



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 22, 2021 – 02:20 PM EST

PDB ID : 6WLP  
Title : Crystal Structure of the ZTL light-state mimic G46S  
Authors : Zoltowski, B.; Green, R.  
Deposited on : 2020-04-20  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.17.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.17.1

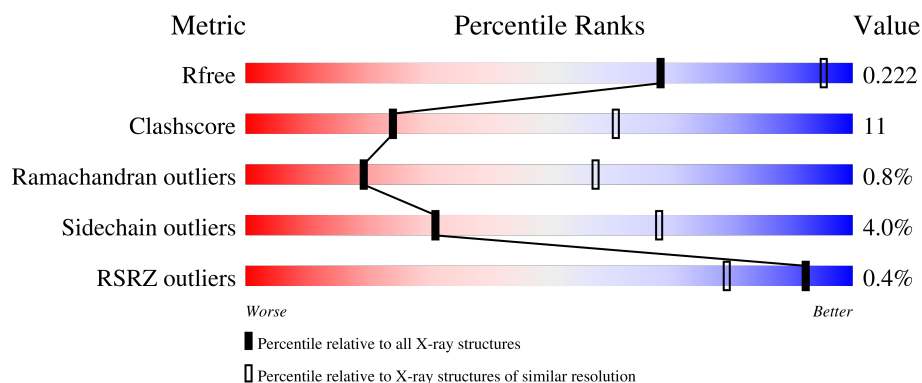
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	190	<div> <div>54%</div> <div>12%</div> <div>.</div> <div>32%</div> </div>
1	B	190	<div> <div>%</div> <div>51%</div> <div>15%</div> <div>..</div> <div>32%</div> </div>
1	C	190	<div> <div>%</div> <div>46%</div> <div>21%</div> <div>.</div> <div>31%</div> </div>
1	D	190	<div> <div>%</div> <div>45%</div> <div>21%</div> <div>.</div> <div>32%</div> </div>
1	E	190	<div> <div>56%</div> <div>10%</div> <div>.</div> <div>32%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	190	<div><div></div><div>48%19%•31%</div></div>
1	G	190	<div>%<div><div></div><div>48%19%•32%</div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14887 atoms, of which 7306 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 Adagio protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	130	Total	C	H	N	O	S	0	0	0
			2058	656	1025	178	192	7			
1	A	130	Total	C	H	N	O	S	0	0	0
			2058	656	1025	178	192	7			
1	C	131	Total	C	H	N	O	S	0	0	0
			2068	661	1028	179	193	7			
1	D	130	Total	C	H	N	O	S	0	0	0
			2037	656	1004	178	192	7			
1	E	130	Total	C	H	N	O	S	0	0	0
			2036	656	1003	178	192	7			
1	F	132	Total	C	H	N	O	S	0	0	0
			2089	670	1037	180	195	7			
1	G	130	Total	C	H	N	O	S	0	0	0
			2054	656	1021	178	192	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	18	SER	GLY	engineered mutation	UNP Q94BT6
B	52	ARG	GLY	engineered mutation	UNP Q94BT6
A	18	SER	GLY	engineered mutation	UNP Q94BT6
A	52	ARG	GLY	engineered mutation	UNP Q94BT6
C	18	SER	GLY	engineered mutation	UNP Q94BT6
C	52	ARG	GLY	engineered mutation	UNP Q94BT6
D	18	SER	GLY	engineered mutation	UNP Q94BT6
D	52	ARG	GLY	engineered mutation	UNP Q94BT6
E	18	SER	GLY	engineered mutation	UNP Q94BT6
E	52	ARG	GLY	engineered mutation	UNP Q94BT6
F	18	SER	GLY	engineered mutation	UNP Q94BT6
F	52	ARG	GLY	engineered mutation	UNP Q94BT6
G	18	SER	GLY	engineered mutation	UNP Q94BT6
G	52	ARG	GLY	engineered mutation	UNP Q94BT6

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- The chemical structure of FMN (Flavin Mononucleotide) is shown. It consists of an isoalloxazine ring system (a tricyclic aromatic system) and a ribityl chain. The ribityl chain is attached to the ring at the N10 position. The ribityl chain is a three-carbon chain with a phosphate group at the end. The phosphate group is shown as a phosphorus atom (P) double-bonded to an oxygen atom (O1P) and single-bonded to three other oxygen atoms (O2P, O3P, O4P). The ribityl chain is shown with stereochemistry: the C2' carbon is bonded to the ring, the C3' carbon has a hydroxyl group (OH) pointing down, and the C4' carbon has a hydroxyl group (OH) pointing up. The ribityl chain is labeled with C1', C2', C3', and C4' for the carbons, and O1P, O2P, O3P, and O4P for the phosphate oxygens. The isoalloxazine ring system is labeled with N1, N3, N5, N10 for the nitrogen atoms and C2, C4, C6, C7, C8, C9, C10 for the carbon atoms. The ribityl chain is attached to the ring at the N10 position. The ribityl chain is shown with stereochemistry: the C2' carbon is bonded to the ring, the C3' carbon has a hydroxyl group (OH) pointing down, and the C4' carbon has a hydroxyl group (OH) pointing up. The ribityl chain is labeled with C1', C2', C3', and C4' for the carbons, and O1P, O2P, O3P, and O4P for the phosphate oxygens.

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $\text{C}_2\text{H}_6\text{O}_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	E	1	Total	C	H	O	0	0
			10	2	6	2		
3	F	1	Total	C	H	O	0	0
			10	2	6	2		

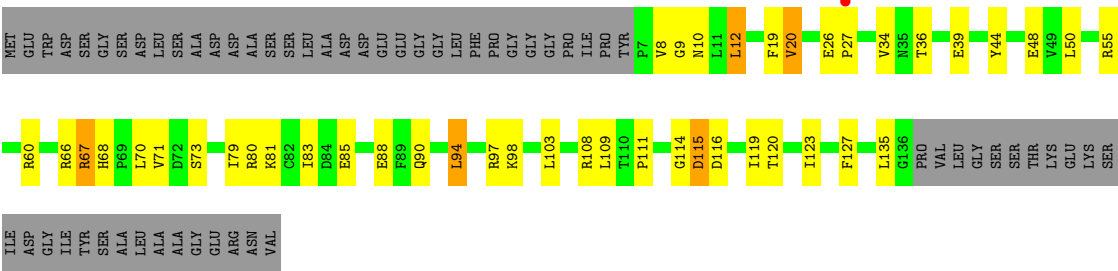
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	18	Total	O	0	0
			18	18		
4	A	13	Total	O	0	0
			13	13		
4	C	10	Total	O	0	0
			10	10		
4	D	10	Total	O	0	0
			10	10		
4	E	15	Total	O	0	0
			15	15		
4	F	15	Total	O	0	0
			15	15		
4	G	6	Total	O	0	0
			6	6		

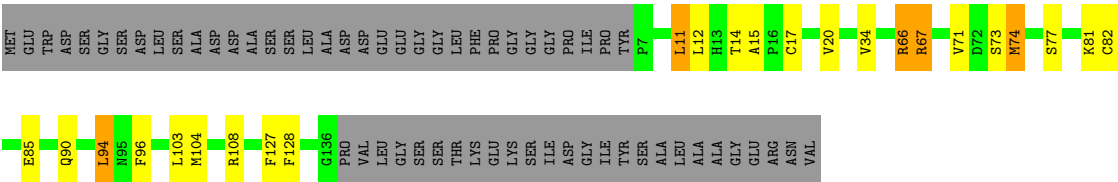


- Molecule 1: Adagio protein 1

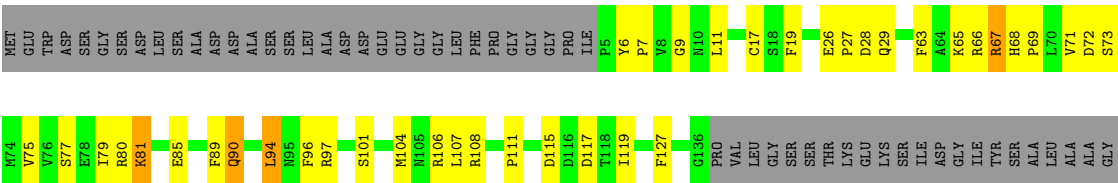




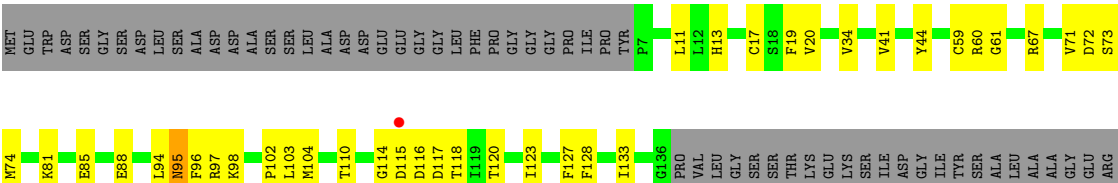
• Molecule 1: Adagio protein 1



• Molecule 1: Adagio protein 1



• Molecule 1: Adagio protein 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	265.07 Å   265.07 Å   265.07 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	46.86 – 3.00 48.39 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.86-3.00) 95.0 (48.39-3.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 3.01 Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.193 , 0.222 0.193 , 0.222	Depositor DCC
$R_{free}$ test set	2005 reflections (3.25%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, EDO

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	0.74	0/1054	0.84	1/1428 (0.1%)
1	B	0.80	0/1054	0.90	3/1428 (0.2%)
1	C	0.76	0/1062	0.95	3/1440 (0.2%)
1	D	0.76	1/1054 (0.1%)	0.83	1/1428 (0.1%)
1	E	0.81	3/1054 (0.3%)	0.93	4/1428 (0.3%)
1	F	0.84	0/1075	0.86	1/1458 (0.1%)
1	G	0.75	1/1054 (0.1%)	0.86	1/1428 (0.1%)
All	All	0.78	5/7407 (0.1%)	0.88	14/10038 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	66	ARG	CB-CG	7.25	1.72	1.52
1	G	17	CYS	CB-SG	-6.60	1.71	1.82
1	E	66	ARG	CG-CD	5.47	1.65	1.51
1	E	17	CYS	CB-SG	-5.21	1.73	1.81
1	D	20	VAL	CB-CG2	-5.09	1.42	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	104	MET	CG-SD-CE	-8.38	86.79	100.20
1	F	104	MET	CG-SD-CE	-7.11	88.83	100.20
1	E	104	MET	CG-SD-CE	-6.83	89.28	100.20
1	E	11	LEU	CB-CG-CD1	-6.60	99.78	111.00
1	B	104	MET	CG-SD-CE	-5.78	90.95	100.20

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	1033	1025	1025	24	0
1	B	1033	1025	1025	22	0
1	C	1040	1028	1032	35	0
1	D	1033	1004	1025	31	0
1	E	1033	1003	1025	18	0
1	F	1052	1037	1042	26	0
1	G	1033	1021	1025	30	0
2	A	31	19	19	1	0
2	B	31	19	19	2	0
2	C	31	19	19	5	0
2	D	31	19	19	3	0
2	E	31	19	19	0	0
2	F	31	19	19	1	0
2	G	31	19	19	0	0
3	A	4	6	6	0	0
3	B	4	6	6	0	0
3	D	4	6	6	0	0
3	E	4	6	6	0	0
3	F	4	6	6	0	0
4	A	13	0	0	0	0
4	B	18	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	15	0	0	0	0
4	F	15	0	0	0	0
4	G	6	0	0	0	0
All	All	7581	7306	7362	164	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 11.

The worst 5 of 164 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:E:103:LEU:HD23	1:E:128:PHE:HB3	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:VAL:HG12	1:B:34:VAL:HG12	1.48	0.93
1:D:20:VAL:HG23	1:D:34:VAL:HG12	1.49	0.93
1:C:106:ARG:NH2	1:G:13:HIS:O	2.06	0.87
1:E:90:GLN:HG2	1:E:108:ARG:HD3	1.57	0.86

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	128/190 (67%)	115 (90%)	11 (9%)	2 (2%)	9	40
1	B	128/190 (67%)	123 (96%)	4 (3%)	1 (1%)	19	57
1	C	129/190 (68%)	121 (94%)	7 (5%)	1 (1%)	19	57
1	D	128/190 (67%)	122 (95%)	6 (5%)	0	100	100
1	E	128/190 (67%)	122 (95%)	6 (5%)	0	100	100
1	F	130/190 (68%)	118 (91%)	12 (9%)	0	100	100
1	G	128/190 (67%)	115 (90%)	10 (8%)	3 (2%)	6	30
All	All	899/1330 (68%)	836 (93%)	56 (6%)	7 (1%)	19	57

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	116	ASP
1	G	60	ARG
1	A	116	ASP
1	C	60	ARG
1	G	133	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	116/161 (72%)	114 (98%)	2 (2%)	60	85
1	B	116/161 (72%)	110 (95%)	6 (5%)	23	59
1	C	117/161 (73%)	113 (97%)	4 (3%)	37	72
1	D	116/161 (72%)	111 (96%)	5 (4%)	29	66
1	E	116/161 (72%)	111 (96%)	5 (4%)	29	66
1	F	118/161 (73%)	109 (92%)	9 (8%)	13	43
1	G	116/161 (72%)	114 (98%)	2 (2%)	60	85
All	All	815/1127 (72%)	782 (96%)	33 (4%)	31	68

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	94	LEU
1	F	115	ASP
1	G	95	ASN
1	D	12	LEU
1	C	108	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	A	5202	-	3,3,3	0.56	0	2,2,2	0.33	0
2	FMN	E	5201	-	31,33,33	1.47	7 (22%)	40,50,50	2.00	8 (20%)
3	EDO	E	5202	-	3,3,3	0.75	0	2,2,2	0.08	0
2	FMN	B	5201	-	31,33,33	1.63	7 (22%)	40,50,50	2.03	11 (27%)
2	FMN	F	5201	-	31,33,33	1.57	6 (19%)	40,50,50	2.05	11 (27%)
3	EDO	D	5202	-	3,3,3	0.64	0	2,2,2	0.24	0
2	FMN	G	5201	-	31,33,33	1.51	6 (19%)	40,50,50	1.92	6 (15%)
3	EDO	B	5202	-	3,3,3	0.71	0	2,2,2	0.35	0
3	EDO	F	5202	-	3,3,3	0.64	0	2,2,2	0.39	0
2	FMN	D	5201	-	31,33,33	1.50	5 (16%)	40,50,50	1.81	10 (25%)
2	FMN	A	5201	-	31,33,33	1.52	7 (22%)	40,50,50	1.85	8 (20%)
2	FMN	C	5201	-	31,33,33	1.53	4 (12%)	40,50,50	1.98	8 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	5202	-	-	0/1/1/1	-
2	FMN	E	5201	-	-	1/18/18/18	0/3/3/3
3	EDO	E	5202	-	-	1/1/1/1	-
2	FMN	B	5201	-	-	2/18/18/18	0/3/3/3
2	FMN	F	5201	-	-	6/18/18/18	0/3/3/3
3	EDO	D	5202	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	G	5201	-	-	6/18/18/18	0/3/3/3
3	EDO	B	5202	-	-	0/1/1/1	-
3	EDO	F	5202	-	-	1/1/1/1	-
2	FMN	D	5201	-	-	8/18/18/18	0/3/3/3
2	FMN	A	5201	-	-	1/18/18/18	0/3/3/3
2	FMN	C	5201	-	-	1/18/18/18	0/3/3/3

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5201	FMN	C10-N1	4.33	1.38	1.33
2	G	5201	FMN	C10-N1	4.23	1.38	1.33
2	D	5201	FMN	C10-N1	4.12	1.38	1.33
2	C	5201	FMN	C10-N1	4.01	1.38	1.33
2	A	5201	FMN	C10-N1	3.99	1.38	1.33

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5201	FMN	C4-N3-C2	6.68	120.78	115.14
2	G	5201	FMN	C1'-N10-C9A	6.58	123.47	118.29
2	E	5201	FMN	C1'-N10-C9A	6.25	123.21	118.29
2	C	5201	FMN	C4-N3-C2	5.92	120.14	115.14
2	D	5201	FMN	C4-N3-C2	5.86	120.09	115.14

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	5201	FMN	C2'-C1'-N10-C9A
2	D	5201	FMN	C1'-C2'-C3'-O3'
2	D	5201	FMN	C1'-C2'-C3'-C4'
2	D	5201	FMN	O2'-C2'-C3'-O3'
2	D	5201	FMN	C5'-O5'-P-O1P

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5201	FMN	2	0

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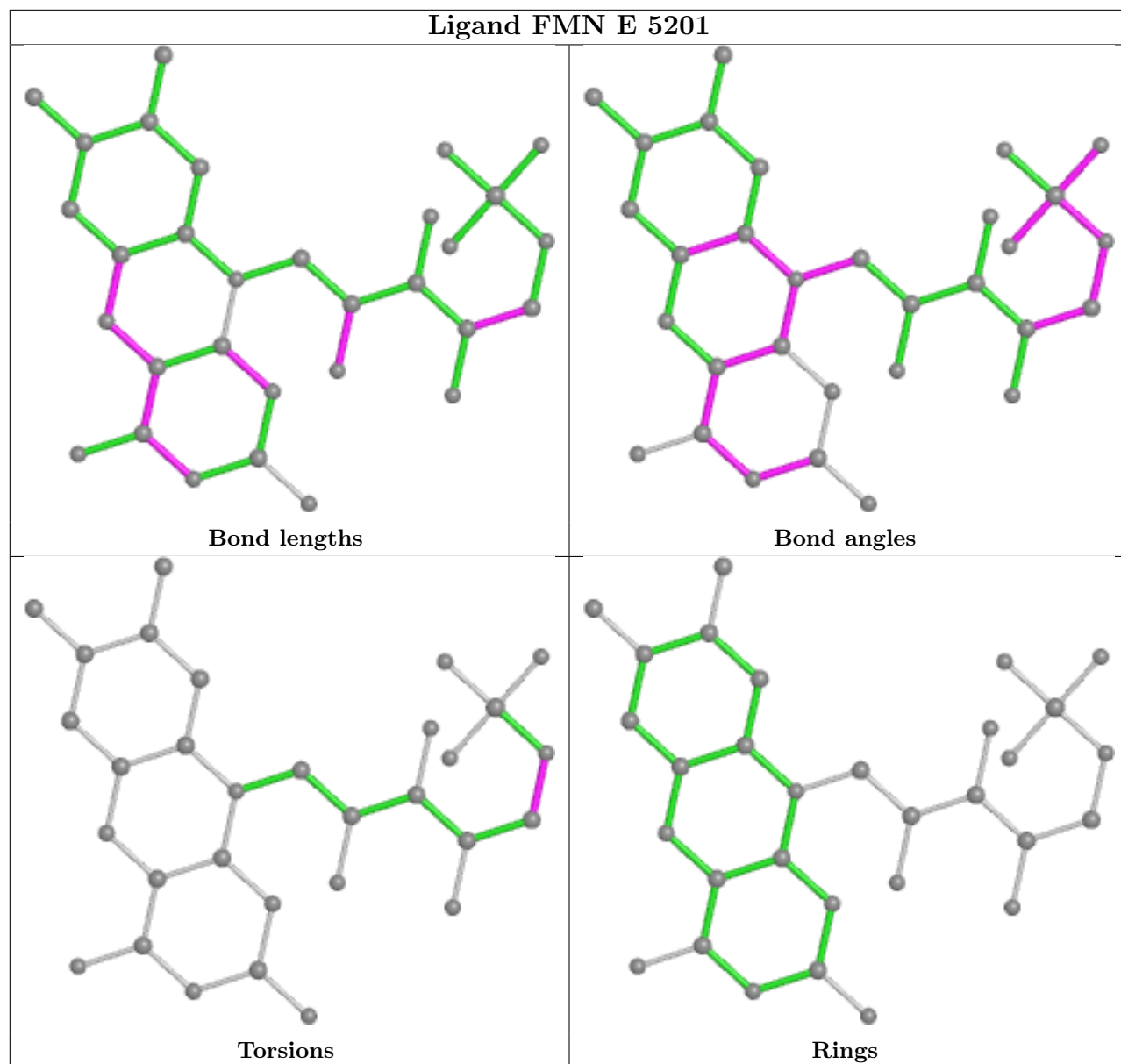
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	5201	FMN	1	0
2	D	5201	FMN	3	0
2	A	5201	FMN	1	0
2	C	5201	FMN	5	0

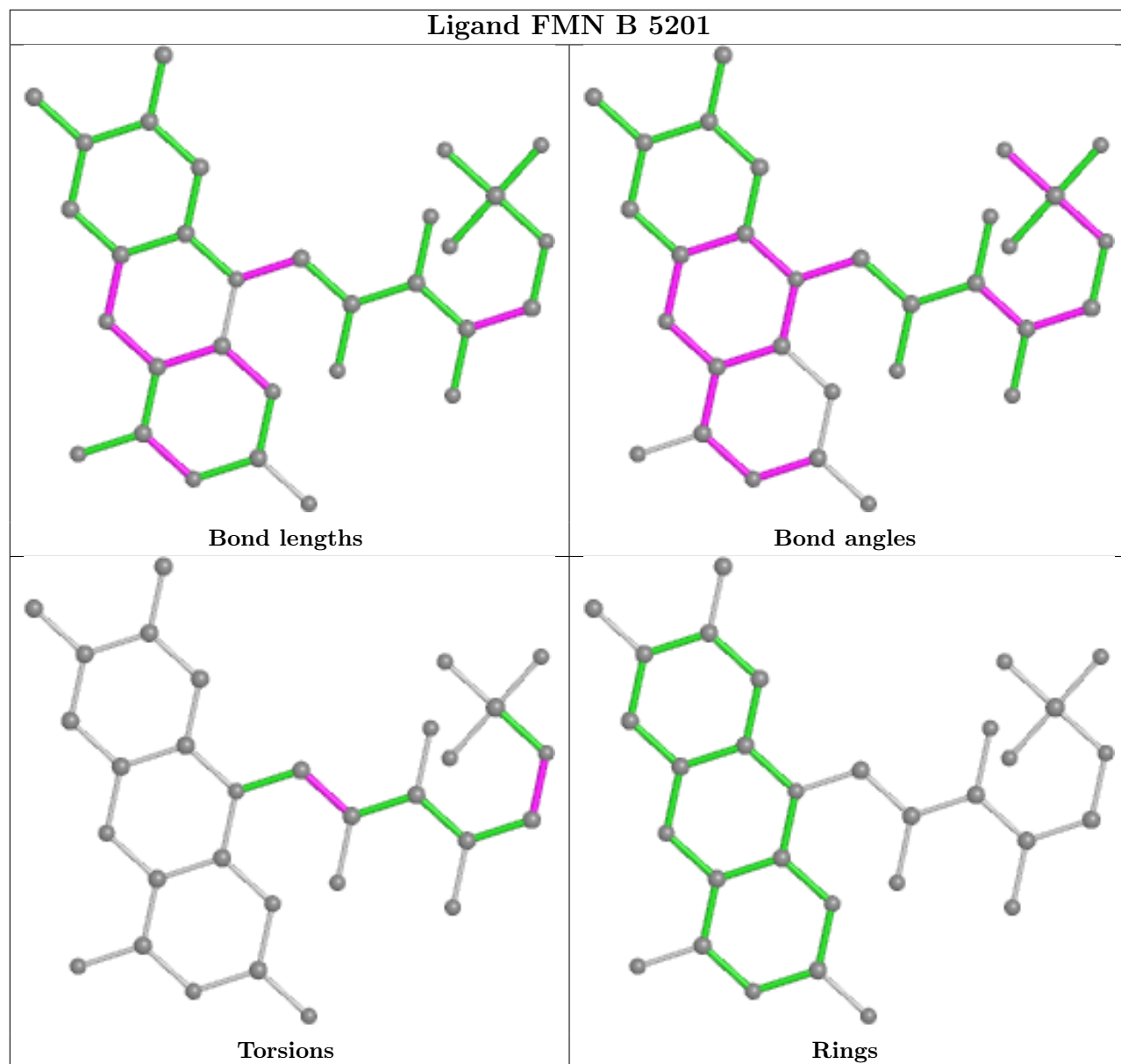
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

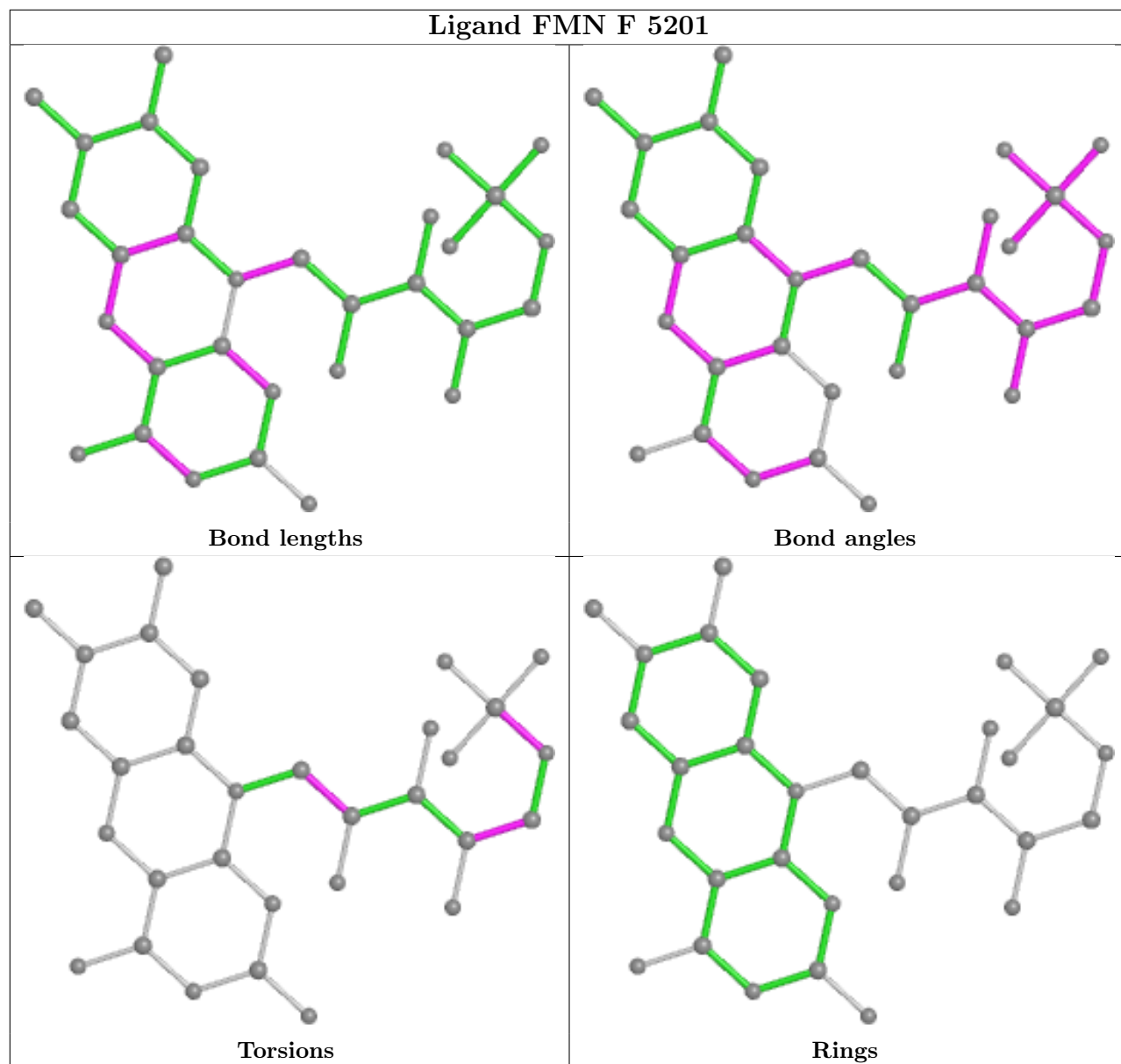


## Ligand FMN E 5201

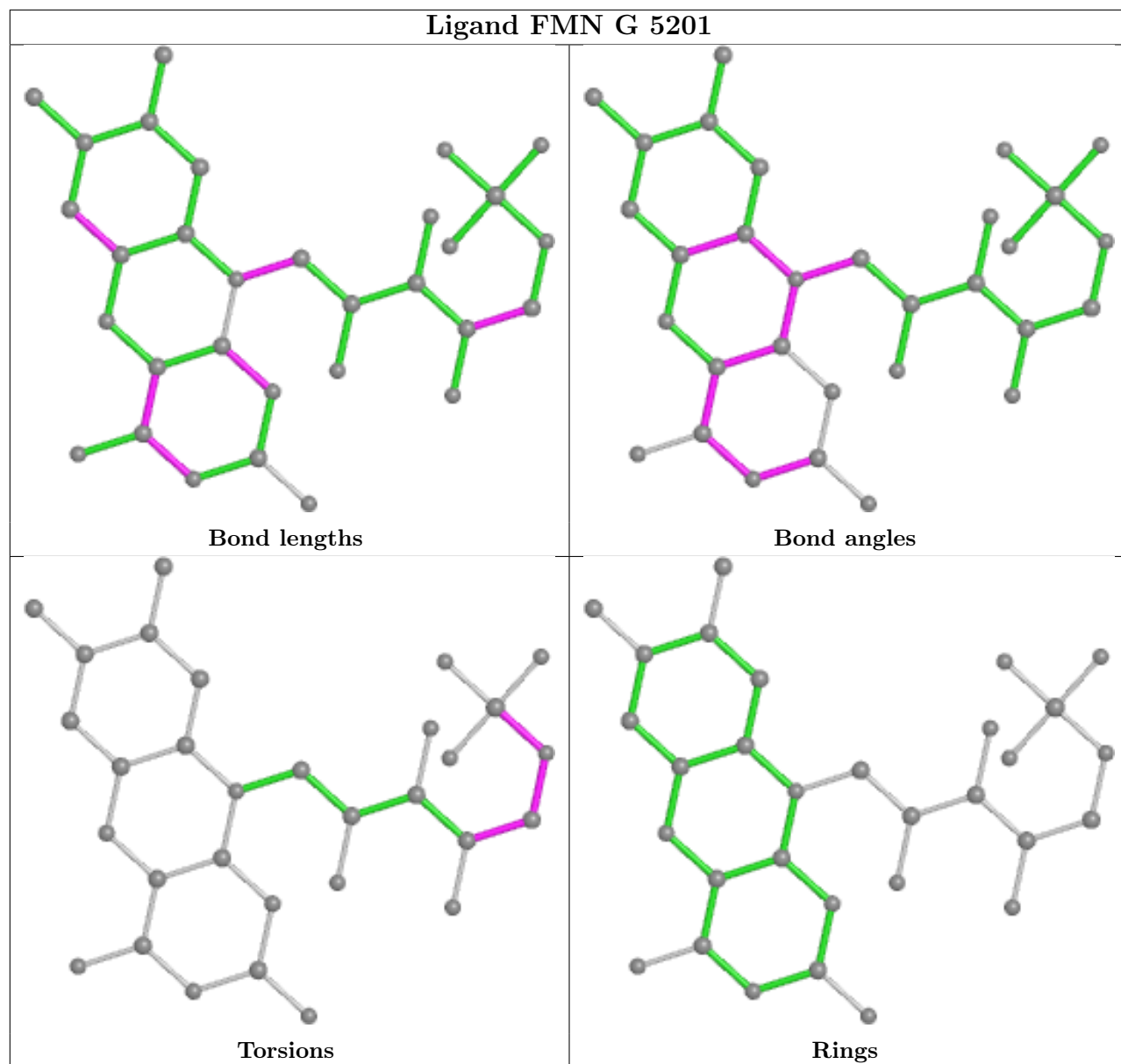


## Ligand FMN B 5201

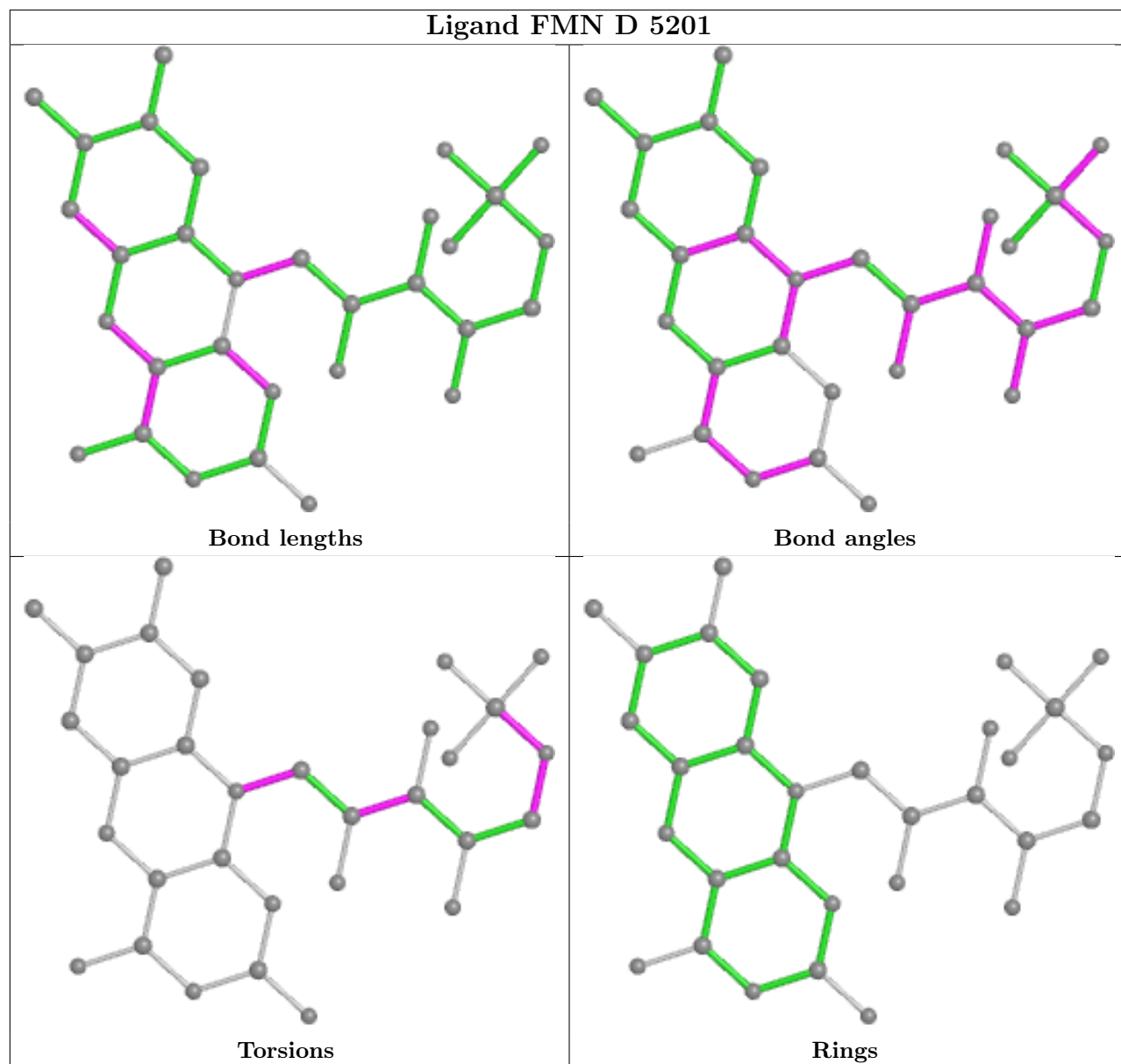




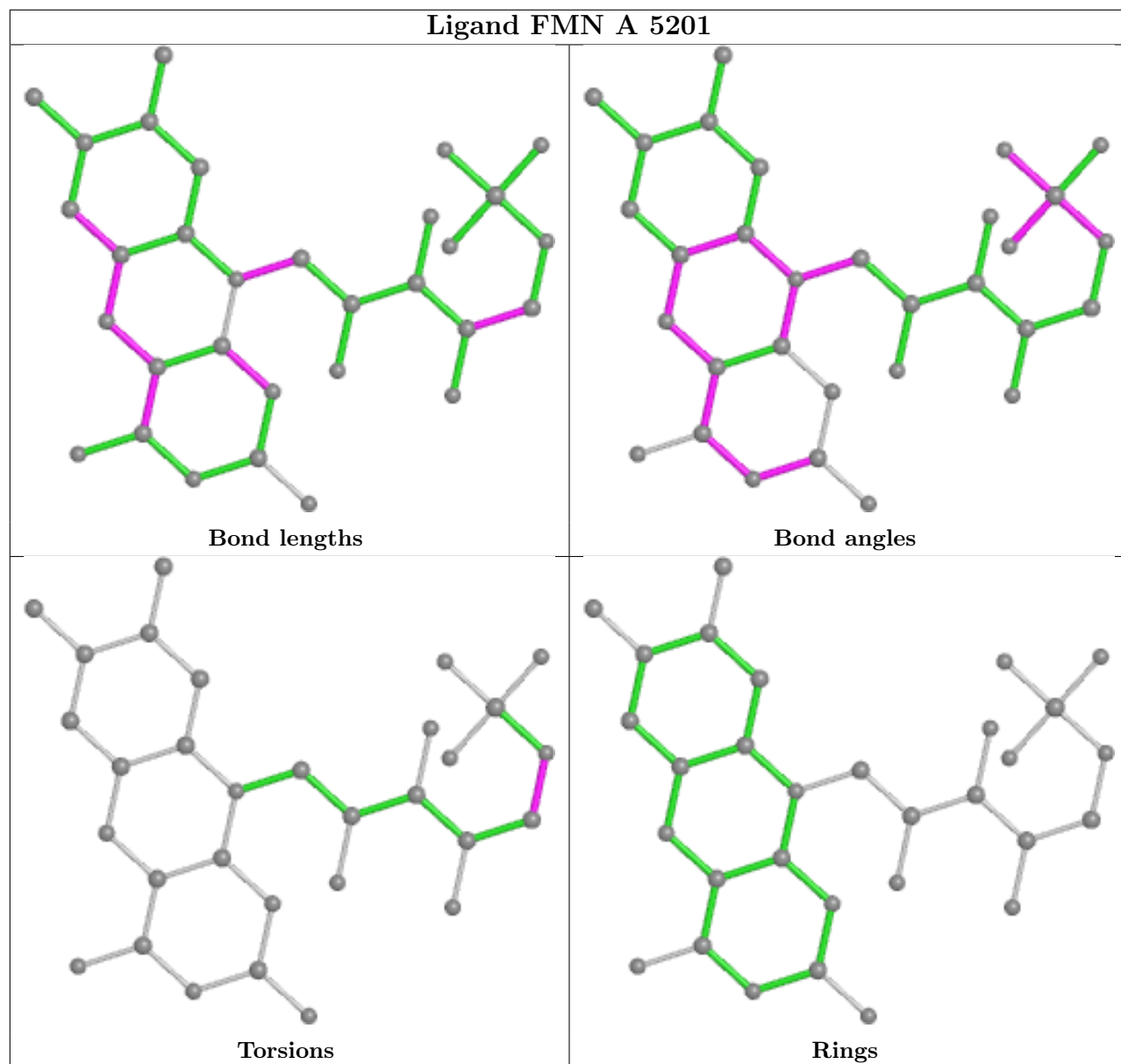
## Ligand FMN G 5201

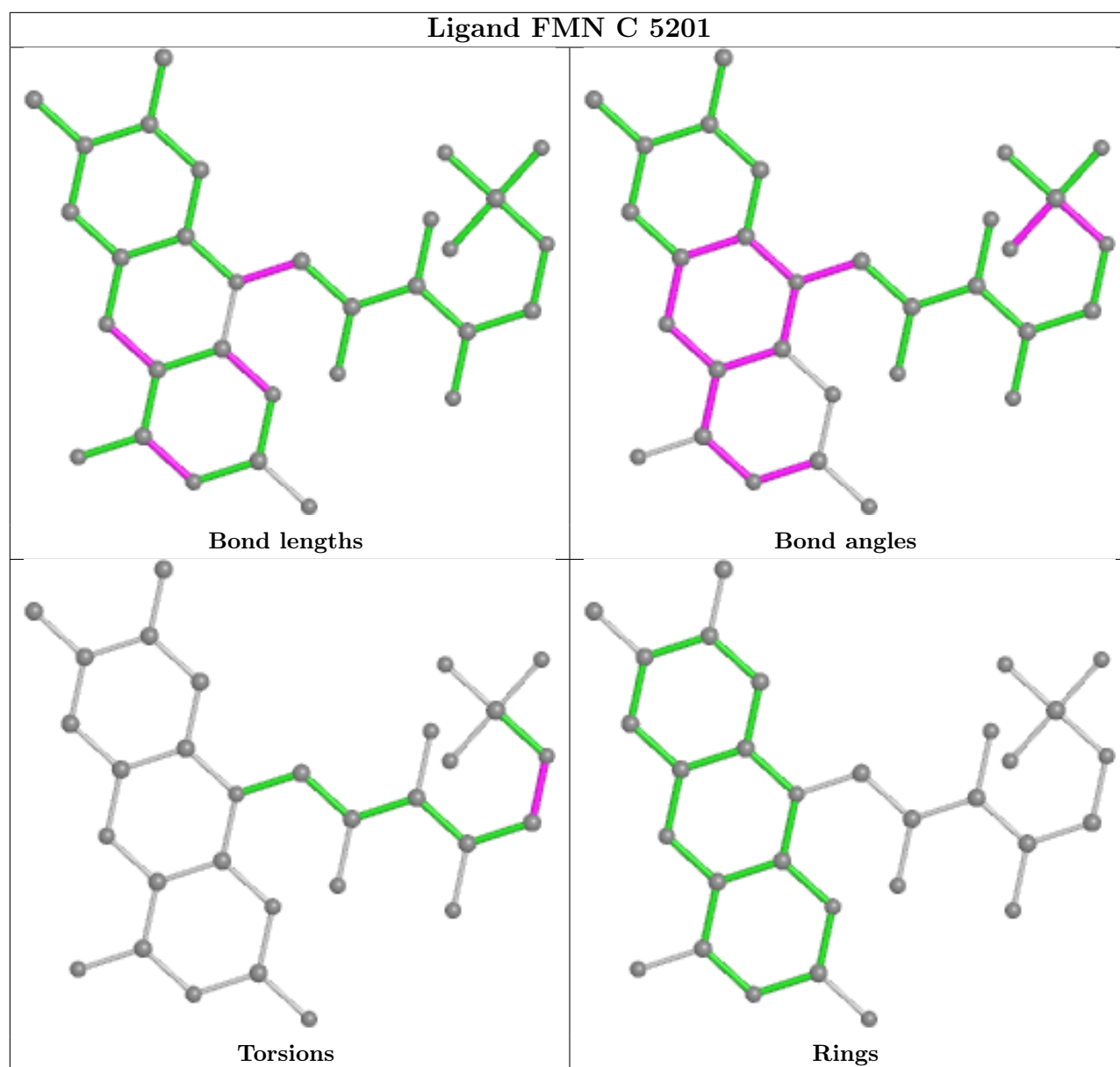


## Ligand FMN D 5201



## Ligand FMN A 5201





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	130/190 (68%)	-0.27	0 <b>100</b> <b>100</b>	41, 55, 89, 113	0
1	B	130/190 (68%)	-0.44	1 (0%) 86 65	30, 45, 71, 97	0
1	C	131/190 (68%)	-0.39	1 (0%) 86 65	37, 56, 80, 132	0
1	D	130/190 (68%)	-0.13	1 (0%) 86 65	42, 55, 79, 111	0
1	E	130/190 (68%)	-0.42	0 <b>100</b> <b>100</b>	30, 47, 78, 149	0
1	F	132/190 (69%)	-0.27	0 <b>100</b> <b>100</b>	33, 49, 85, 109	0
1	G	130/190 (68%)	-0.17	1 (0%) 86 65	41, 59, 107, 140	0
All	All	913/1330 (68%)	-0.30	4 (0%) <b>92</b> <b>79</b>	30, 53, 87, 149	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	115	ASP	2.7
1	C	115	ASP	2.7
1	B	115	ASP	2.3
1	D	27	PRO	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands

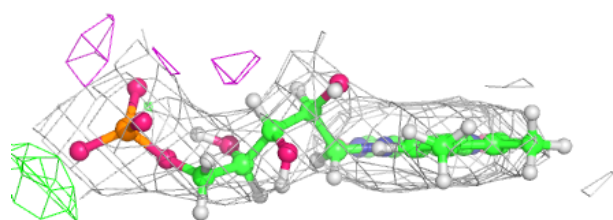
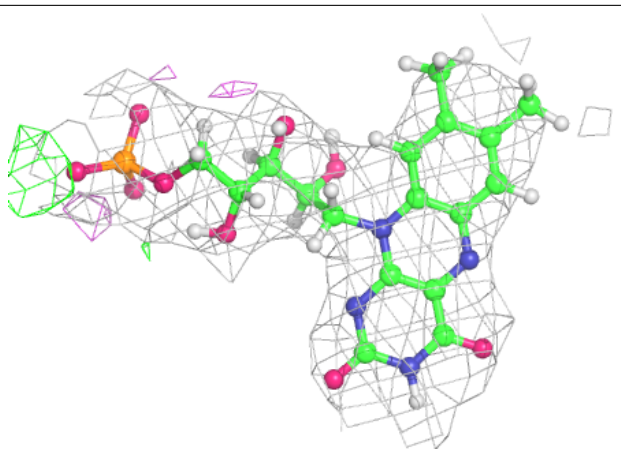
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	D	5202	4/4	0.87	0.22	61,73,82,82	0
3	EDO	E	5202	4/4	0.88	0.15	53,63,71,71	0
3	EDO	A	5202	4/4	0.89	0.32	60,73,88,88	0
3	EDO	B	5202	4/4	0.92	0.19	47,56,67,67	0
3	EDO	F	5202	4/4	0.94	0.16	50,61,79,79	0
2	FMN	F	5201	31/31	0.96	0.18	35,46,60,67	0
2	FMN	G	5201	31/31	0.97	0.21	45,62,77,81	0
2	FMN	D	5201	31/31	0.97	0.23	41,55,72,76	0
2	FMN	A	5201	31/31	0.98	0.19	39,51,68,69	0
2	FMN	E	5201	31/31	0.98	0.18	32,46,59,60	0
2	FMN	C	5201	31/31	0.98	0.16	46,58,75,84	0
2	FMN	B	5201	31/31	0.99	0.18	33,47,60,65	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.

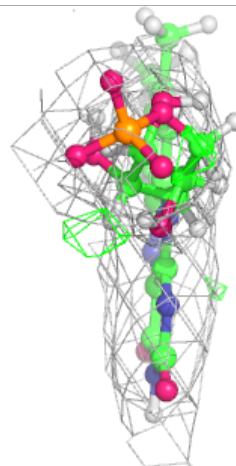
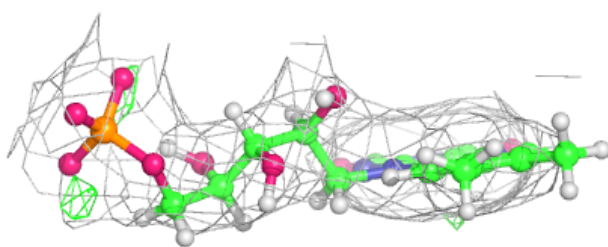
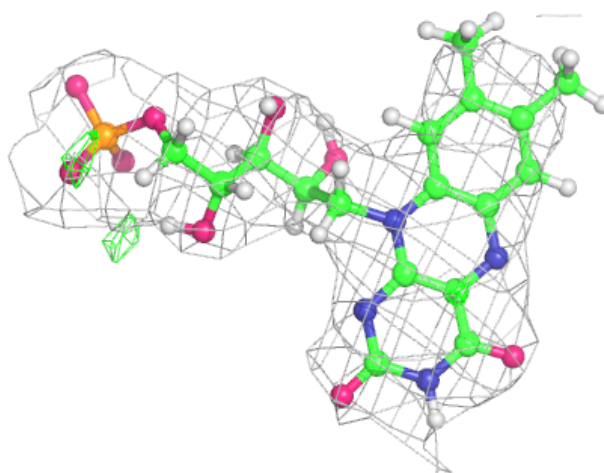
**Electron density around FMN F 5201:**

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



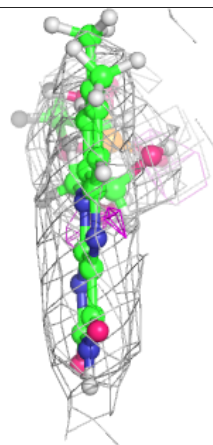
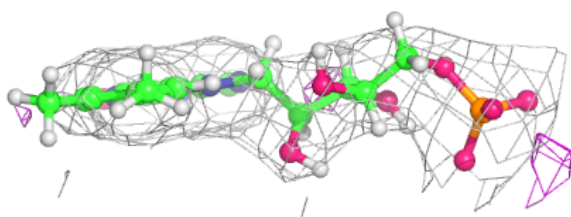
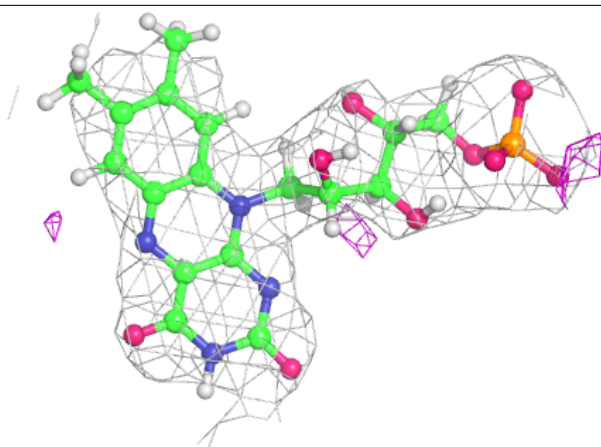
**Electron density around FMN G 5201:**

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



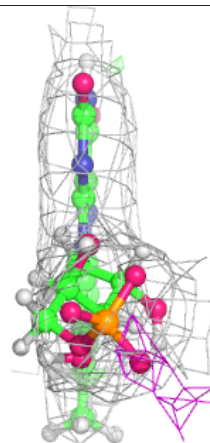
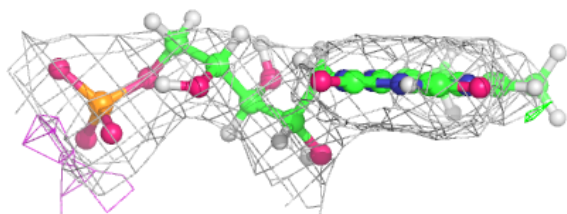
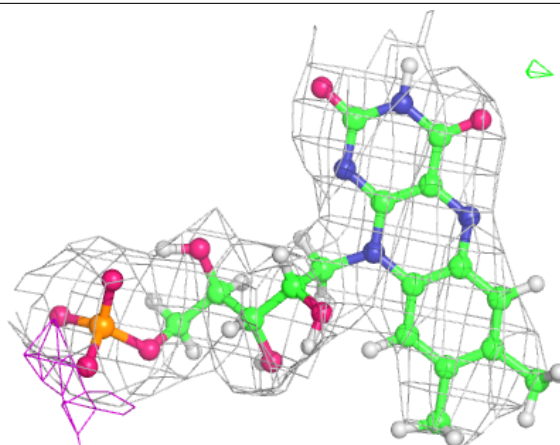
**Electron density around FMN D 5201:**

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



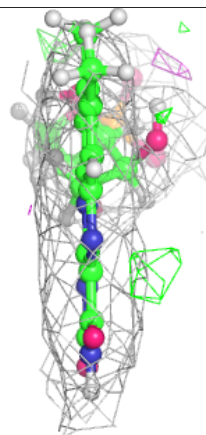
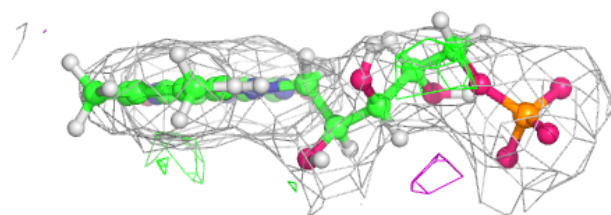
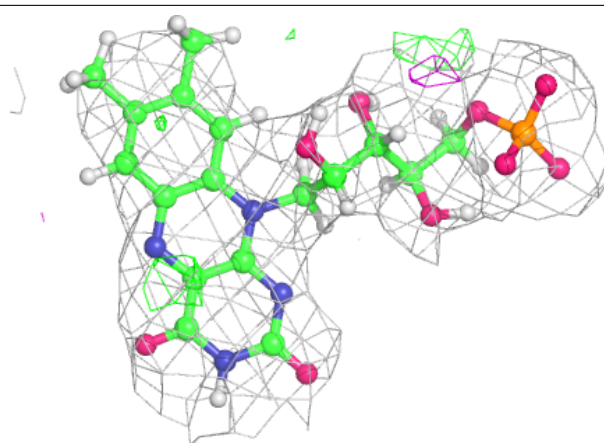
**Electron density around FMN A 5201:**

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



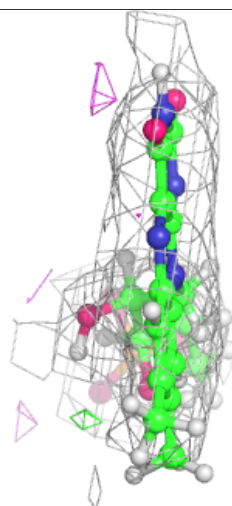
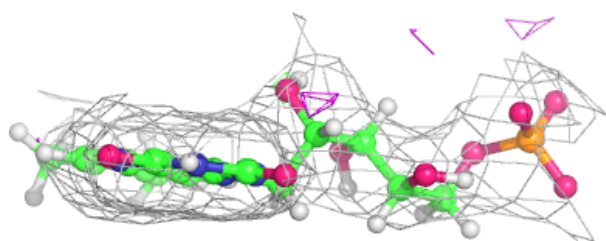
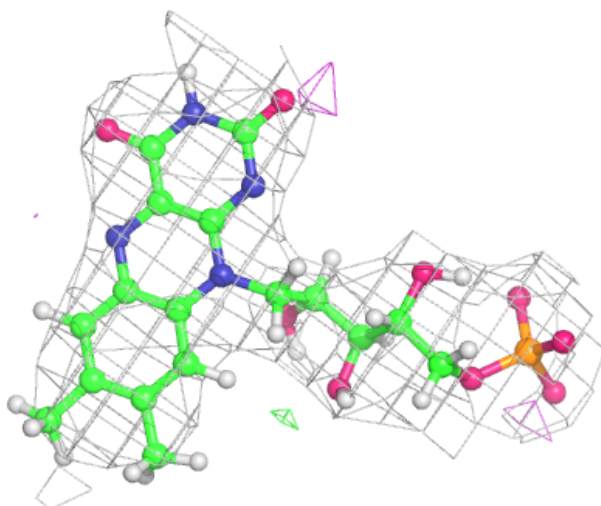
**Electron density around FMN E 5201:**

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



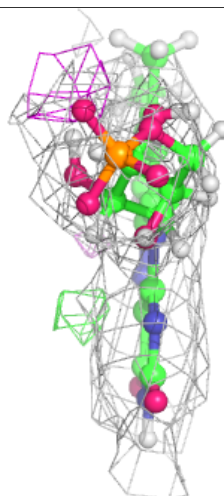
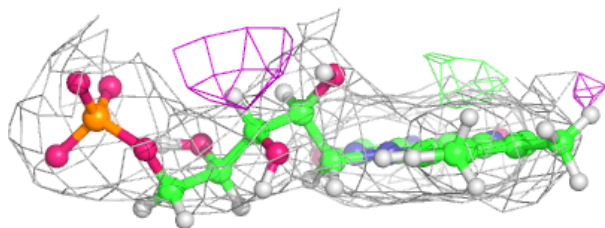
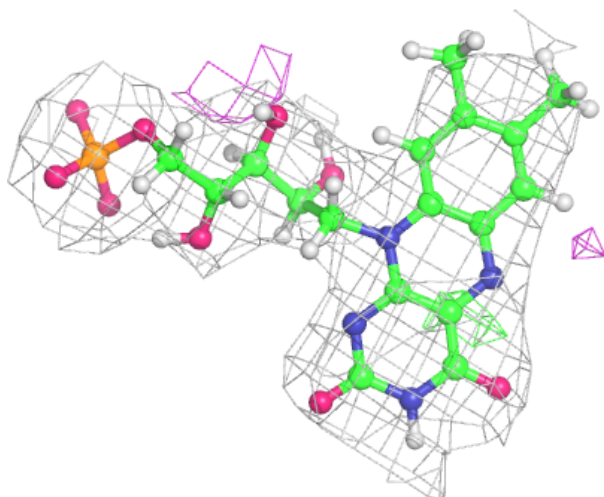
**Electron density around FMN C 5201:**

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



**Electron density around FMN B 5201:**

$2mF_o-DF_c$  (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.