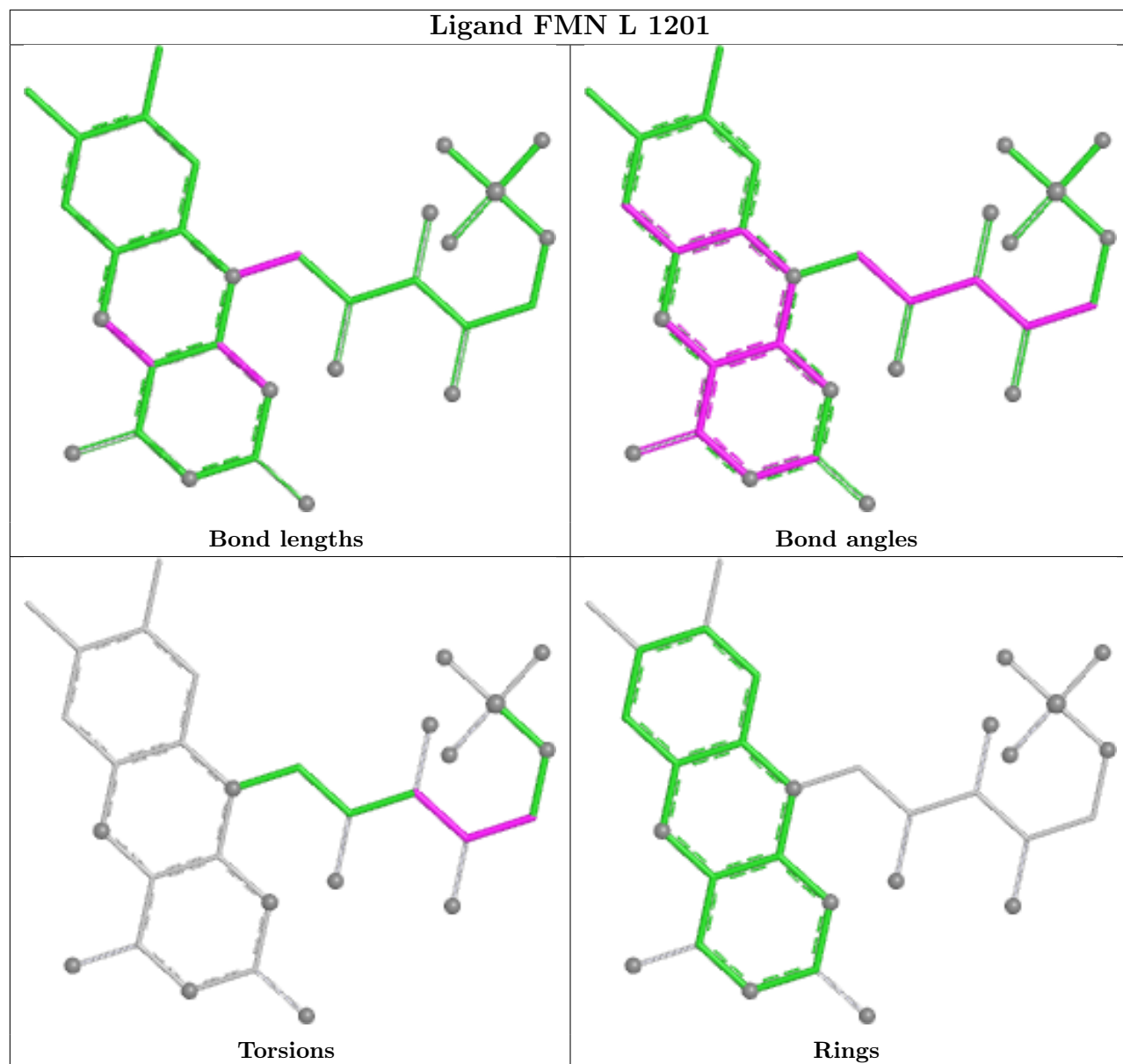
Ligand FMN P 5201



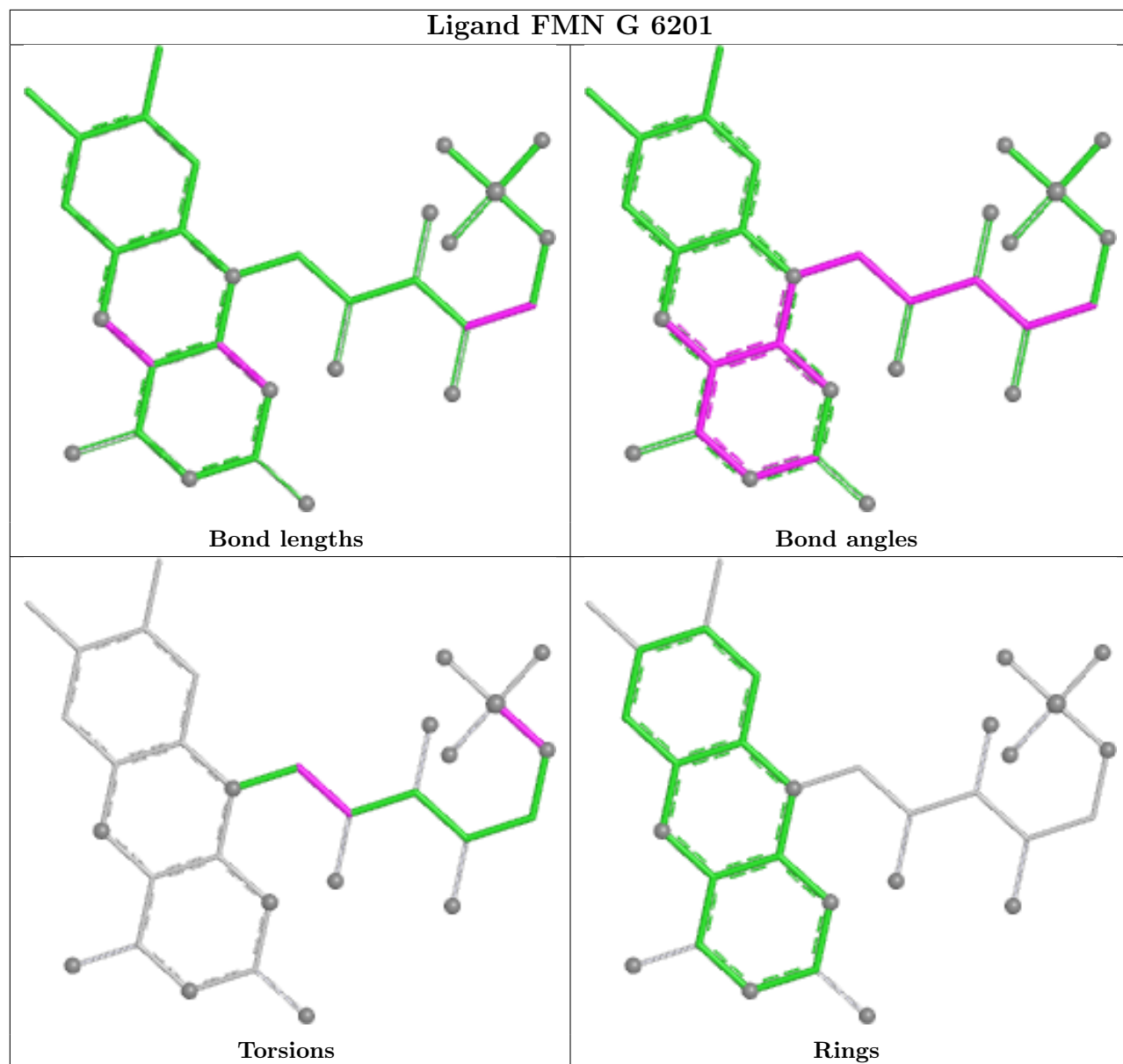
Ligand FMN Q 6201



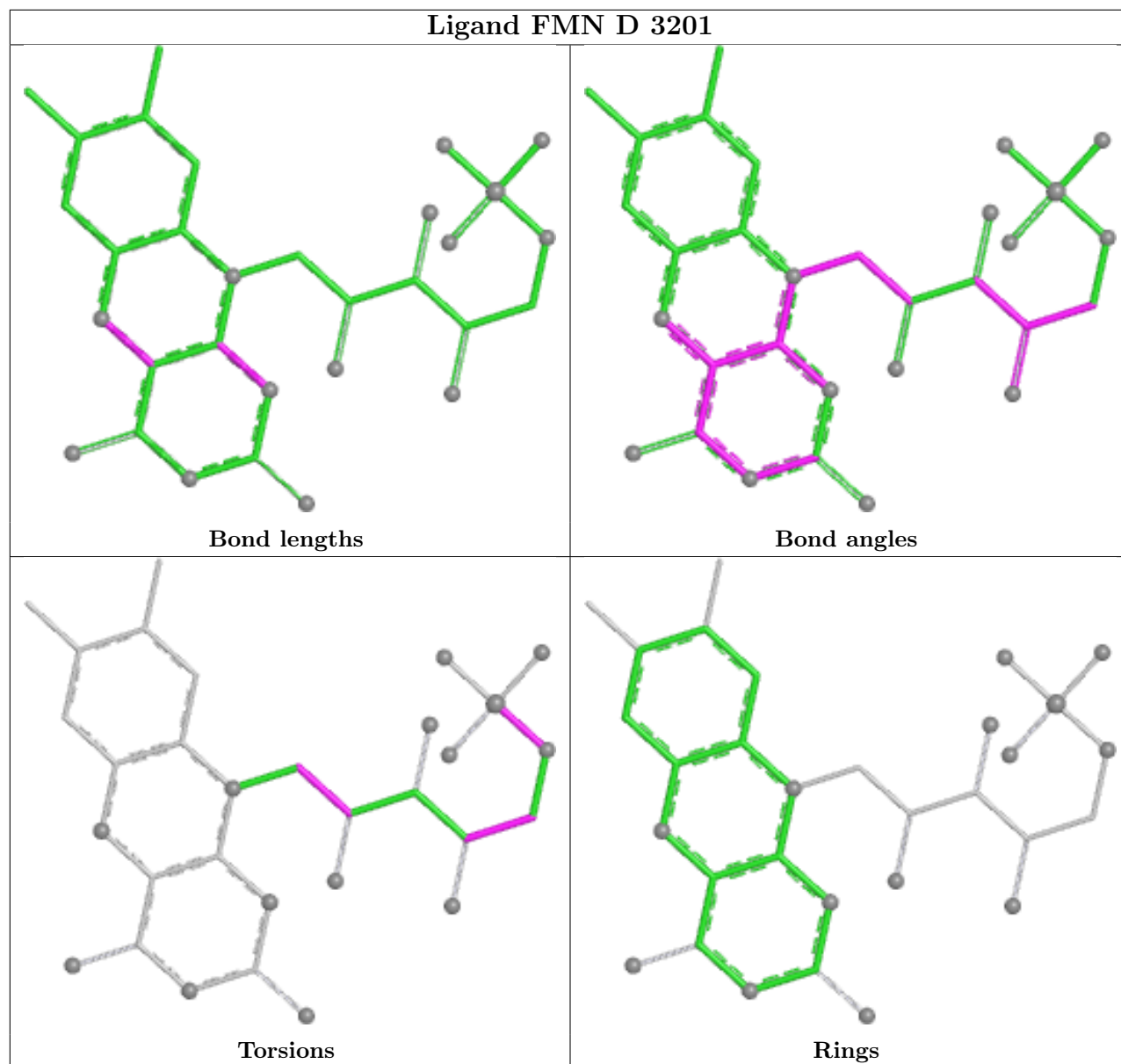
Ligand FMN L 1201

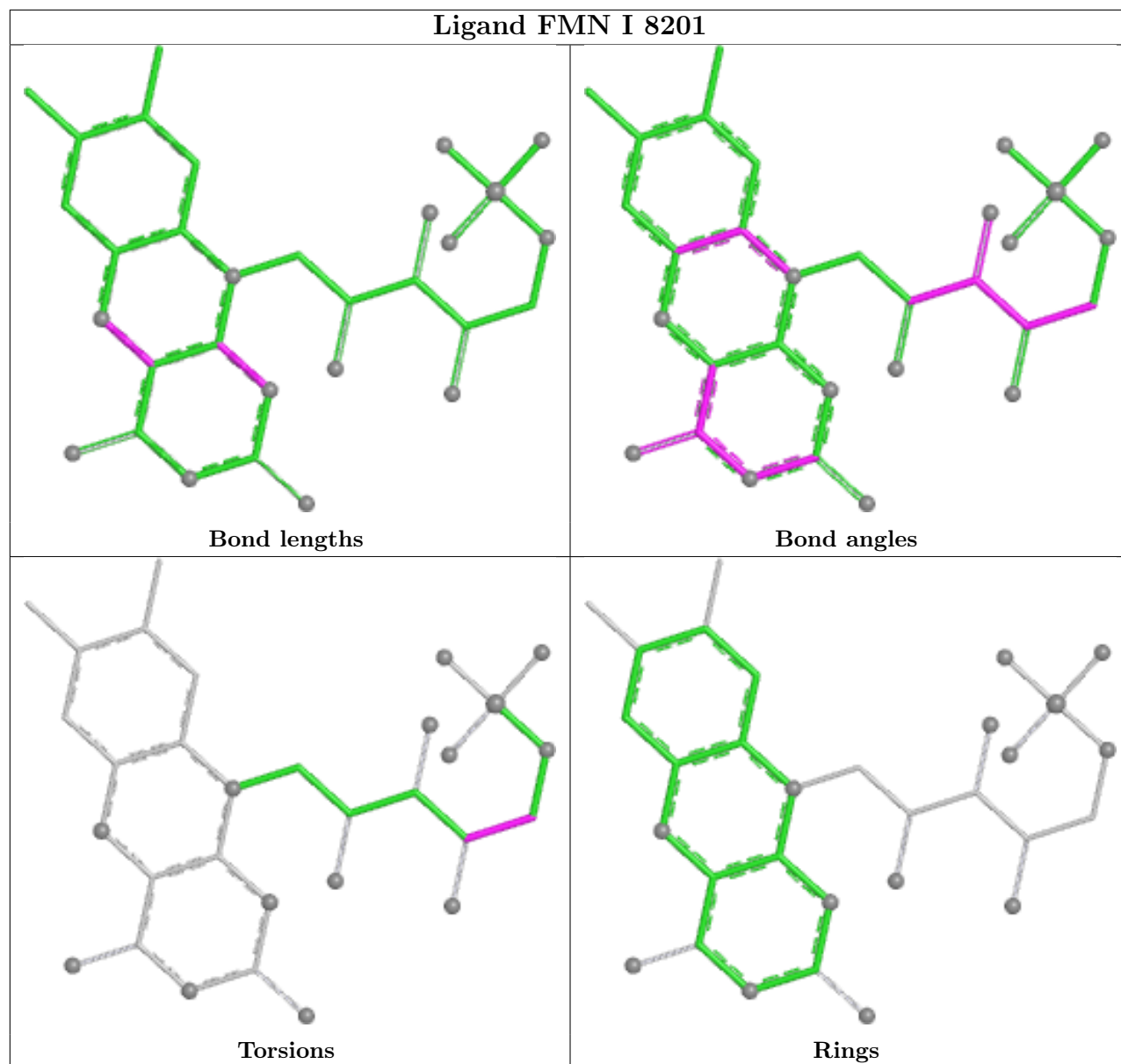


Ligand FMN G 6201

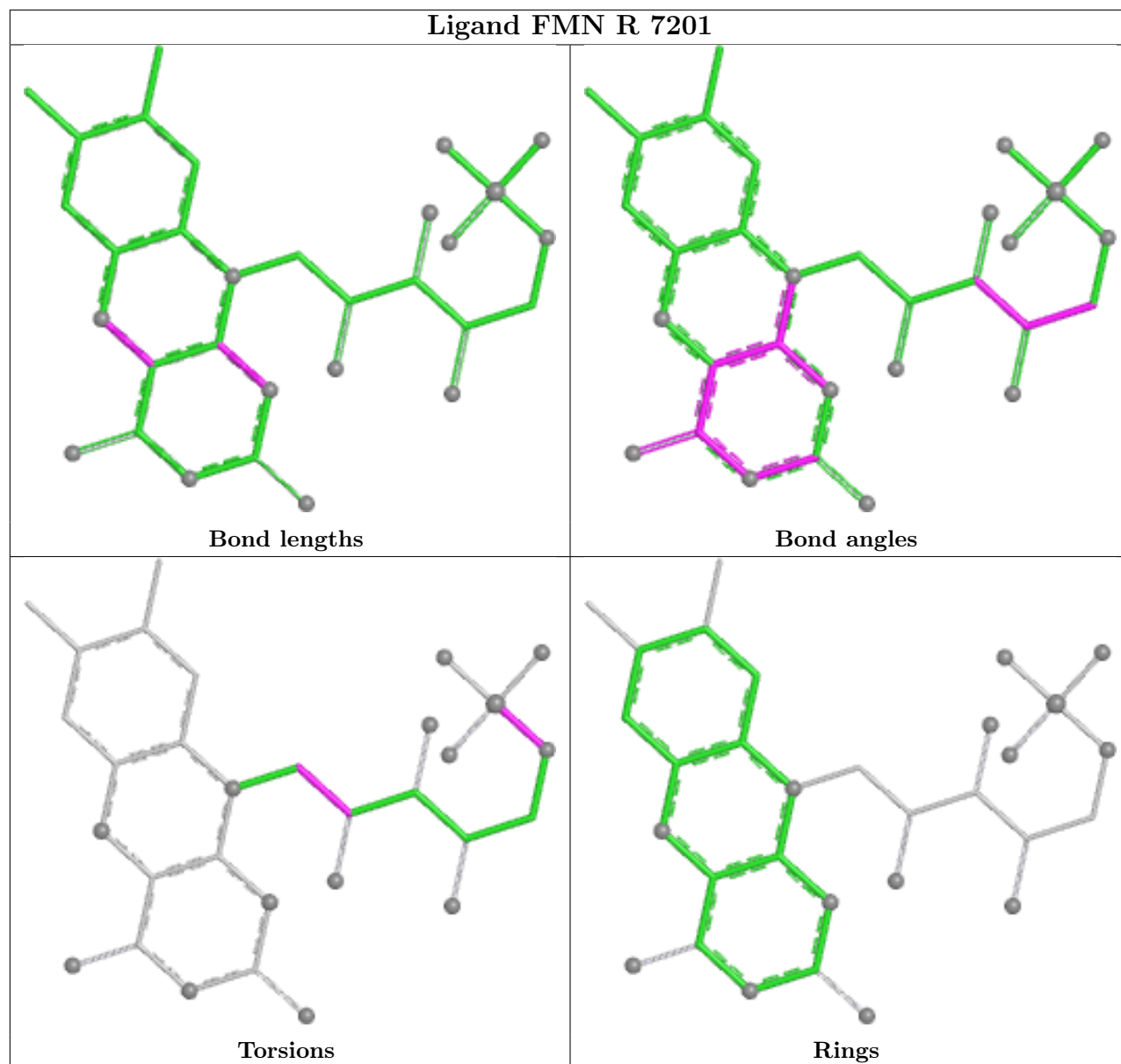


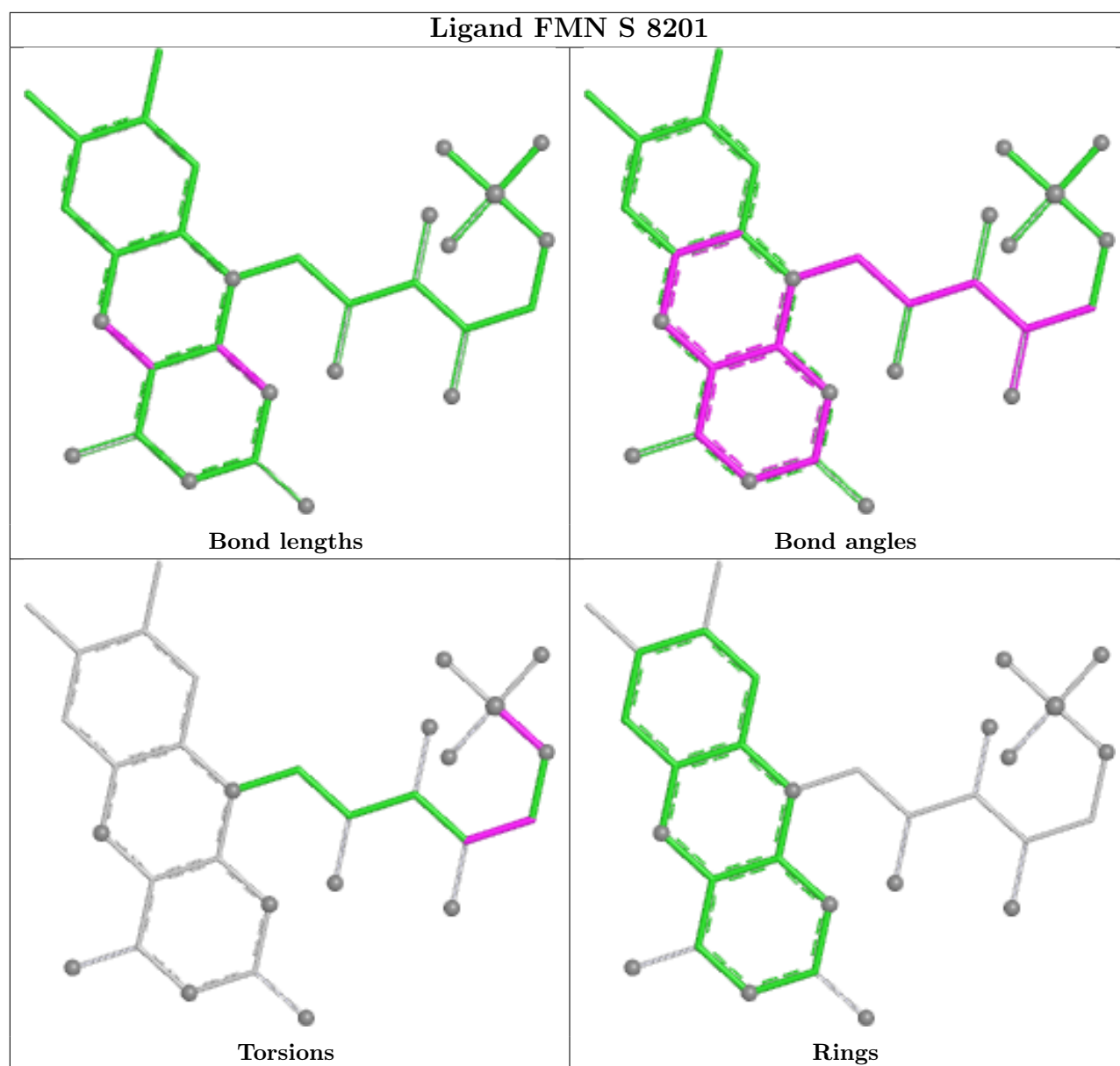
Ligand FMN D 3201



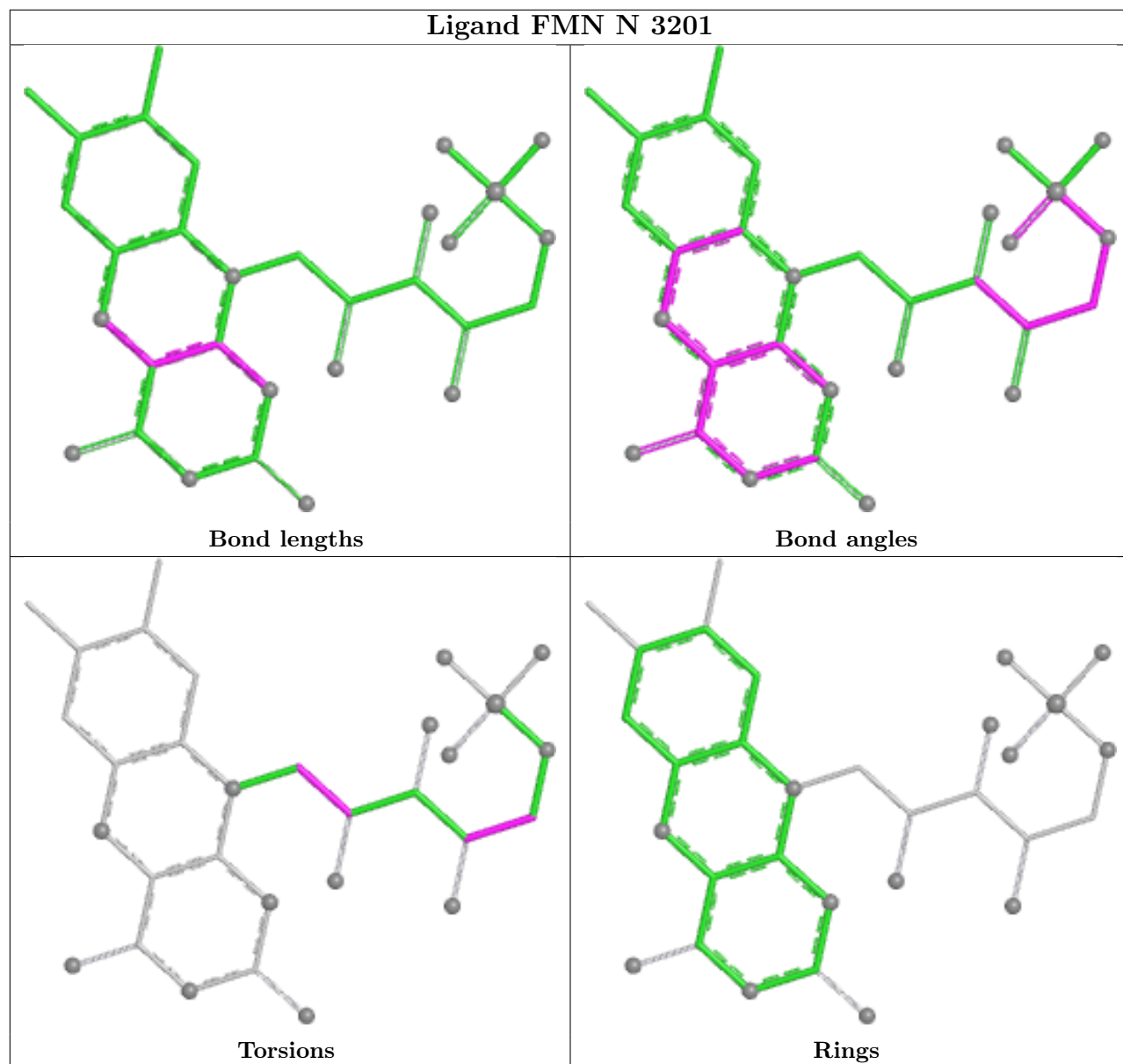


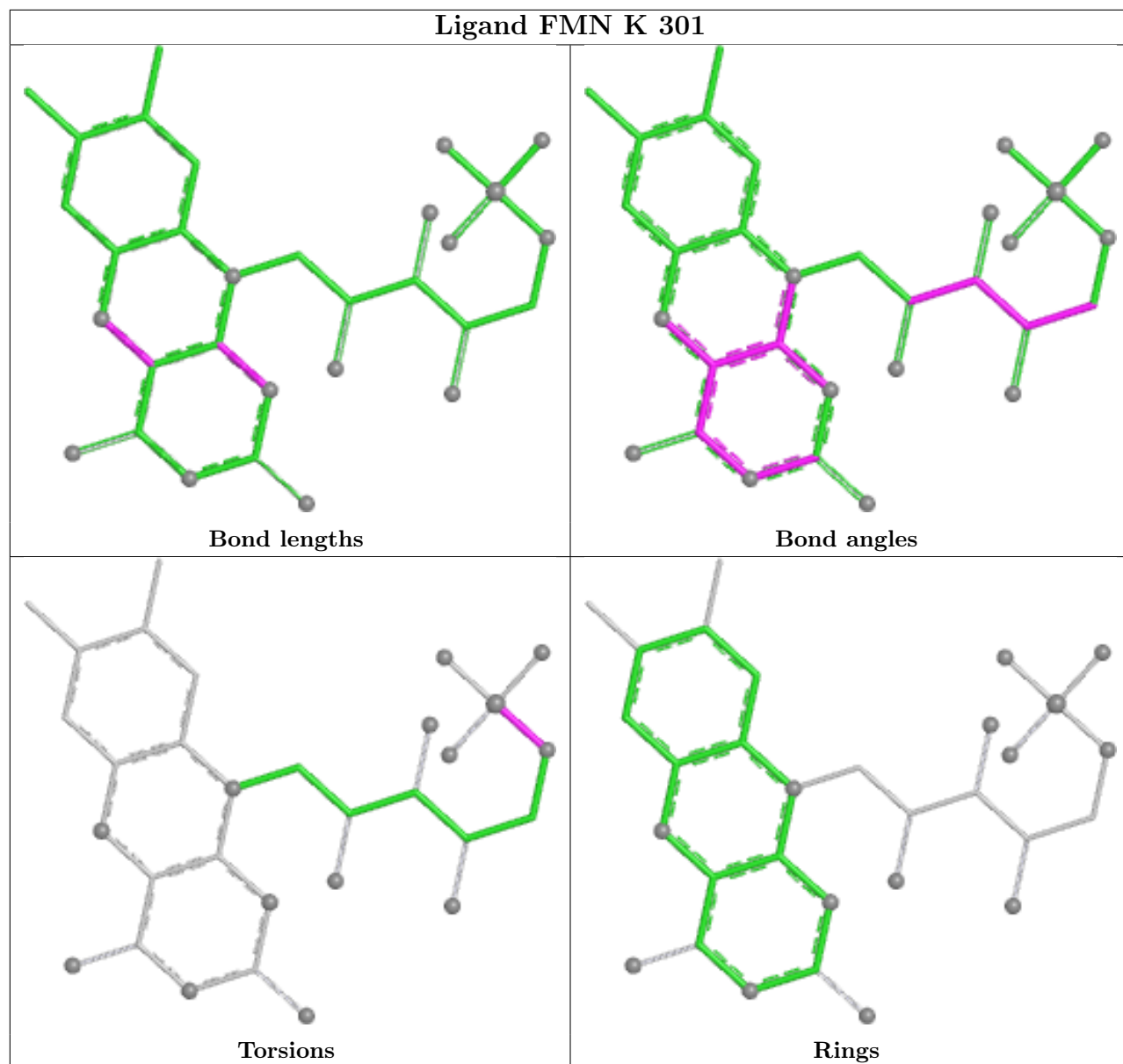
Ligand FMN R 7201



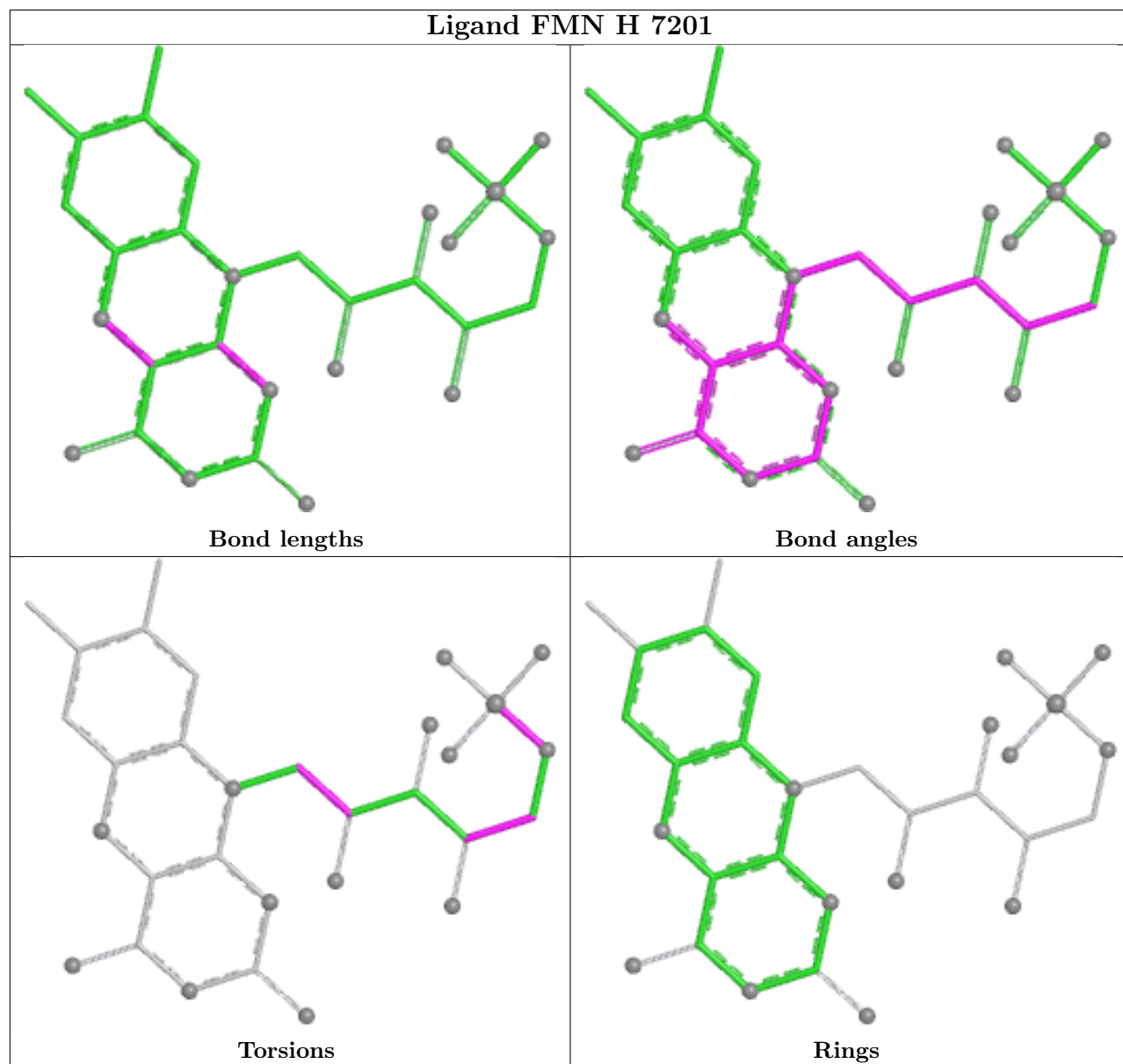


Ligand FMN N 3201

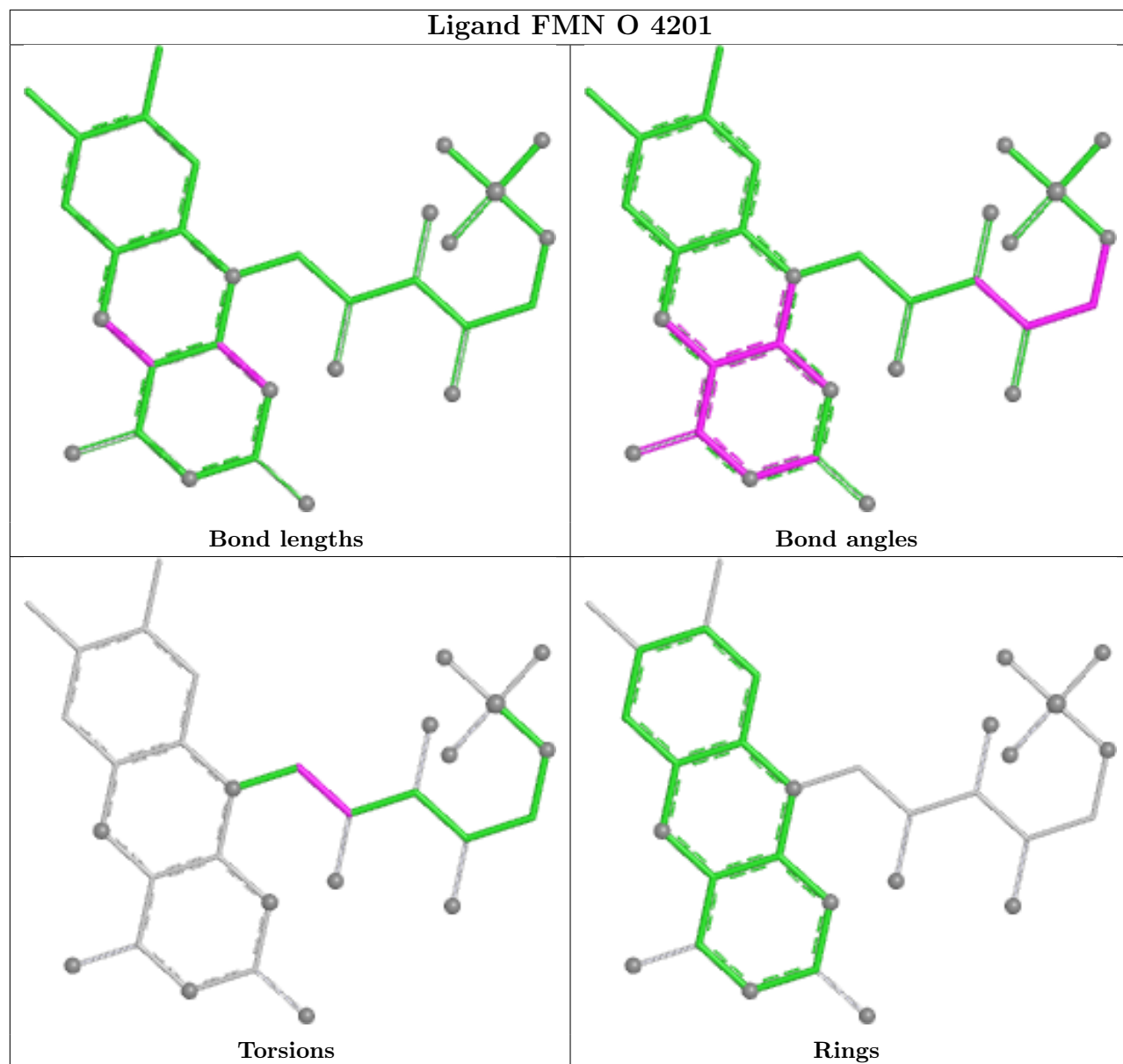




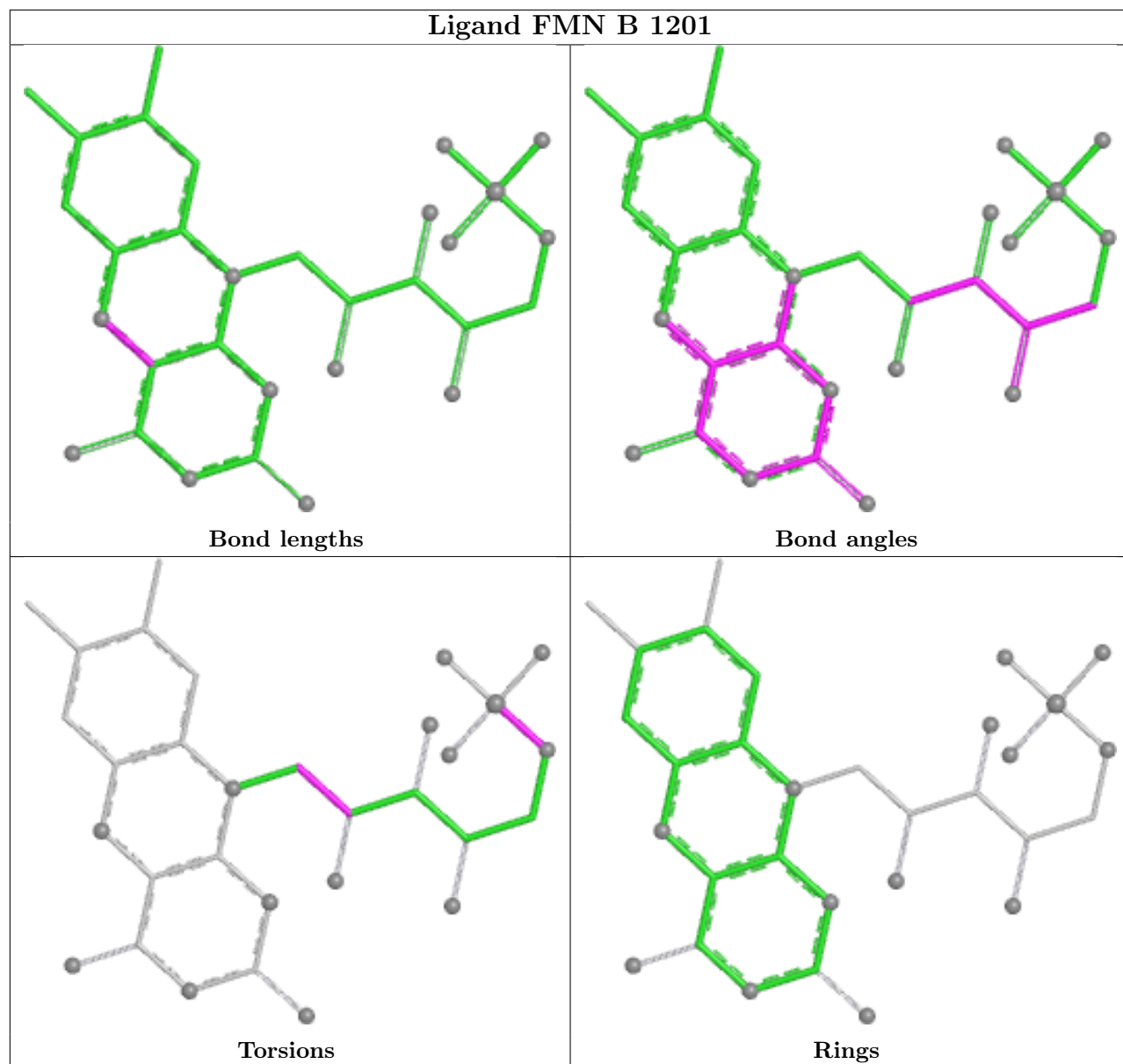
Ligand FMN H 7201



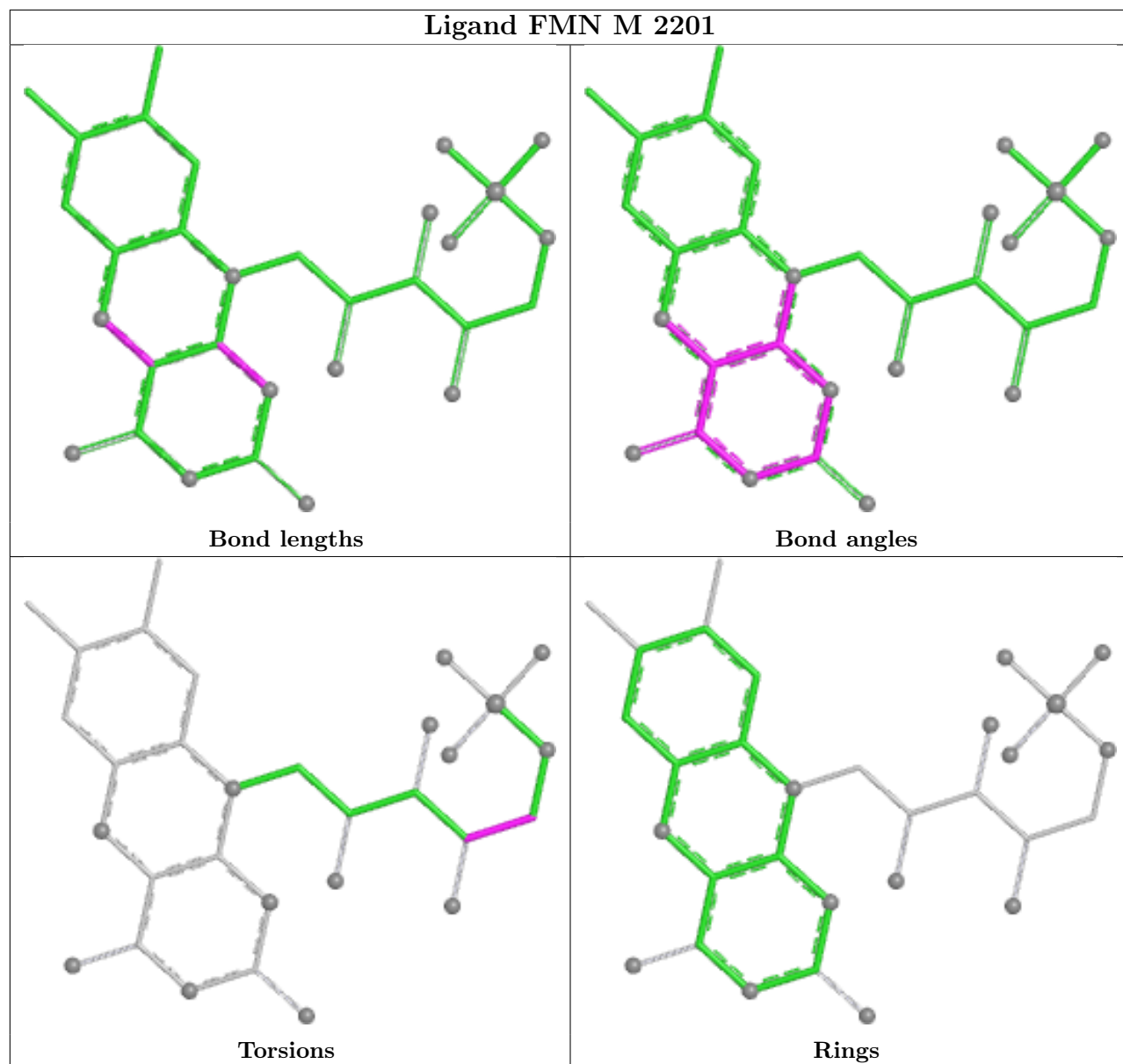
Ligand FMN O 4201



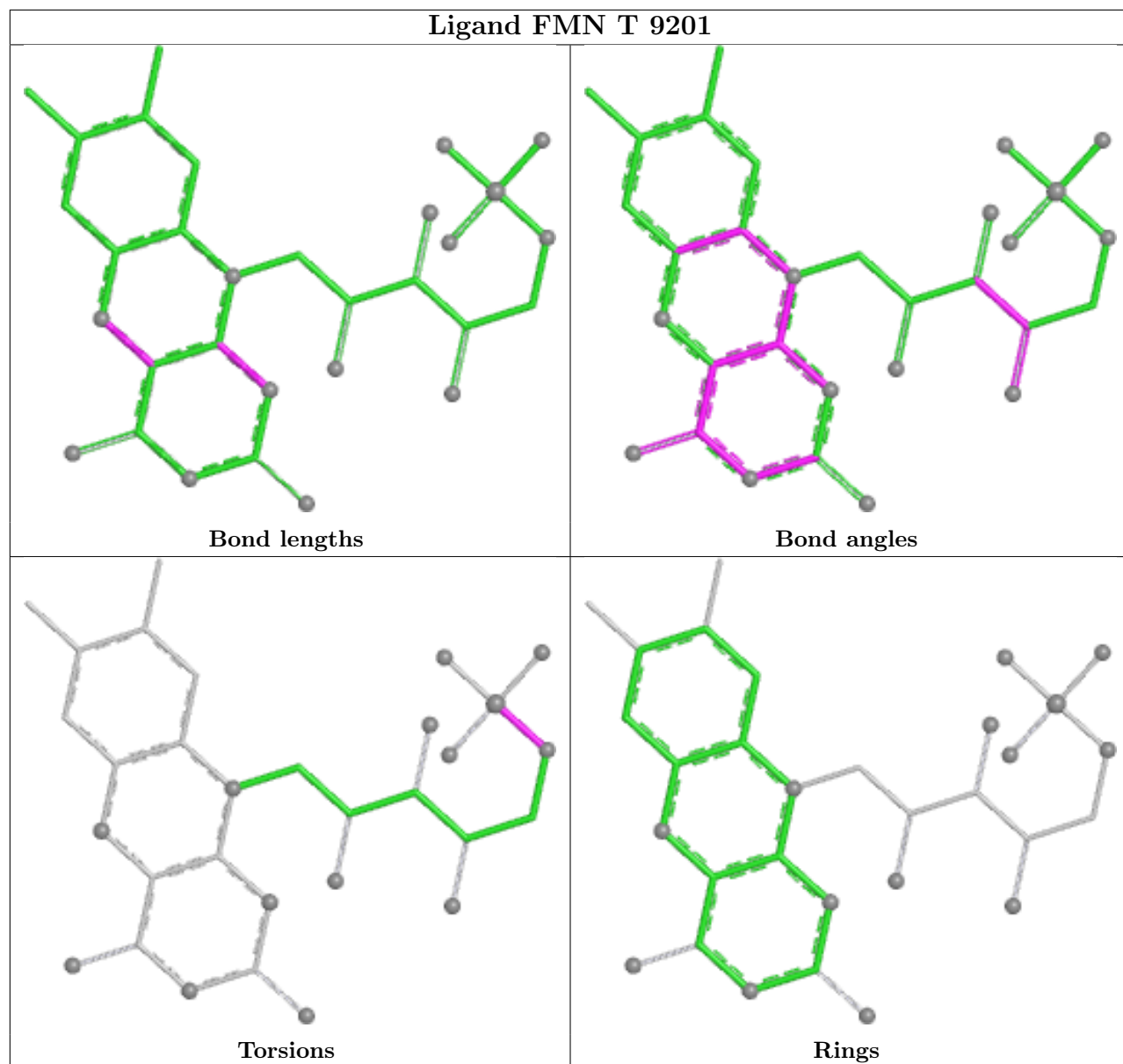
Ligand FMN B 1201

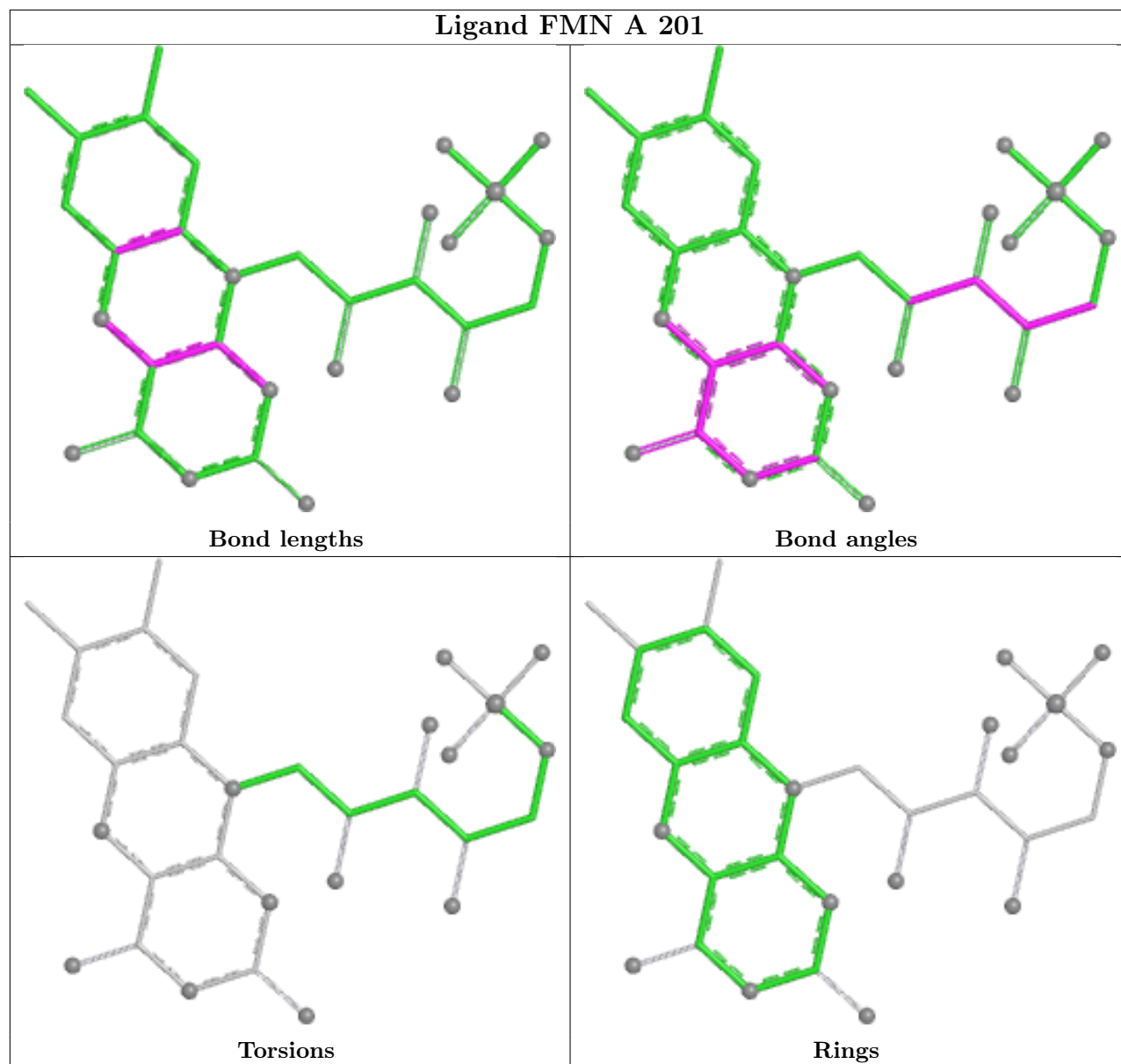


Ligand FMN M 2201

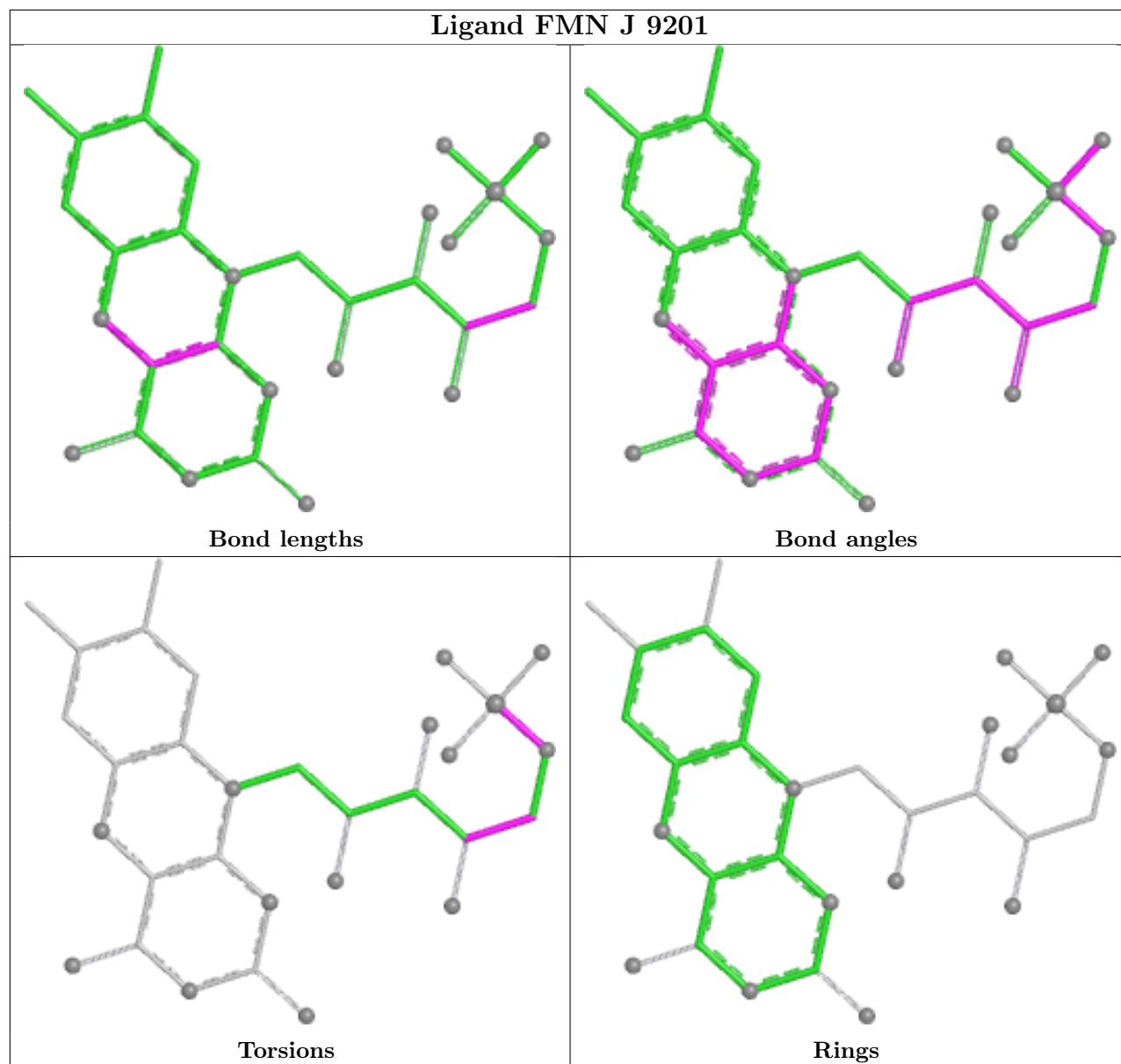


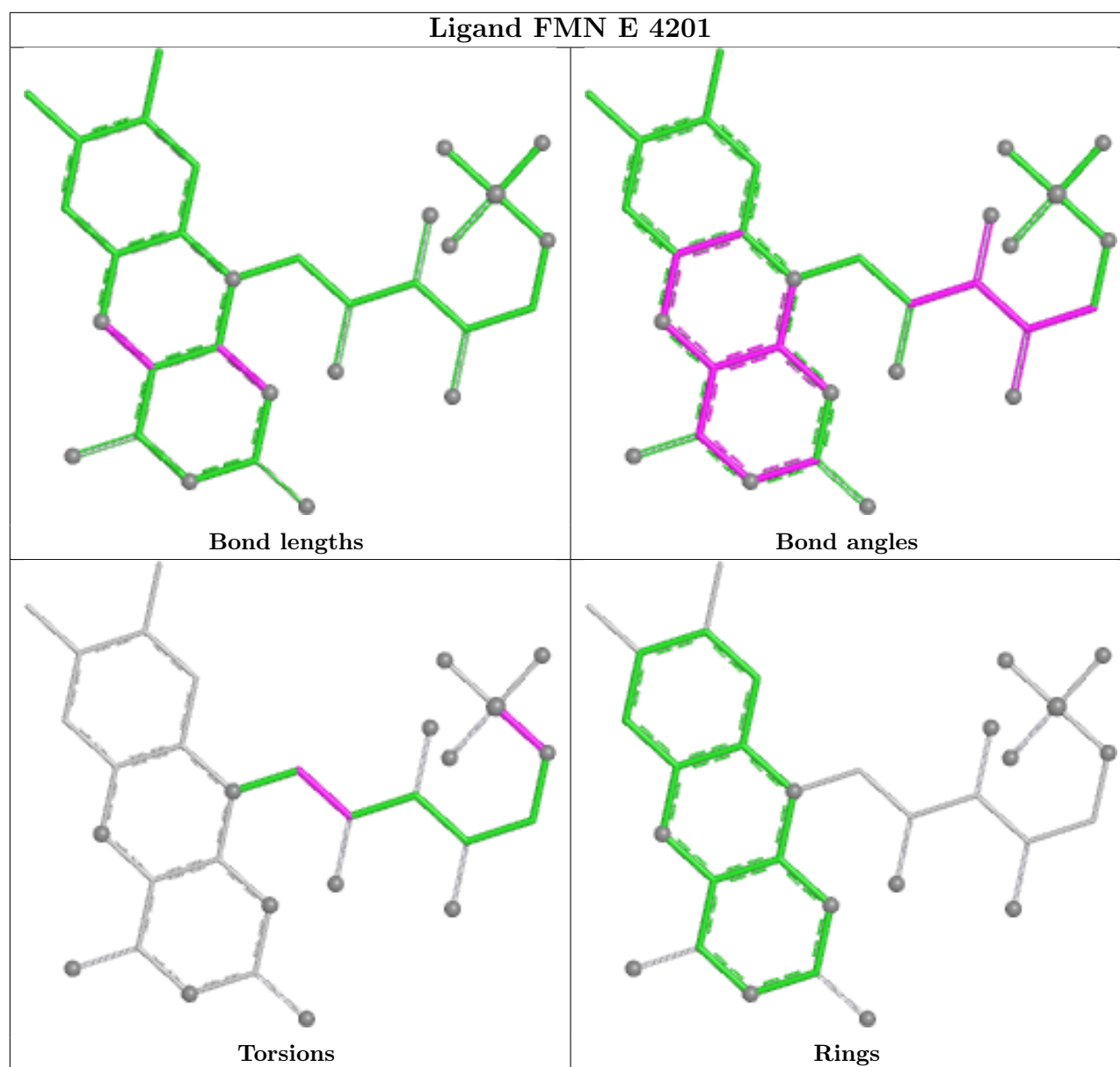
Ligand FMN T 9201





Ligand FMN J 9201





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	140/163 (85%)	0.09	5 (3%)	46	47	32, 48, 76, 93	0
1	B	141/163 (86%)	-0.07	4 (2%)	55	56	32, 44, 62, 79	0
1	C	140/163 (85%)	-0.03	0	100	100	35, 48, 72, 87	0
1	D	141/163 (86%)	-0.10	4 (2%)	55	56	33, 42, 64, 84	0
1	E	142/163 (87%)	-0.29	2 (1%)	73	74	29, 41, 59, 73	0
1	F	143/163 (87%)	-0.08	3 (2%)	63	64	32, 45, 65, 96	0
1	G	140/163 (85%)	-0.08	0	100	100	33, 45, 66, 73	0
1	H	141/163 (86%)	-0.06	3 (2%)	63	64	35, 47, 62, 80	0
1	I	141/163 (86%)	-0.16	1 (0%)	84	86	34, 44, 62, 73	0
1	J	141/163 (86%)	-0.15	2 (1%)	73	74	30, 43, 66, 84	0
1	K	140/163 (85%)	0.44	7 (5%)	34	33	37, 56, 75, 82	0
1	L	141/163 (86%)	0.62	10 (7%)	22	21	45, 60, 83, 95	0
1	M	140/163 (85%)	0.62	4 (2%)	53	55	45, 65, 88, 97	0
1	N	140/163 (85%)	0.32	4 (2%)	53	55	40, 55, 73, 85	0
1	O	140/163 (85%)	0.87	9 (6%)	25	24	46, 66, 88, 99	0
1	P	141/163 (86%)	0.64	8 (5%)	29	29	43, 66, 85, 118	0
1	Q	140/163 (85%)	-0.09	2 (1%)	73	74	38, 49, 62, 74	0
1	R	140/163 (85%)	0.32	4 (2%)	53	55	41, 57, 79, 87	0
1	S	141/163 (86%)	0.31	9 (6%)	25	24	38, 56, 83, 106	0
1	T	140/163 (85%)	0.41	2 (1%)	73	74	42, 57, 82, 101	0
All	All	2813/3260 (86%)	0.18	83 (2%)	52	54	29, 51, 79, 118	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	1000	HIS	4.9
1	K	101	MET	4.8
1	D	3140	SER	4.1
1	O	4001	MET	4.1
1	O	4018	TYR	4.0

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($\text{\AA}^2$)	Q<0.9
2	FMN	O	4201	31/31	0.81	0.14	74,79,106,118	0
2	FMN	P	5201	31/31	0.81	0.13	69,75,111,119	0
2	FMN	M	2201	31/31	0.86	0.15	60,68,104,115	0
2	FMN	T	9201	31/31	0.87	0.11	62,76,90,93	0
2	FMN	K	301	31/31	0.88	0.10	57,67,112,121	0
2	FMN	D	3201	31/31	0.89	0.10	40,48,87,93	0
2	FMN	F	5201	31/31	0.89	0.10	36,49,88,98	0
2	FMN	G	6201	31/31	0.89	0.11	40,45,92,97	0
2	FMN	R	7201	31/31	0.89	0.12	49,59,89,100	0
2	FMN	C	2201	31/31	0.89	0.11	44,52,85,95	0
2	FMN	L	1201	31/31	0.90	0.12	48,58,95,115	0
2	FMN	S	8201	31/31	0.90	0.11	43,55,94,101	0
2	FMN	I	8201	31/31	0.90	0.11	35,44,92,108	0
2	FMN	J	9201	31/31	0.91	0.10	36,42,68,70	0
2	FMN	E	4201	31/31	0.91	0.10	31,41,79,86	0
2	FMN	A	201	31/31	0.91	0.10	44,52,87,90	0
2	FMN	Q	6201	31/31	0.92	0.09	41,45,76,79	0
2	FMN	N	3201	31/31	0.92	0.09	44,51,71,74	0
2	FMN	H	7201	31/31	0.92	0.09	38,49,86,99	0

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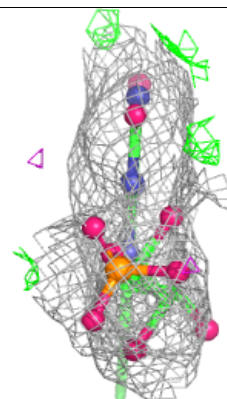
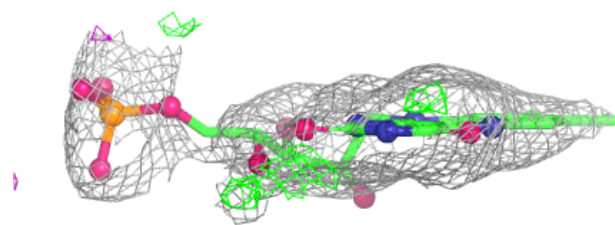
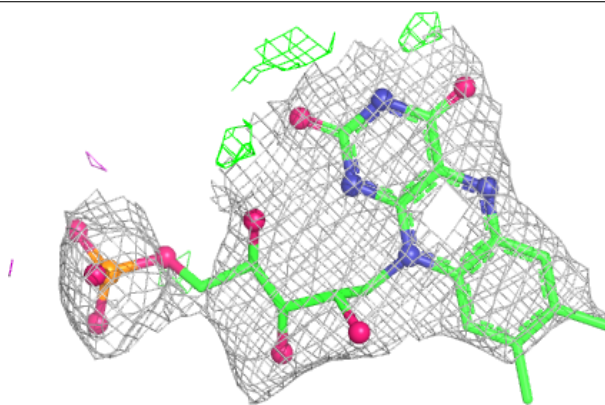
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMN	B	1201	31/31	0.92	0.09	35,43,86,103	0

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.

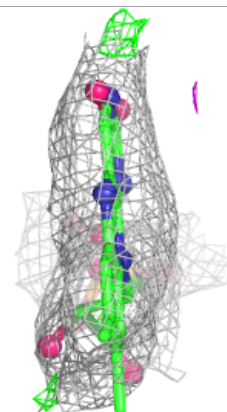
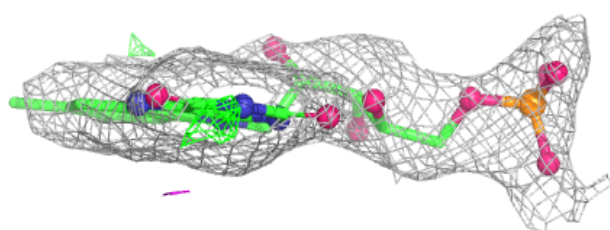
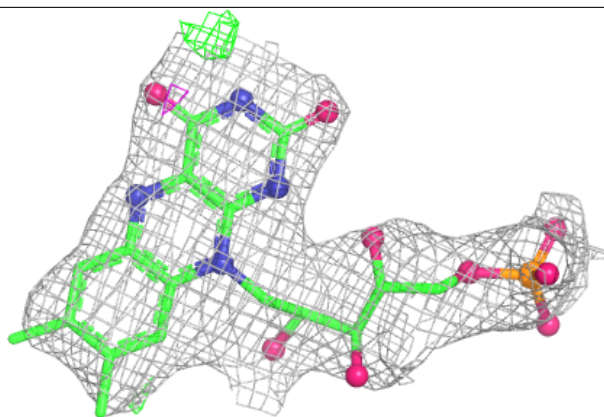
Electron density around FMN O 4201:

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

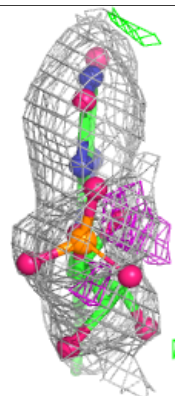
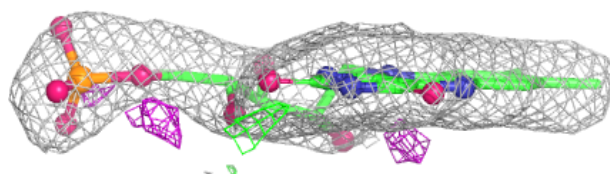
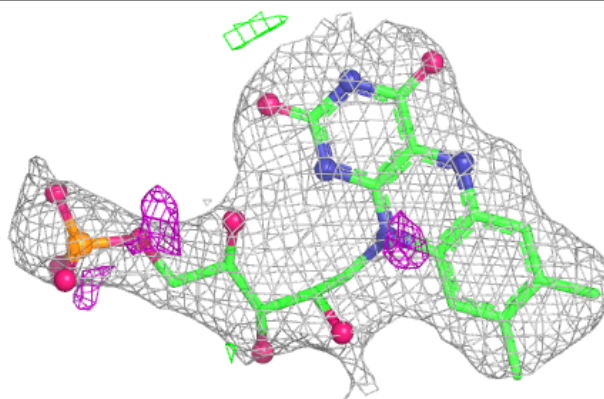


Electron density around FMN P 5201:

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

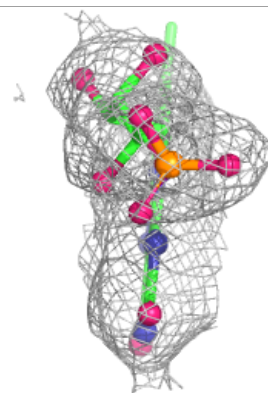
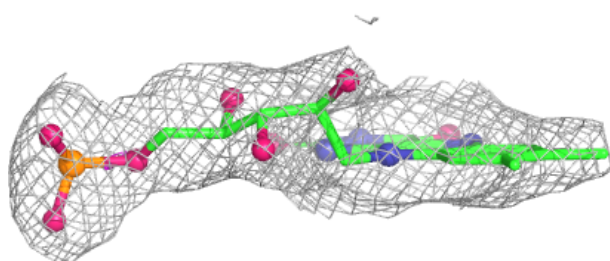
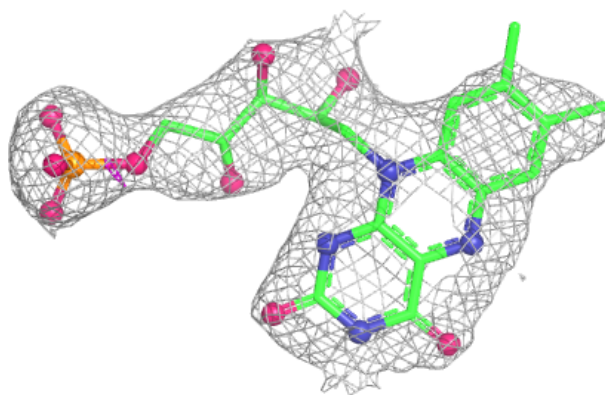
**Electron density around FMN M 2201:**

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

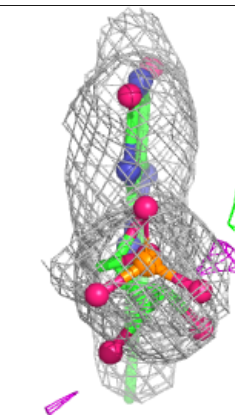
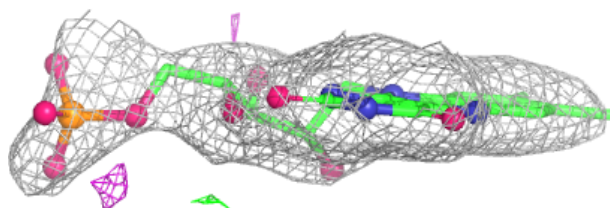
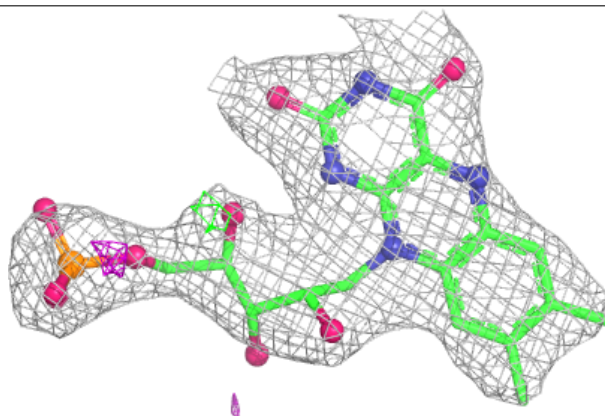


Electron density around FMN T 9201:

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

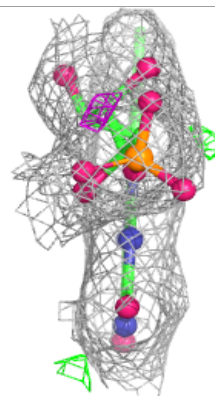
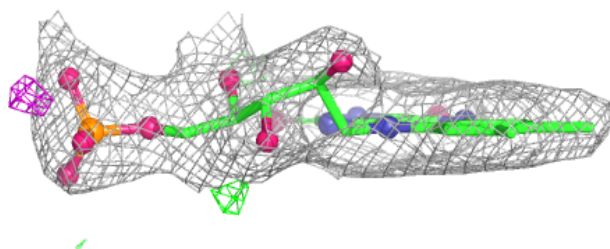
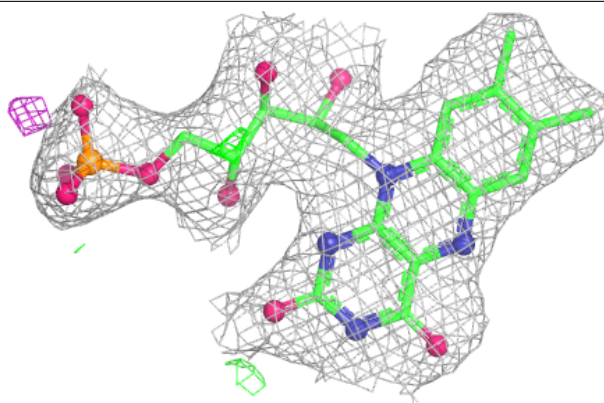
**Electron density around FMN K 301:**

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and green (positive)

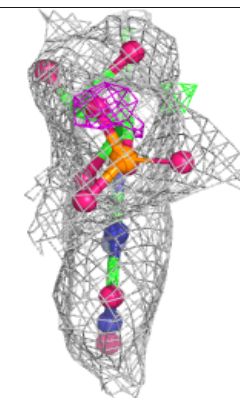
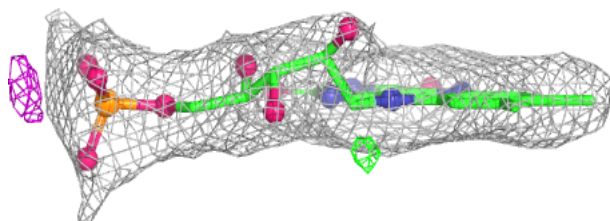
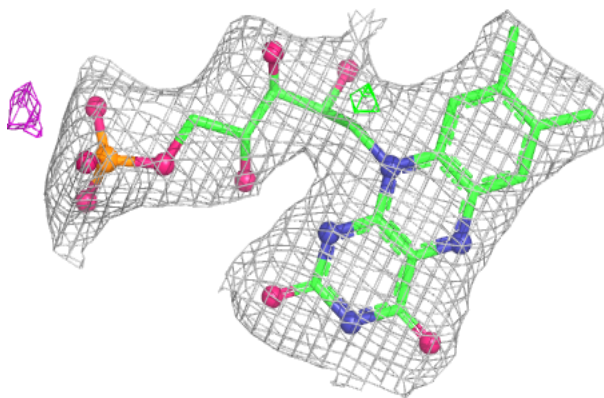


Electron density around FMN D 3201:

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

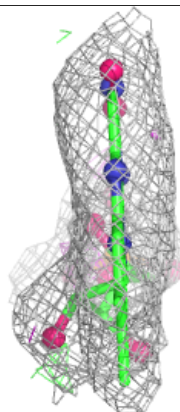
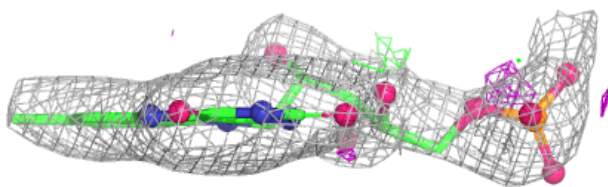
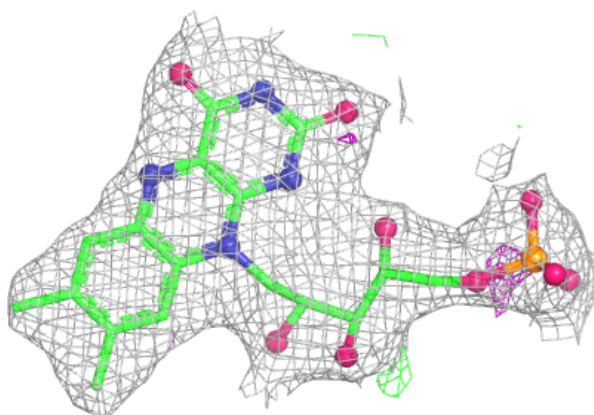
**Electron density around FMN F 5201:**

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

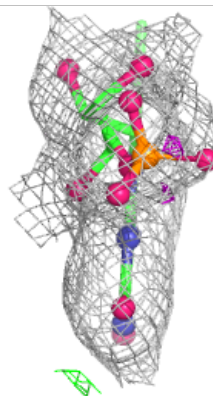
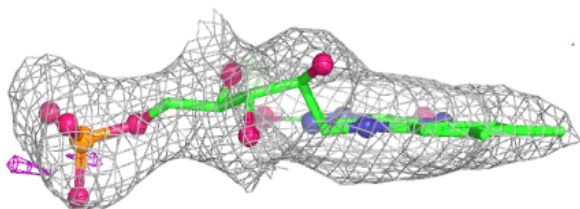
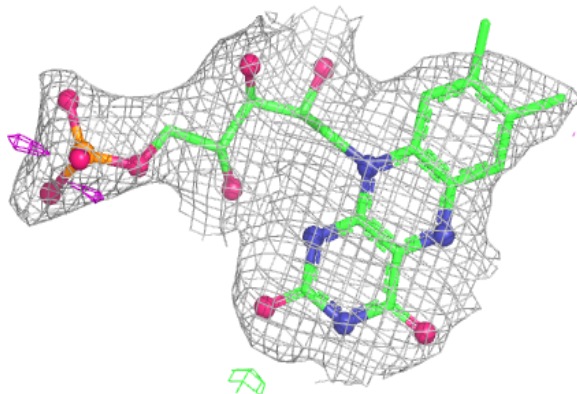


Electron density around FMN G 6201:

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

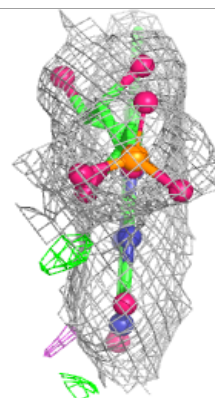
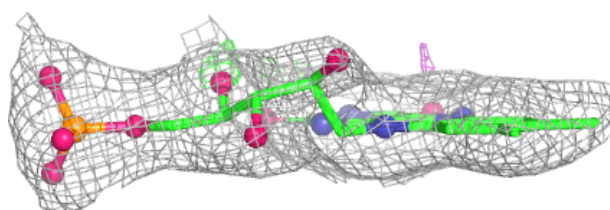
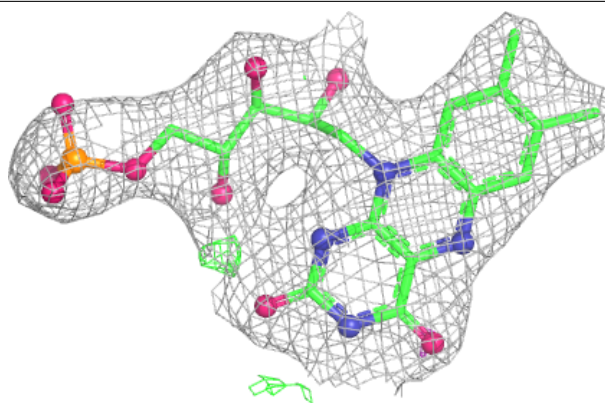
**Electron density around FMN R 7201:**

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

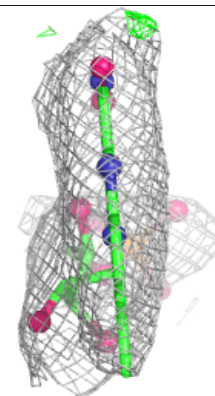
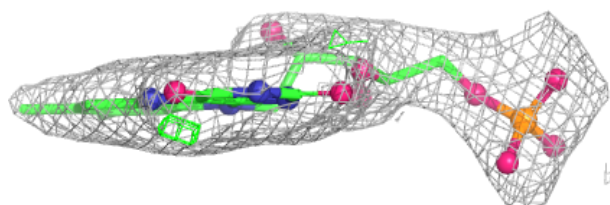
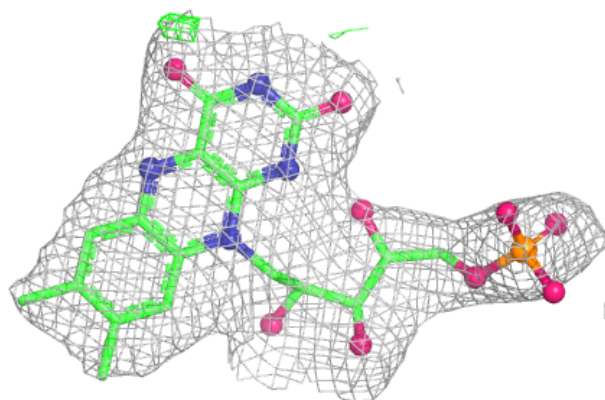


Electron density around FMN C 2201:

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

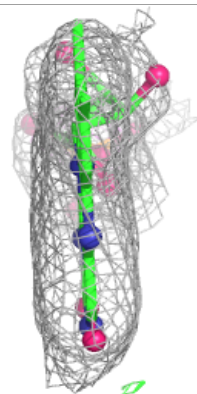
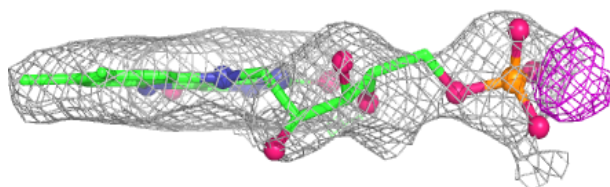
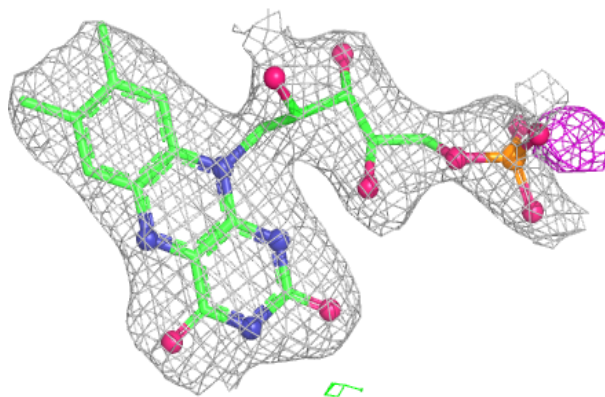
**Electron density around FMN L 1201:**

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

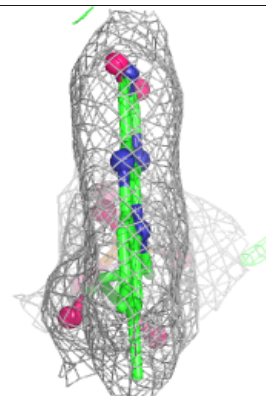
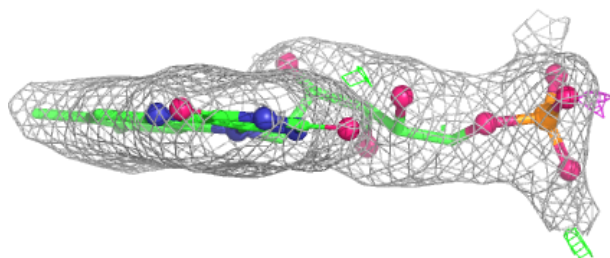
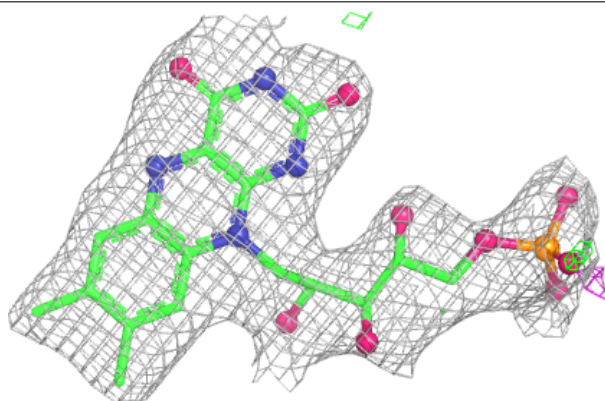


Electron density around FMN S 8201:

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

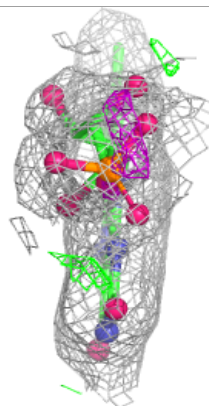
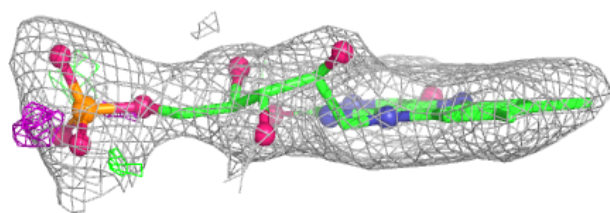
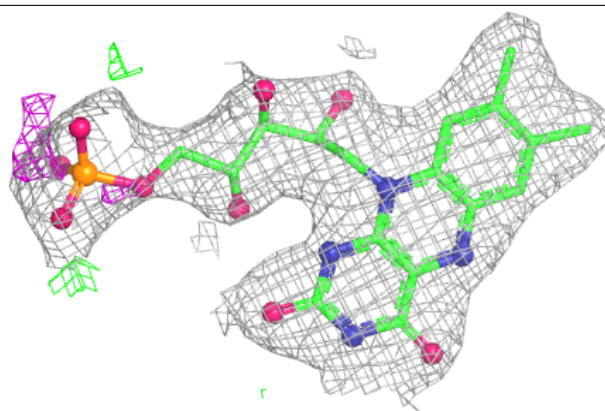
**Electron density around FMN I 8201:**

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

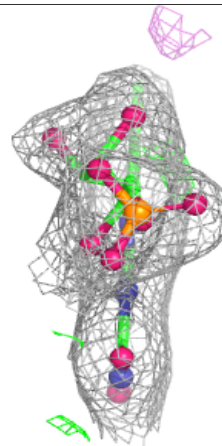
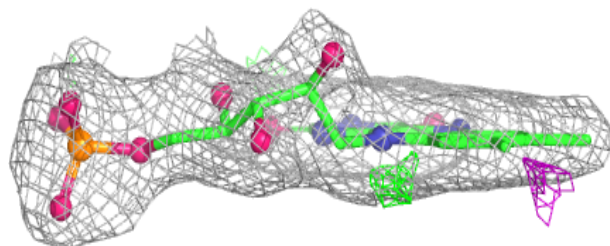
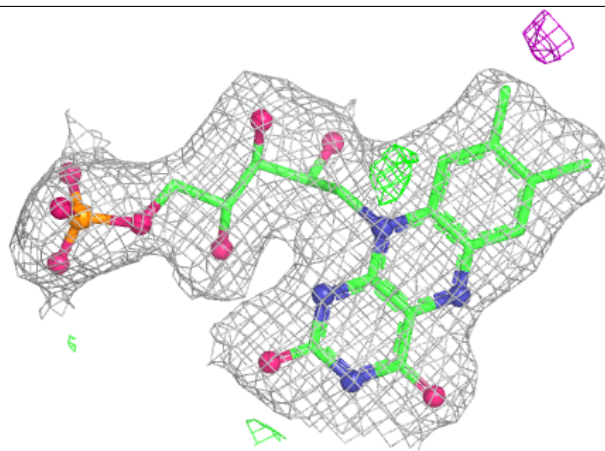


Electron density around FMN J 9201:

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

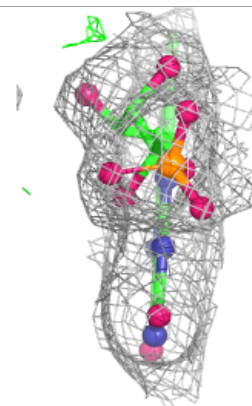
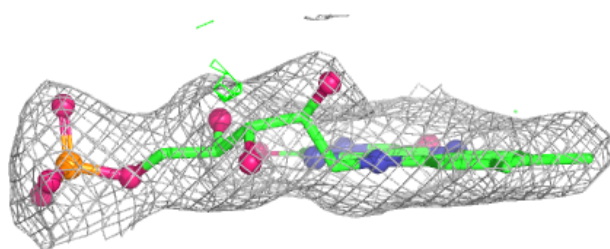
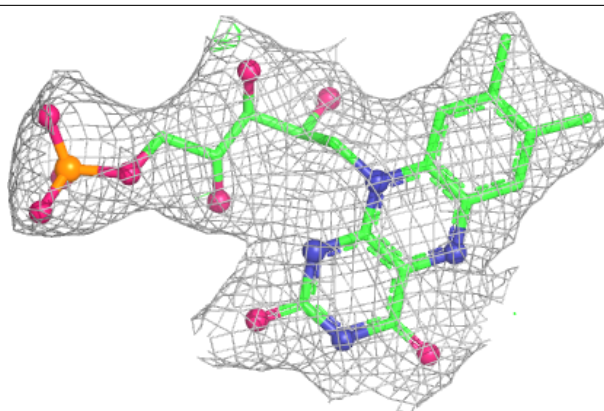
**Electron density around FMN E 4201:**

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

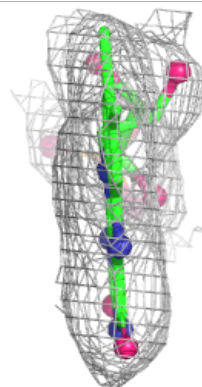
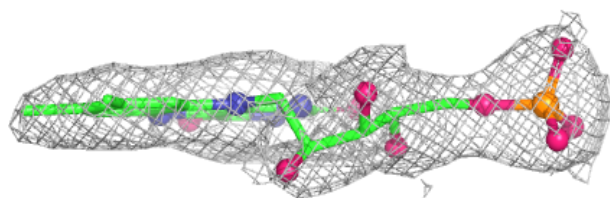
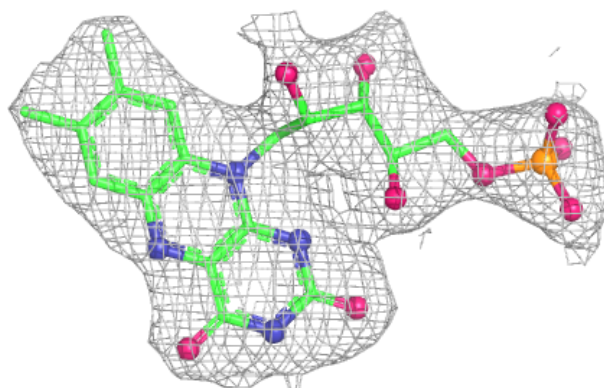


Electron density around FMN A 201:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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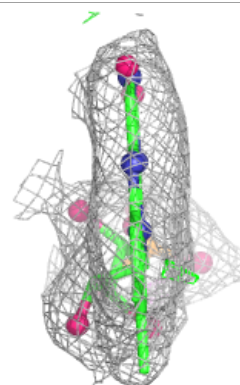
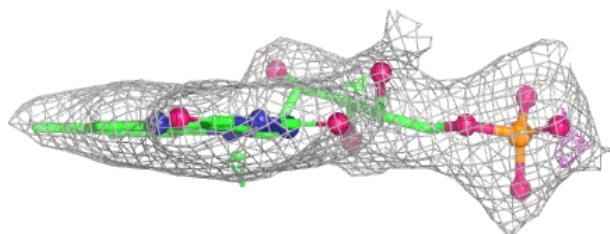
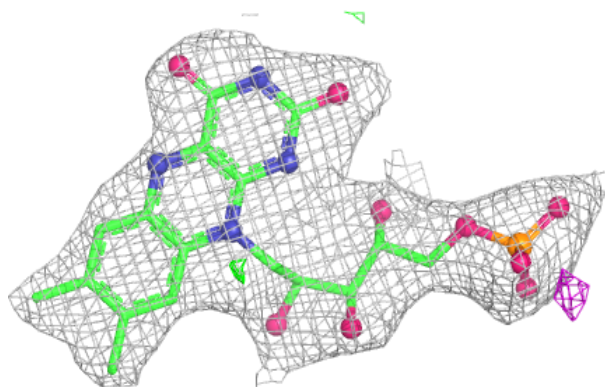
**Electron density around FMN Q 6201:**

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

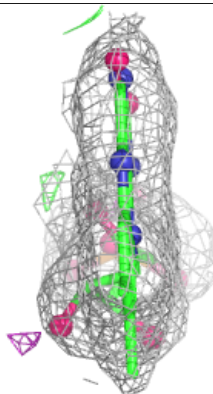
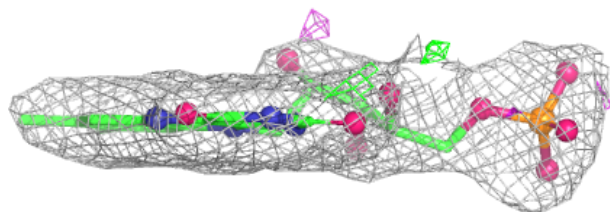
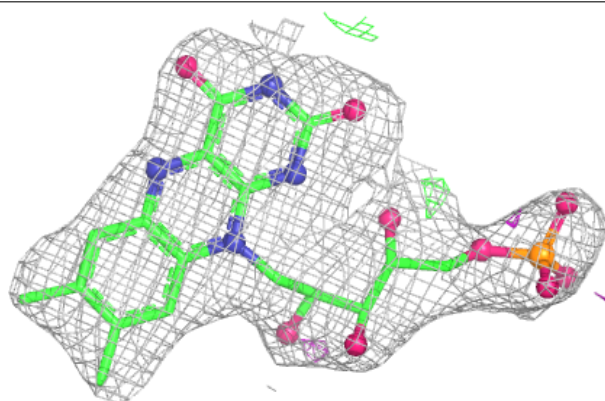


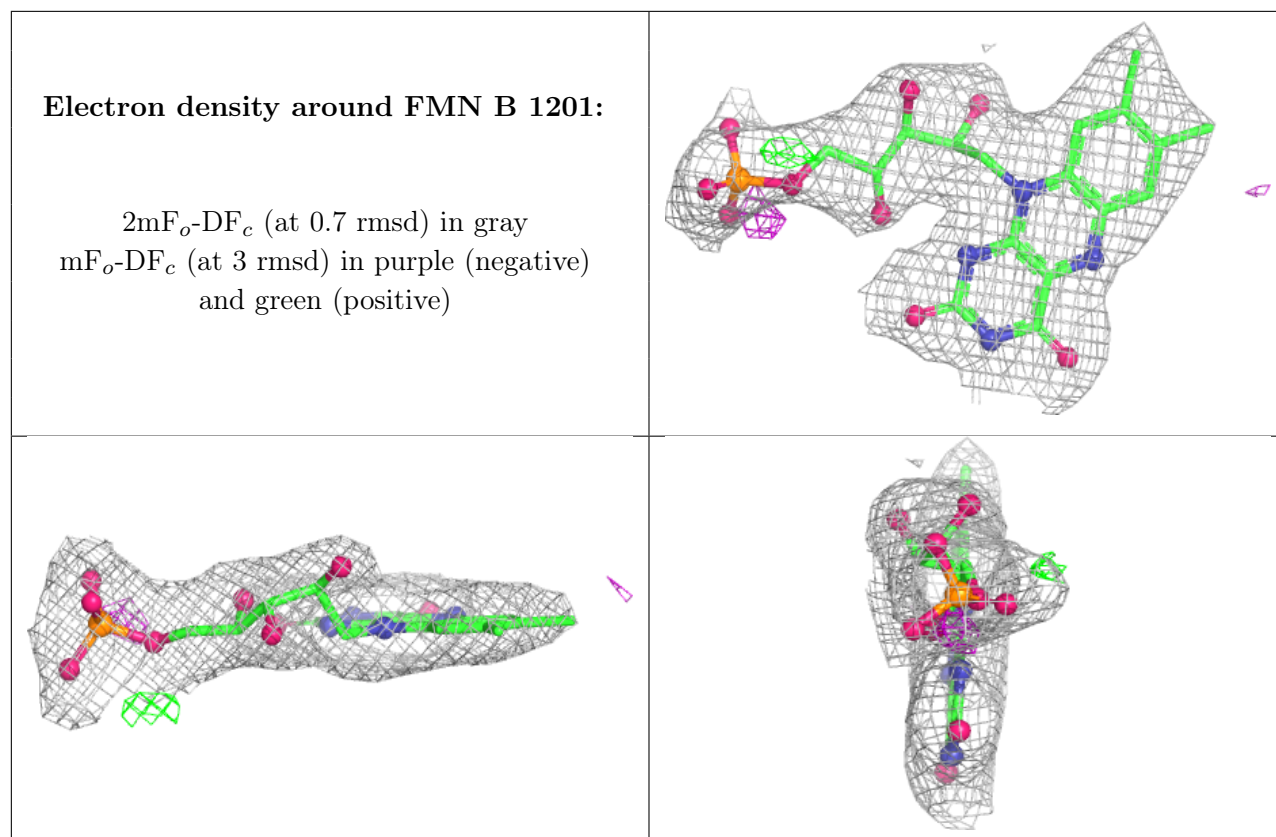
Electron density around FMN N 3201:

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

**Electron density around FMN H 7201:**

$2mF_o-DF_c$ (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.