



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 11:37 am BST

PDB ID : 3QJG
Title : Epidermin biosynthesis protein EpiD from Staphylococcus aureus
Authors : Osipiuk, J.; Makowska-Grzyska, M.; Kwon, K.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2011-01-28
Resolution : 2.04 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

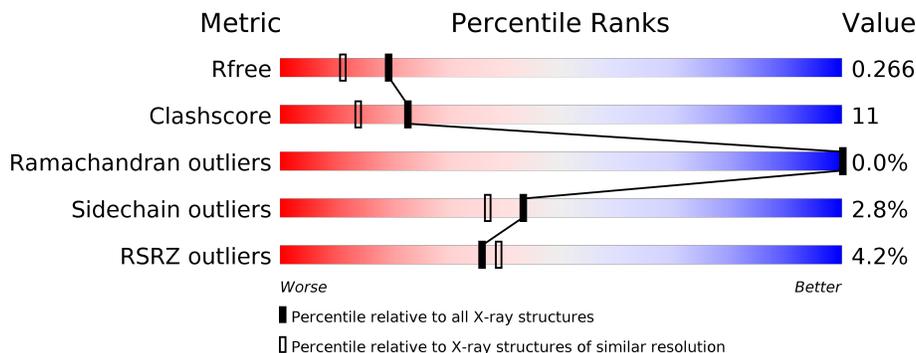
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	175	
1	B	175	
1	C	175	
1	D	175	
1	E	175	
1	F	175	

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Mol	Chain	Length	Quality of chain
1	G	175	<p>2% 82% 15% .</p>
1	H	175	<p>2% 80% 17% ..</p>
1	I	175	<p>10% 81% 15% ..</p>
1	J	175	<p>4% 78% 17% ..</p>
1	K	175	<p>3% 78% 18% ..</p>
1	L	175	<p>6% 78% 18% ..</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18797 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 Epidermin biosynthesis protein EpiD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	171	1424	922	228	267	7	0	9	0
1	B	170	1399	902	224	266	7	0	6	0
1	C	170	1377	885	224	261	7	0	2	0
1	D	170	1418	917	231	263	7	0	9	0
1	E	170	1398	904	223	264	7	0	6	0
1	F	170	1404	907	227	263	7	0	7	0
1	G	170	1410	910	229	264	7	0	7	0
1	H	170	1400	907	225	261	7	0	6	0
1	I	170	1429	927	224	271	7	0	11	0
1	J	170	1431	926	231	267	7	0	11	0
1	K	170	1428	926	234	261	7	0	11	0
1	L	170	1397	900	224	266	7	0	6	0

There are 36 discrepancies between the modelled and reference sequences:

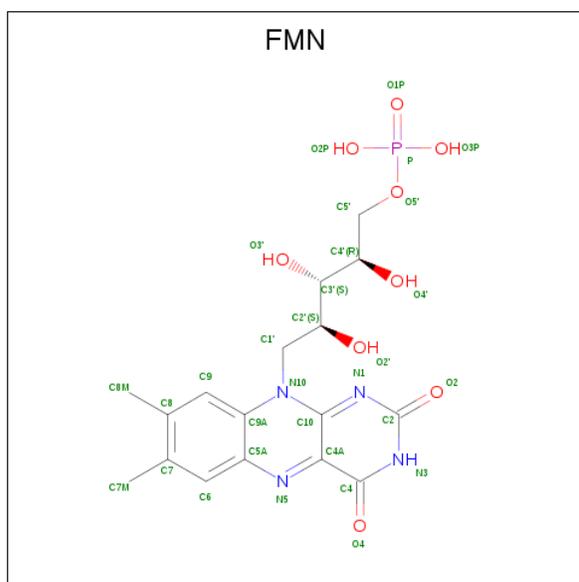
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q5HEV4
A	-1	ASN	-	EXPRESSION TAG	UNP Q5HEV4
A	0	ALA	-	EXPRESSION TAG	UNP Q5HEV4
B	-2	SER	-	EXPRESSION TAG	UNP Q5HEV4
B	-1	ASN	-	EXPRESSION TAG	UNP Q5HEV4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	EXPRESSION TAG	UNP Q5HEV4
C	-2	SER	-	EXPRESSION TAG	UNP Q5HEV4
C	-1	ASN	-	EXPRESSION TAG	UNP Q5HEV4
C	0	ALA	-	EXPRESSION TAG	UNP Q5HEV4
D	-2	SER	-	EXPRESSION TAG	UNP Q5HEV4
D	-1	ASN	-	EXPRESSION TAG	UNP Q5HEV4
D	0	ALA	-	EXPRESSION TAG	UNP Q5HEV4
E	-2	SER	-	EXPRESSION TAG	UNP Q5HEV4
E	-1	ASN	-	EXPRESSION TAG	UNP Q5HEV4
E	0	ALA	-	EXPRESSION TAG	UNP Q5HEV4
F	-2	SER	-	EXPRESSION TAG	UNP Q5HEV4
F	-1	ASN	-	EXPRESSION TAG	UNP Q5HEV4
F	0	ALA	-	EXPRESSION TAG	UNP Q5HEV4
G	-2	SER	-	EXPRESSION TAG	UNP Q5HEV4
G	-1	ASN	-	EXPRESSION TAG	UNP Q5HEV4
G	0	ALA	-	EXPRESSION TAG	UNP Q5HEV4
H	-2	SER	-	EXPRESSION TAG	UNP Q5HEV4
H	-1	ASN	-	EXPRESSION TAG	UNP Q5HEV4
H	0	ALA	-	EXPRESSION TAG	UNP Q5HEV4
I	-2	SER	-	EXPRESSION TAG	UNP Q5HEV4
I	-1	ASN	-	EXPRESSION TAG	UNP Q5HEV4
I	0	ALA	-	EXPRESSION TAG	UNP Q5HEV4
J	-2	SER	-	EXPRESSION TAG	UNP Q5HEV4
J	-1	ASN	-	EXPRESSION TAG	UNP Q5HEV4
J	0	ALA	-	EXPRESSION TAG	UNP Q5HEV4
K	-2	SER	-	EXPRESSION TAG	UNP Q5HEV4
K	-1	ASN	-	EXPRESSION TAG	UNP Q5HEV4
K	0	ALA	-	EXPRESSION TAG	UNP Q5HEV4
L	-2	SER	-	EXPRESSION TAG	UNP Q5HEV4
L	-1	ASN	-	EXPRESSION TAG	UNP Q5HEV4
L	0	ALA	-	EXPRESSION TAG	UNP Q5HEV4

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	2	Total Cl 2 2	0	0
3	A	2	Total Cl 2 2	0	0
3	D	2	Total Cl 2 2	0	0

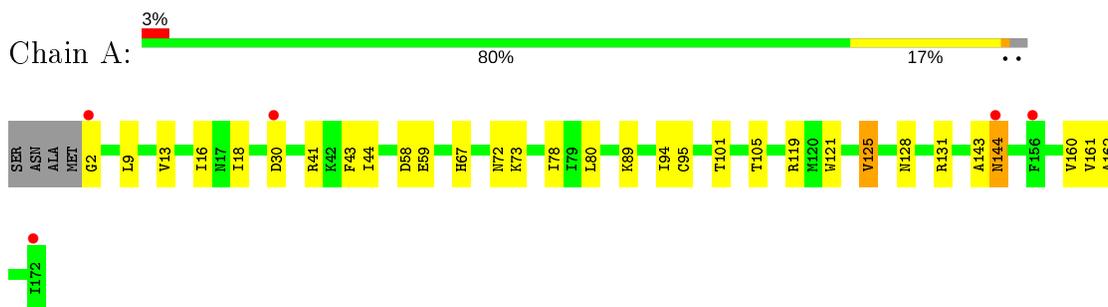
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	157	Total O 157 157	0	0
4	B	149	Total O 149 149	0	0
4	C	128	Total O 128 128	0	0
4	D	166	Total O 166 166	0	0
4	E	98	Total O 98 98	0	0
4	F	100	Total O 100 100	0	0
4	G	154	Total O 154 154	0	0
4	H	125	Total O 125 125	0	0
4	I	102	Total O 102 102	0	0
4	J	131	Total O 131 131	0	1
4	K	111	Total O 111 111	0	0
4	L	83	Total O 83 83	0	0

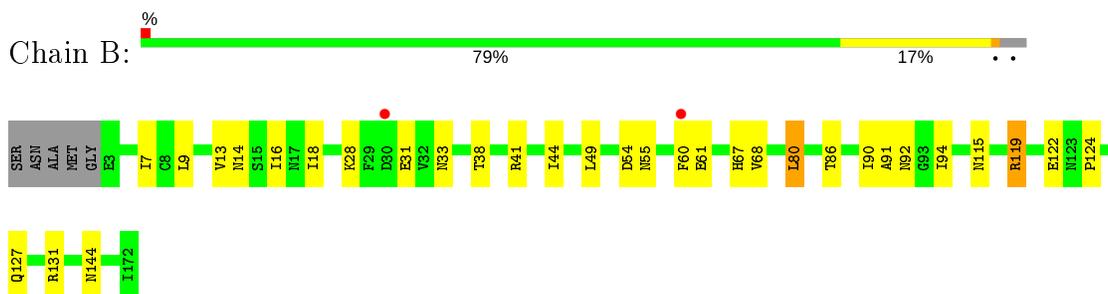
3 Residue-property plots [i](#)

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

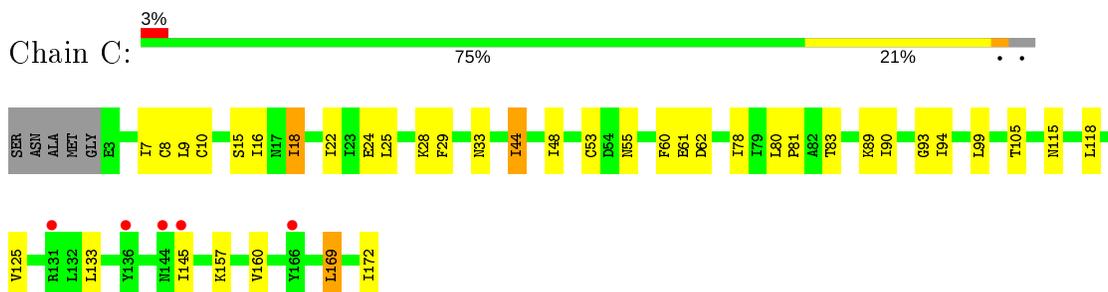
- Molecule 1: Epidermin biosynthesis protein EpiD



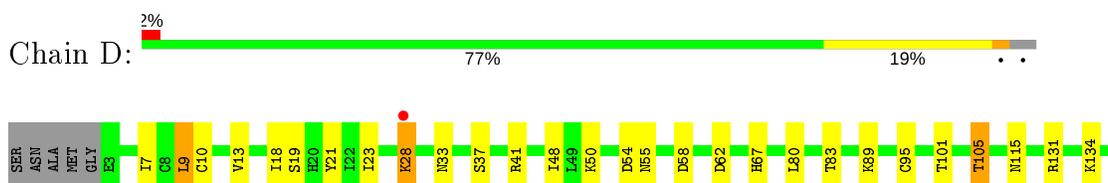
- Molecule 1: Epidermin biosynthesis protein EpiD



- Molecule 1: Epidermin biosynthesis protein EpiD

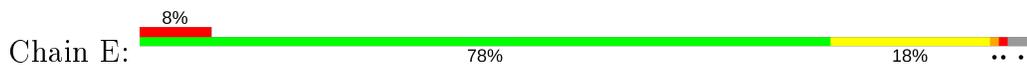


- Molecule 1: Epidermin biosynthesis protein EpiD

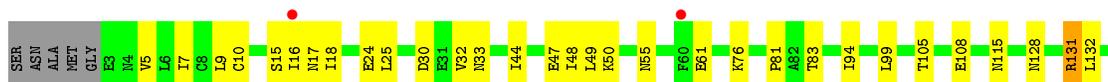
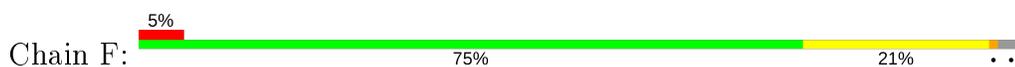




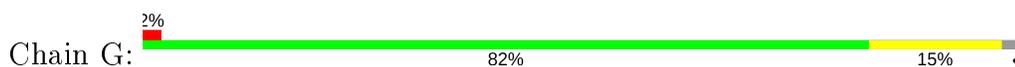
- Molecule 1: Epidermin biosynthesis protein EpiD



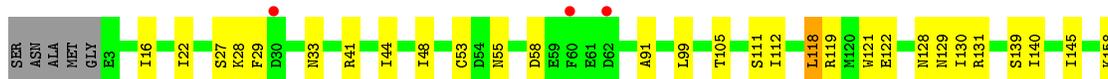
- Molecule 1: Epidermin biosynthesis protein EpiD



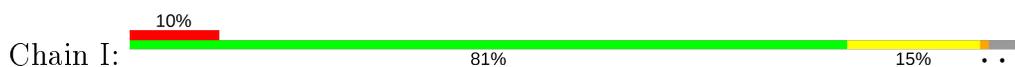
- Molecule 1: Epidermin biosynthesis protein EpiD

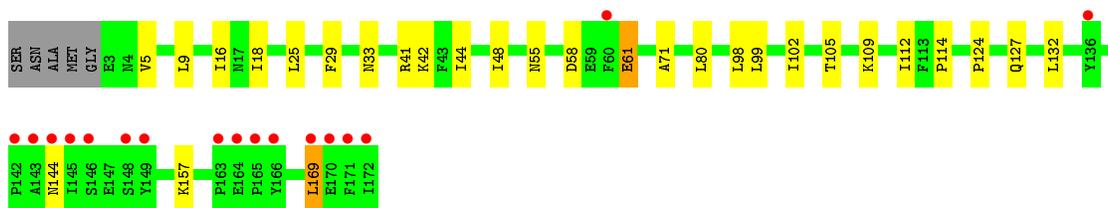


- Molecule 1: Epidermin biosynthesis protein EpiD

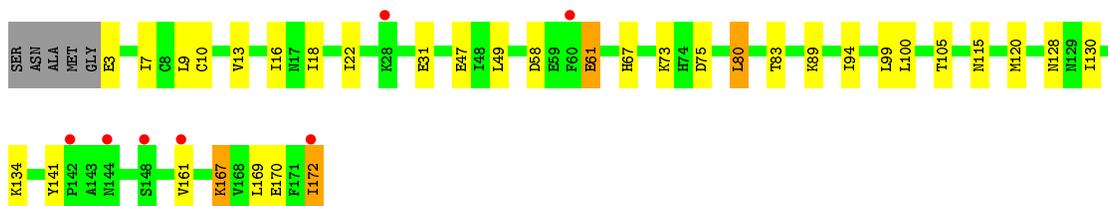
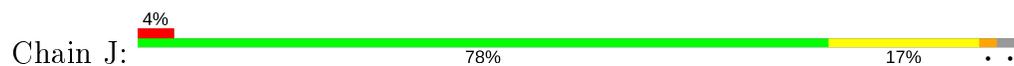


- Molecule 1: Epidermin biosynthesis protein EpiD

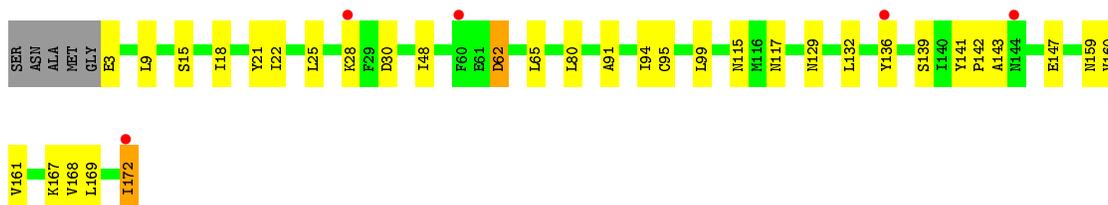
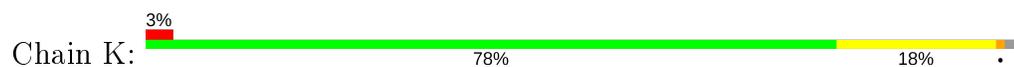




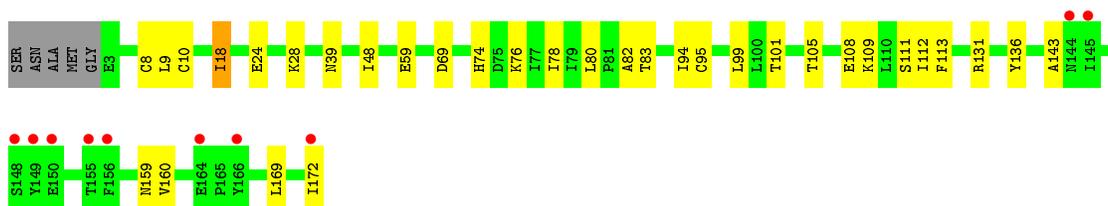
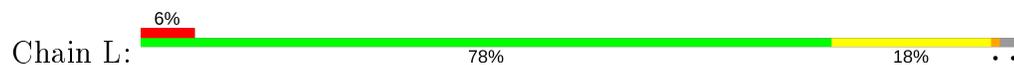
- Molecule 1: Epidermin biosynthesis protein EpiD



- Molecule 1: Epidermin biosynthesis protein EpiD



- Molecule 1: Epidermin biosynthesis protein EpiD



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.99Å 111.26Å 154.57Å 90.00° 97.25° 90.00°	Depositor
Resolution (Å)	45.80 – 2.04 45.75 – 2.04	Depositor EDS
% Data completeness (in resolution range)	95.0 (45.80-2.04) 95.0 (45.75-2.04)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.05Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.208 , 0.263 0.212 , 0.266	Depositor DCC
R_{free} test set	8182 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtrriage
Anisotropy	1.195	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18797	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0001e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.95	1/1477 (0.1%)	0.88	0/2003
1	B	0.86	0/1446	0.81	1/1961 (0.1%)
1	C	0.90	0/1411	0.81	0/1913
1	D	0.83	0/1473	0.82	1/1993 (0.1%)
1	E	0.74	0/1444	0.77	4/1959 (0.2%)
1	F	0.76	0/1453	0.75	0/1971
1	G	0.72	0/1460	0.74	0/1978
1	H	0.76	0/1447	0.78	0/1962
1	I	0.76	0/1491	0.81	1/2023 (0.0%)
1	J	0.76	0/1493	0.77	1/2024 (0.0%)
1	K	0.76	0/1489	0.75	0/2014
1	L	0.73	0/1443	0.73	0/1957
All	All	0.80	1/17527 (0.0%)	0.79	8/23758 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	VAL	CB-CG2	6.65	1.66	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	119	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	E	101	THR	CA-CB-CG2	-5.88	104.17	112.40
1	B	119	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	E	99	LEU	CB-CG-CD1	-5.54	101.59	111.00
1	D	58	ASP	CB-CG-OD2	-5.17	113.64	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1424	0	1444	37	0
1	B	1399	0	1402	25	1
1	C	1377	0	1378	50	0
1	D	1418	0	1455	37	0
1	E	1398	0	1415	40	0
1	F	1404	0	1426	43	0
1	G	1410	0	1425	21	0
1	H	1400	0	1420	25	0
1	I	1429	0	1448	39	0
1	J	1431	0	1458	38	0
1	K	1428	0	1481	45	0
1	L	1397	0	1406	37	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	0	0
2	D	31	0	19	1	0
2	E	31	0	19	0	0
2	F	31	0	19	0	0
2	G	31	0	19	0	0
2	H	31	0	19	0	0
2	I	31	0	19	0	0
2	J	31	0	19	1	0
2	K	31	0	19	0	0
2	L	31	0	19	0	0
3	A	2	0	0	0	0
3	D	2	0	0	0	0
3	J	2	0	0	0	0
4	A	157	0	0	3	0
4	B	149	0	0	4	0
4	C	128	0	0	2	0
4	D	166	0	0	7	1
4	E	98	0	0	2	0
4	F	100	0	0	3	0
4	G	154	0	0	6	0
4	H	125	0	0	5	0
4	I	102	0	0	2	0
4	J	131	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	111	0	0	1	0
4	L	83	0	0	4	0
All	All	18797	0	17386	397	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 397 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:C:9:LEU:HD21	1:C:18:ILE:CD1	1.78	1.12
1:A:9:LEU:HD21	1:A:18:ILE:HG13	1.11	1.06
1:J:9[B]:LEU:HD21	1:J:18[B]:ILE:HG13	1.05	1.03
1:A:9:LEU:CD2	1:A:18:ILE:HG13	1.87	1.03
1:C:9:LEU:CD2	1:C:18:ILE:HD13	1.87	1.02

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:GLU:OE2	4:D:195:HOH:O[4_546]	2.07	0.13

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	178/175 (102%)	173 (97%)	5 (3%)	0	100	100
1	B	174/175 (99%)	166 (95%)	8 (5%)	0	100	100
1	C	170/175 (97%)	164 (96%)	6 (4%)	0	100	100
1	D	177/175 (101%)	170 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	174/175 (99%)	169 (97%)	5 (3%)	0	100	100
1	F	175/175 (100%)	172 (98%)	2 (1%)	1 (1%)	25	15
1	G	175/175 (100%)	171 (98%)	4 (2%)	0	100	100
1	H	174/175 (99%)	166 (95%)	8 (5%)	0	100	100
1	I	179/175 (102%)	175 (98%)	4 (2%)	0	100	100
1	J	179/175 (102%)	175 (98%)	4 (2%)	0	100	100
1	K	179/175 (102%)	174 (97%)	5 (3%)	0	100	100
1	L	174/175 (99%)	167 (96%)	7 (4%)	0	100	100
All	All	2108/2100 (100%)	2042 (97%)	65 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	30	ASP

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	166/160 (104%)	164 (99%)	2 (1%)	71	70
1	B	163/160 (102%)	159 (98%)	4 (2%)	47	40
1	C	159/160 (99%)	153 (96%)	6 (4%)	33	26
1	D	166/160 (104%)	157 (95%)	9 (5%)	22	13
1	E	163/160 (102%)	156 (96%)	7 (4%)	29	22
1	F	164/160 (102%)	155 (94%)	9 (6%)	21	13
1	G	164/160 (102%)	164 (100%)	0	100	100
1	H	163/160 (102%)	161 (99%)	2 (1%)	71	70
1	I	168/160 (105%)	163 (97%)	5 (3%)	41	34
1	J	168/160 (105%)	161 (96%)	7 (4%)	30	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	168/160 (105%)	163 (97%)	5 (3%)	41	34
1	L	163/160 (102%)	157 (96%)	6 (4%)	34	27
All	All	1975/1920 (103%)	1913 (97%)	62 (3%)	43	33

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	61[A]	GLU
1	F	131[B]	ARG
1	L	24[A]	GLU
1	F	108	GLU
1	F	148	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	144	ASN
1	F	72	ASN
1	K	72	ASN
1	F	33	ASN
1	H	17	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	G	501	-	31,33,33	1.86	5 (16%)	40,50,50	2.15	10 (25%)
2	FMN	E	501	-	31,33,33	1.56	5 (16%)	40,50,50	2.12	8 (20%)
2	FMN	C	501	-	31,33,33	2.02	8 (25%)	40,50,50	2.54	12 (30%)
2	FMN	A	501	-	31,33,33	1.40	5 (16%)	40,50,50	2.45	12 (30%)
2	FMN	L	501	-	31,33,33	1.82	7 (22%)	40,50,50	2.44	9 (22%)
2	FMN	J	501	-	31,33,33	1.55	4 (12%)	40,50,50	2.23	10 (25%)
2	FMN	H	501	-	31,33,33	1.70	6 (19%)	40,50,50	1.50	5 (12%)
2	FMN	F	501	-	31,33,33	1.76	4 (12%)	40,50,50	2.17	12 (30%)
2	FMN	D	501	-	31,33,33	1.68	7 (22%)	40,50,50	1.87	6 (15%)
2	FMN	B	501	-	31,33,33	1.73	8 (25%)	40,50,50	2.24	11 (27%)
2	FMN	K	501	-	31,33,33	1.79	6 (19%)	40,50,50	2.10	12 (30%)
2	FMN	I	501	-	31,33,33	1.69	7 (22%)	40,50,50	2.70	9 (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	G	501	-	-	0/18/18/18	0/3/3/3
2	FMN	E	501	-	-	0/18/18/18	0/3/3/3
2	FMN	C	501	-	-	3/18/18/18	0/3/3/3
2	FMN	A	501	-	-	1/18/18/18	0/3/3/3
2	FMN	L	501	-	-	1/18/18/18	0/3/3/3
2	FMN	J	501	-	-	5/18/18/18	0/3/3/3
2	FMN	H	501	-	-	0/18/18/18	0/3/3/3
2	FMN	F	501	-	-	3/18/18/18	0/3/3/3
2	FMN	D	501	-	-	4/18/18/18	0/3/3/3
2	FMN	B	501	-	-	0/18/18/18	0/3/3/3
2	FMN	K	501	-	-	3/18/18/18	0/3/3/3
2	FMN	I	501	-	-	2/18/18/18	0/3/3/3

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	FMN	C10-N1	6.36	1.41	1.33
2	G	501	FMN	C4A-N5	5.31	1.40	1.33
2	K	501	FMN	C10-N1	5.15	1.39	1.33
2	C	501	FMN	C5A-N5	4.97	1.43	1.35
2	B	501	FMN	C4A-N5	4.81	1.40	1.33

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	501	FMN	C1'-N10-C9A	10.93	126.89	118.29
2	E	501	FMN	C1'-N10-C9A	9.36	125.66	118.29
2	B	501	FMN	C4-N3-C2	9.28	122.98	115.14
2	L	501	FMN	C1'-N10-C9A	8.73	125.17	118.29
2	J	501	FMN	C4-N3-C2	8.58	122.38	115.14

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	FMN	C5'-O5'-P-O2P
2	C	501	FMN	C5'-O5'-P-O3P
2	A	501	FMN	C5'-O5'-P-O3P
2	J	501	FMN	C5'-O5'-P-O1P
2	J	501	FMN	C5'-O5'-P-O2P

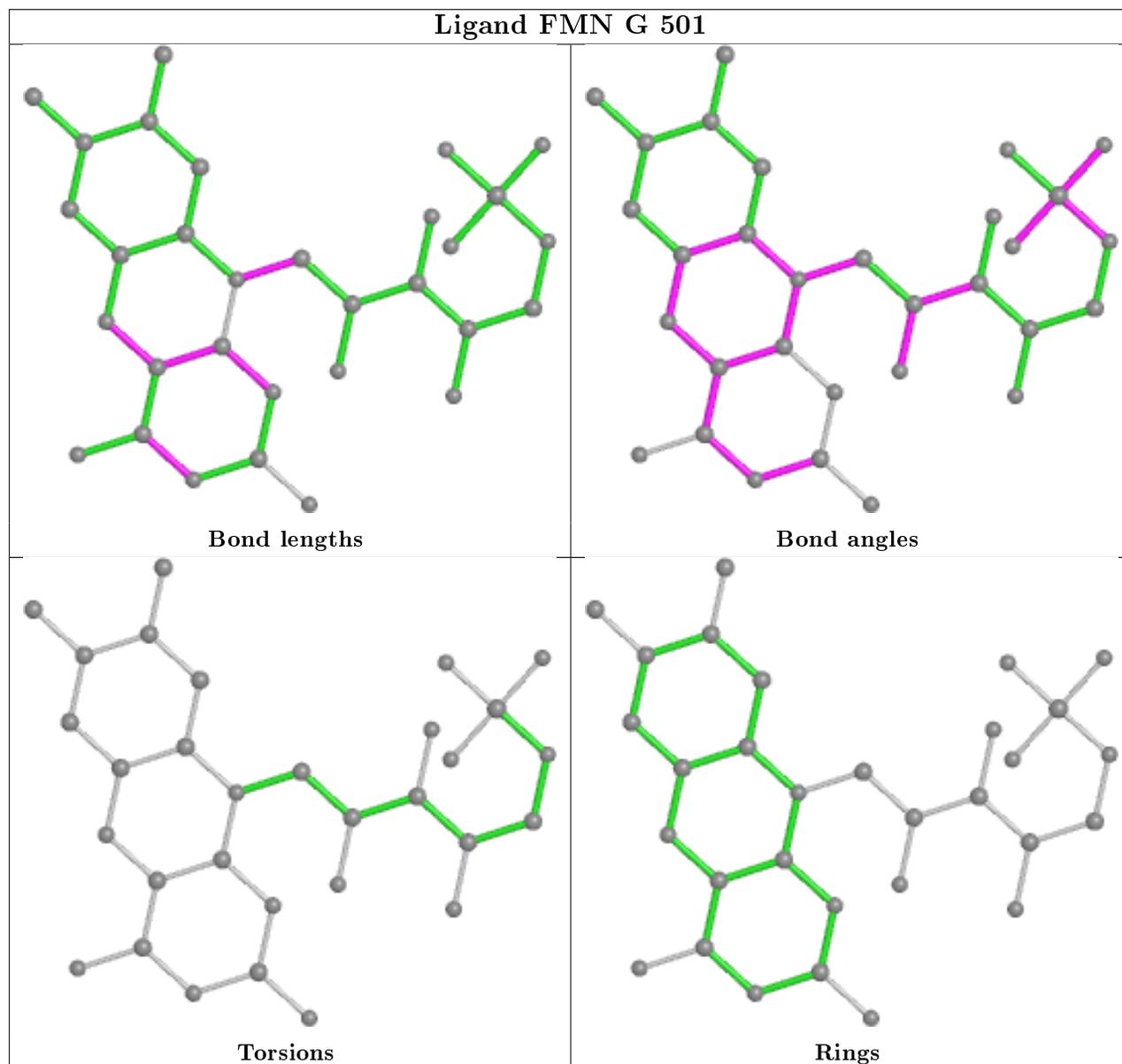
There are no ring outliers.

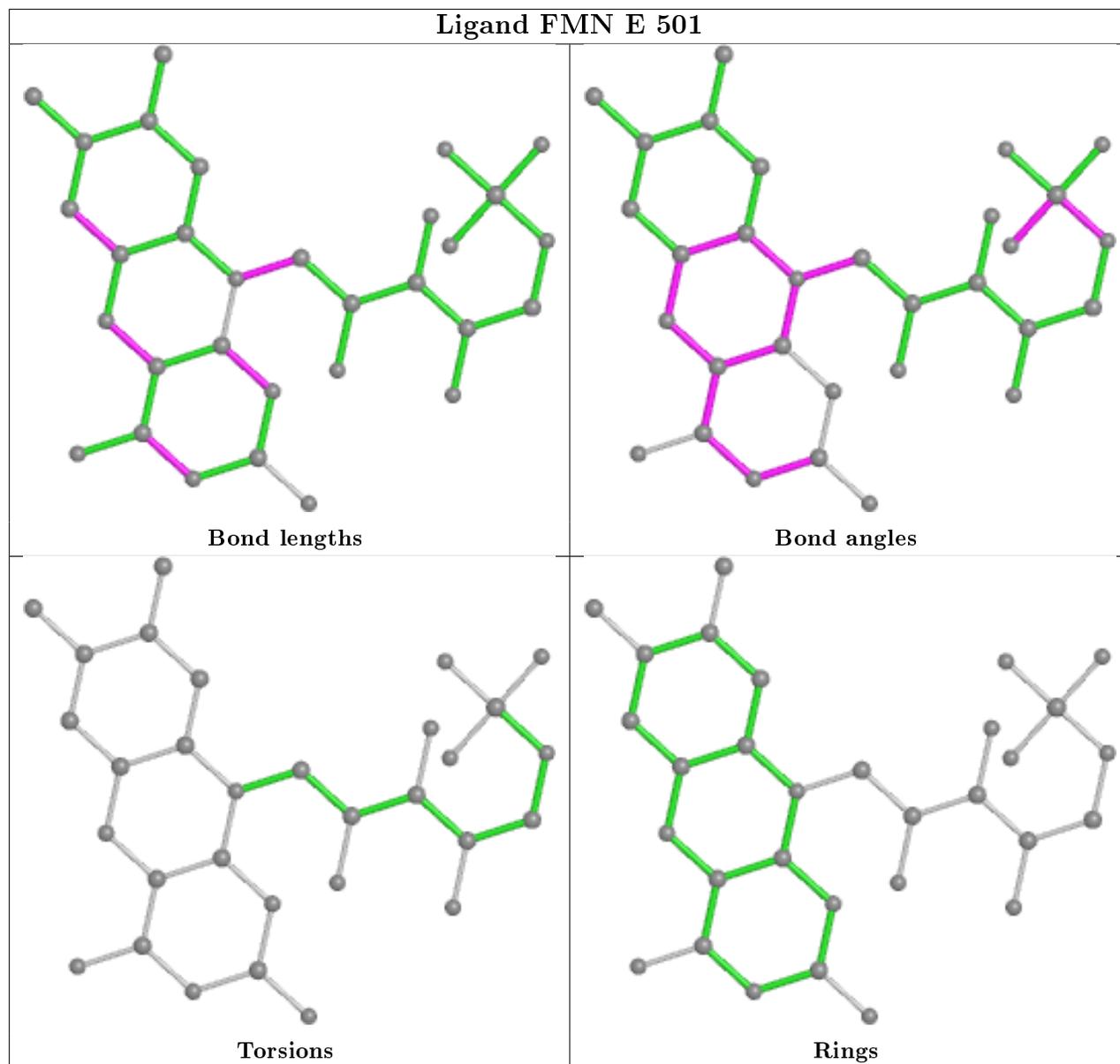
2 monomers are involved in 2 short contacts:

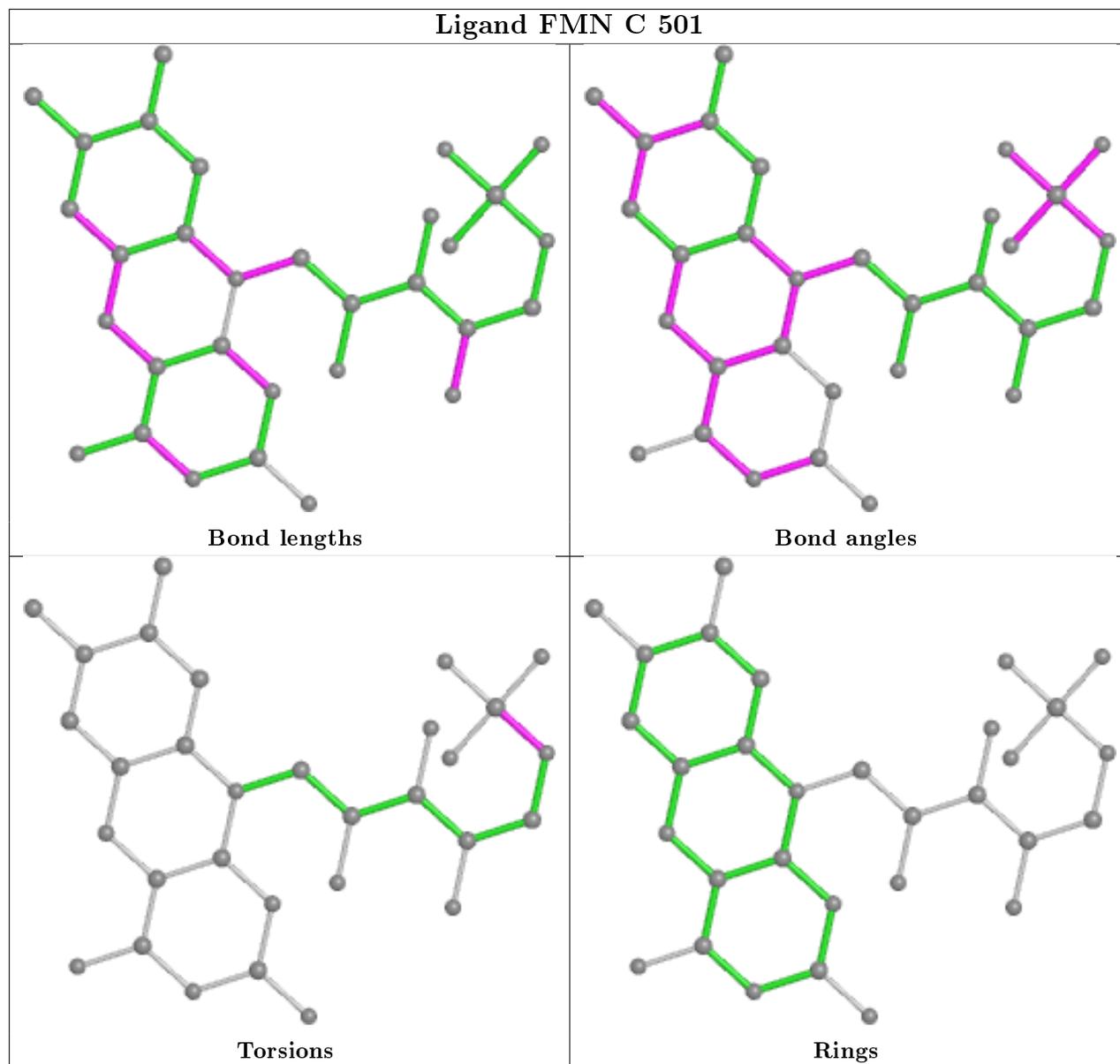
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	501	FMN	1	0
2	D	501	FMN	1	0

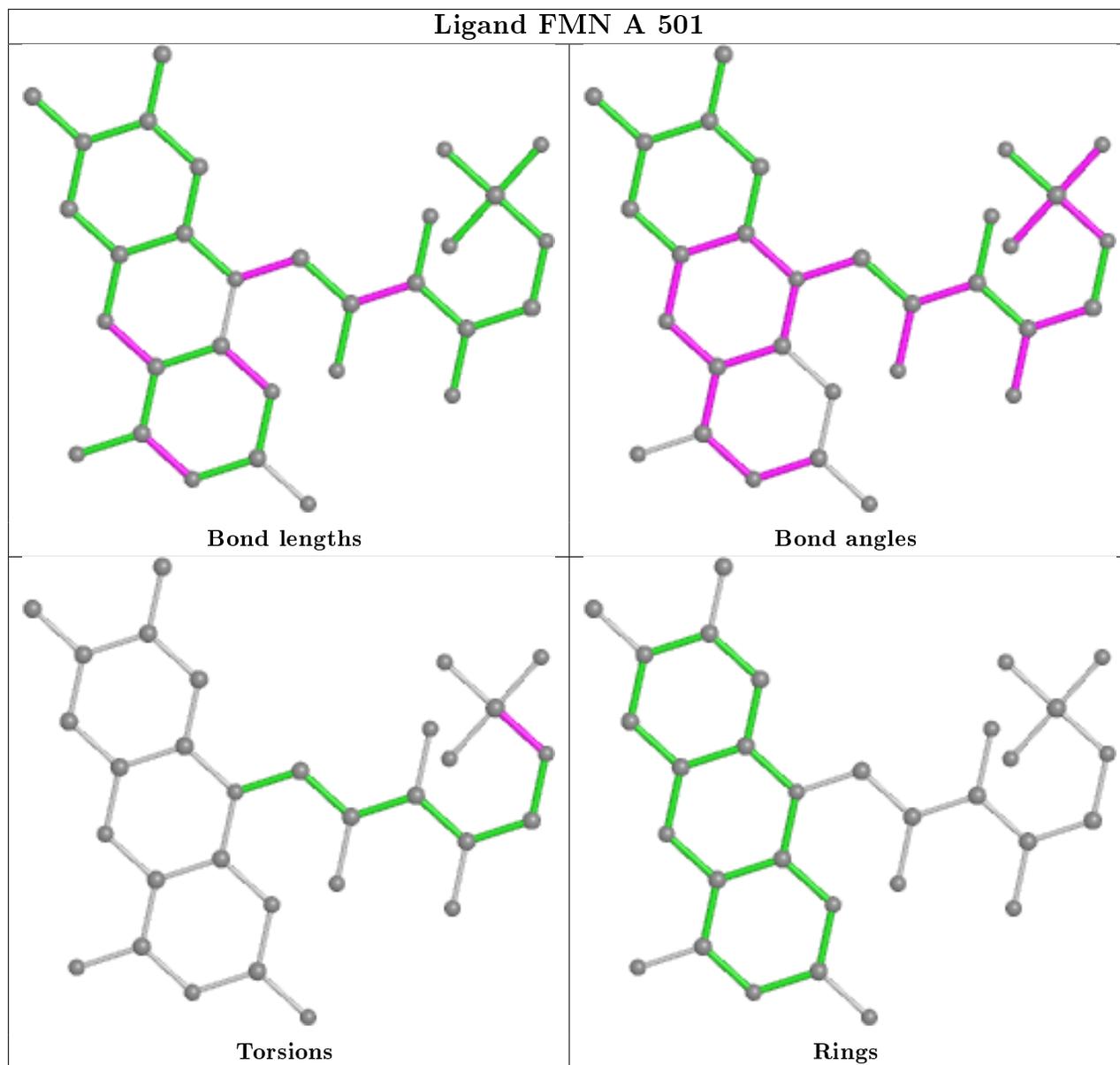
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

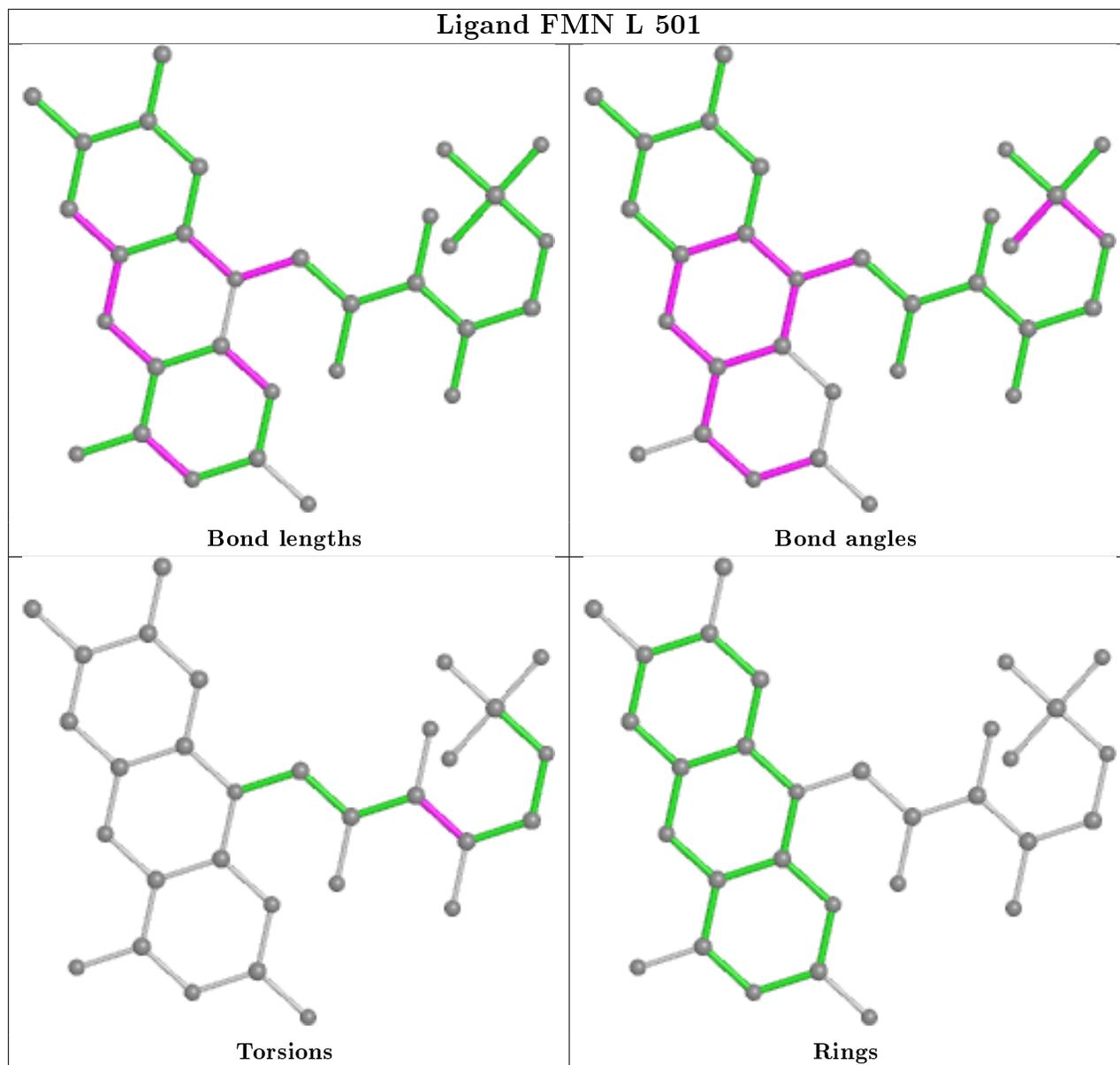
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

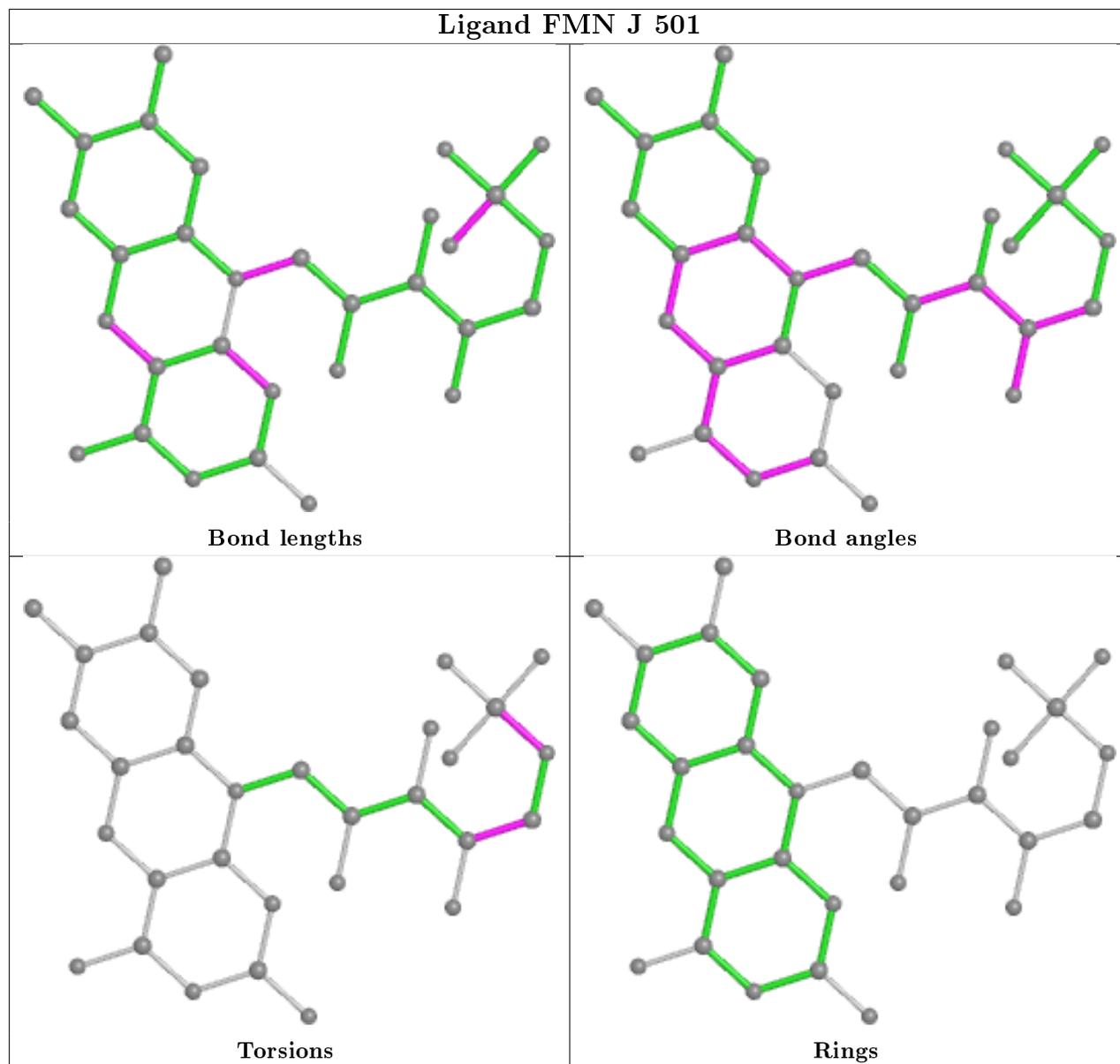


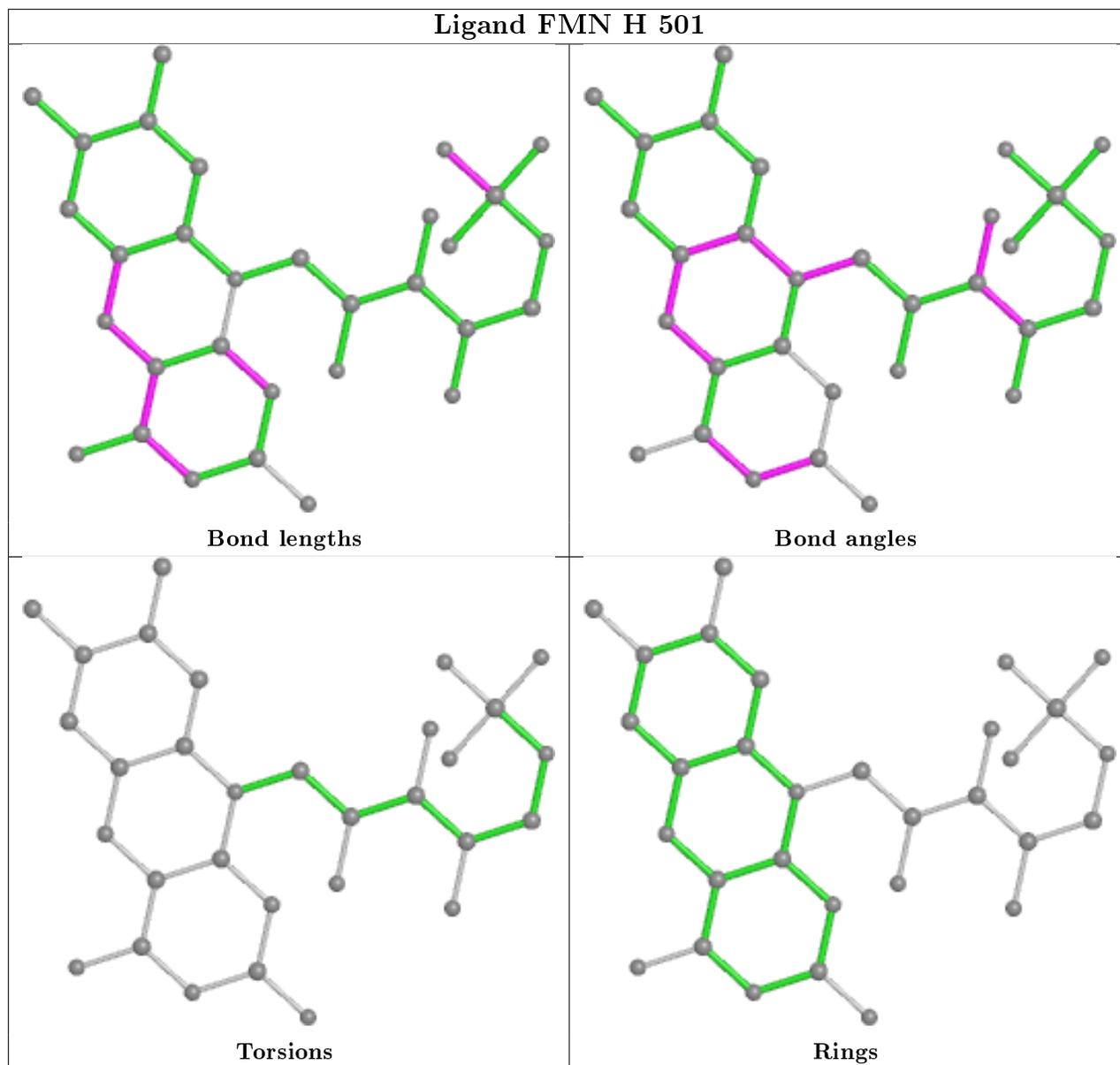


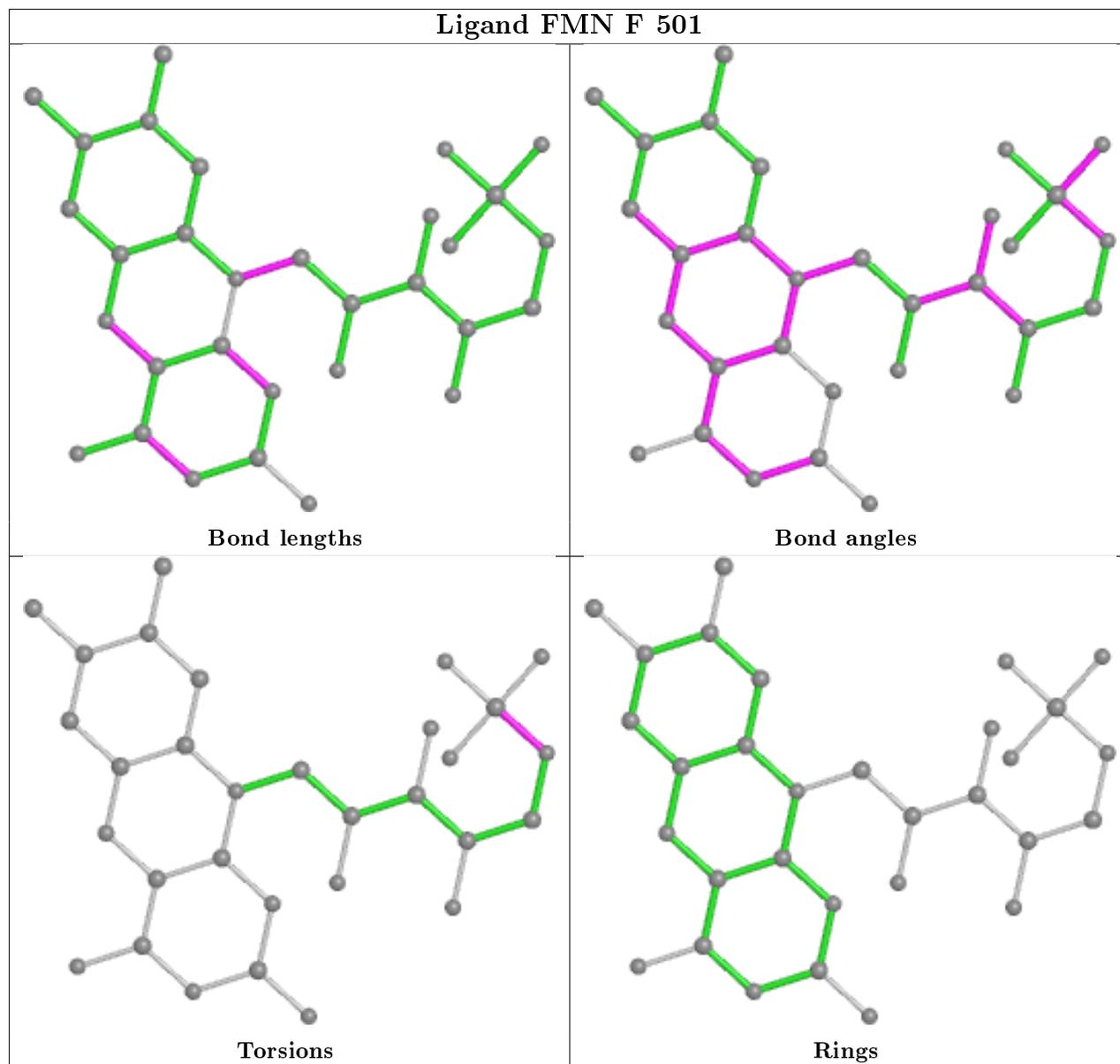


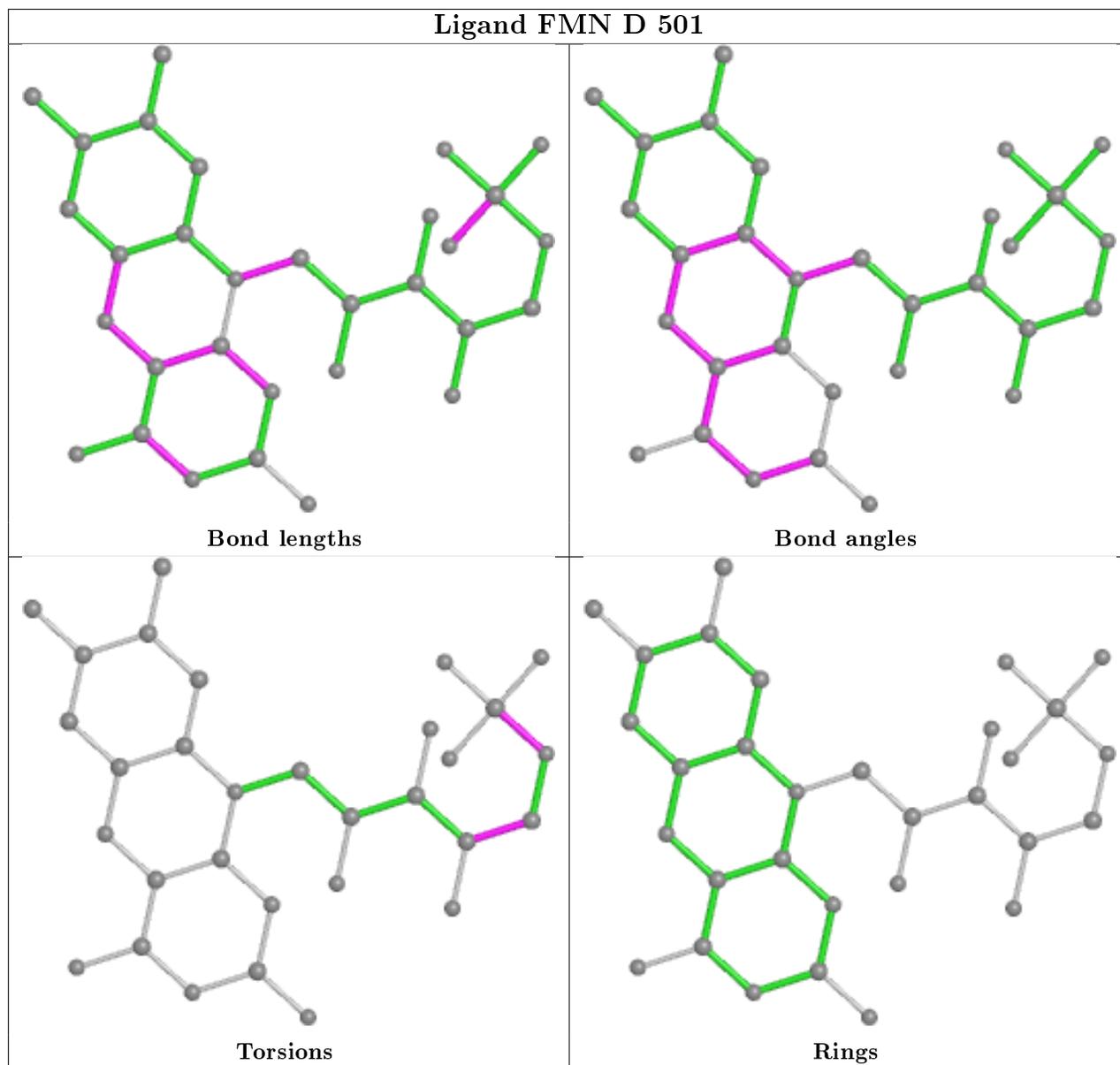


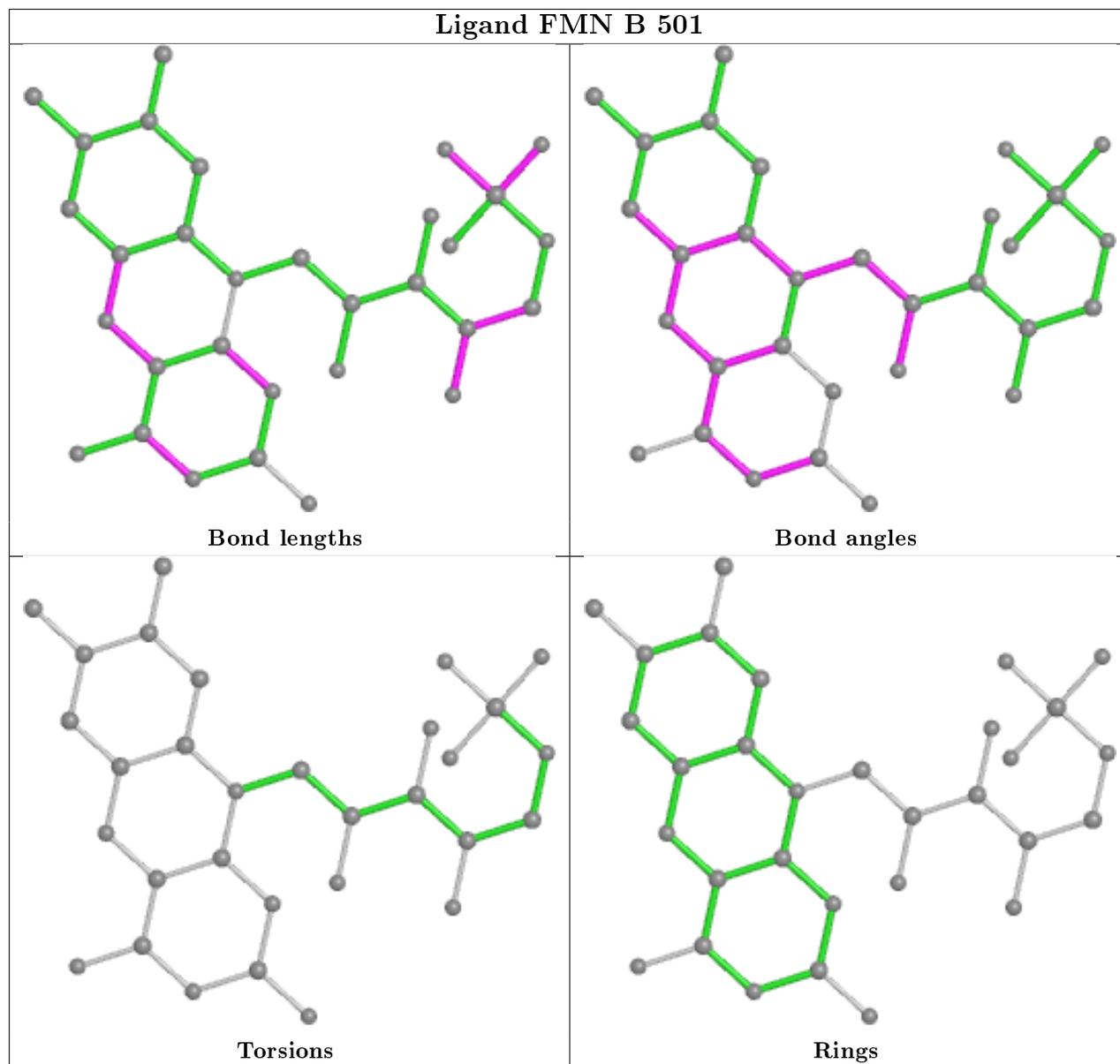


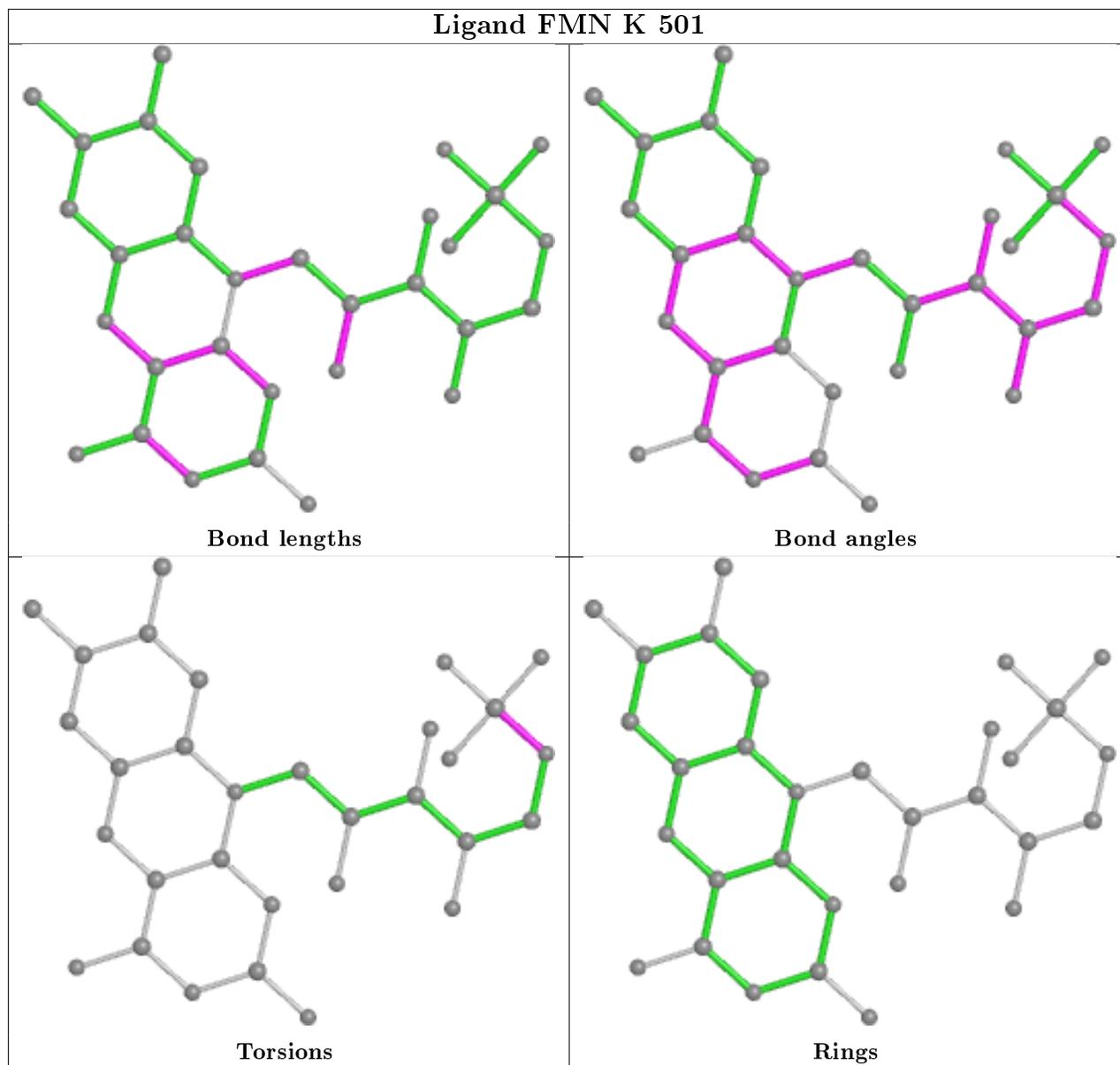


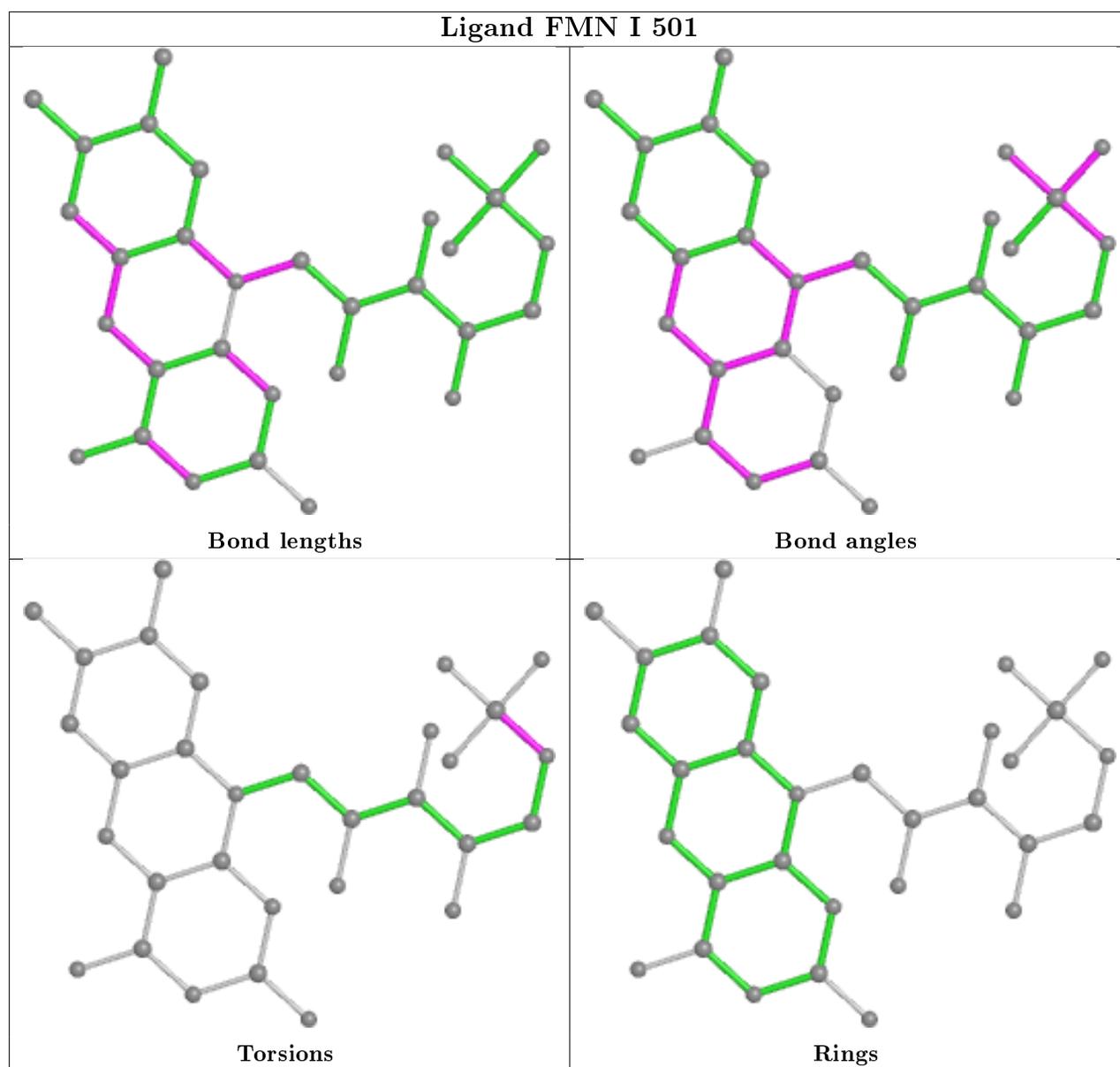












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	171/175 (97%)	0.20	5 (2%) 51 56	12, 25, 40, 49	0
1	B	170/175 (97%)	0.16	2 (1%) 79 81	16, 26, 38, 44	0
1	C	170/175 (97%)	0.34	5 (2%) 51 56	15, 28, 46, 53	0
1	D	170/175 (97%)	0.07	4 (2%) 59 63	18, 28, 42, 47	0
1	E	170/175 (97%)	0.36	14 (8%) 11 12	19, 35, 59, 69	0
1	F	170/175 (97%)	0.35	9 (5%) 26 28	22, 34, 50, 57	0
1	G	170/175 (97%)	0.15	4 (2%) 59 63	20, 29, 43, 52	0
1	H	170/175 (97%)	0.10	4 (2%) 59 63	20, 30, 43, 49	0
1	I	170/175 (97%)	0.41	17 (10%) 7 7	18, 31, 53, 60	0
1	J	170/175 (97%)	0.21	7 (4%) 37 40	19, 30, 45, 52	0
1	K	170/175 (97%)	0.18	5 (2%) 51 56	22, 33, 47, 56	0
1	L	170/175 (97%)	0.48	10 (5%) 22 24	21, 35, 60, 66	0
All	All	2041/2100 (97%)	0.25	86 (4%) 36 39	12, 30, 49, 69	0

The worst 5 of 86 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	166	TYR	5.5
1	L	155	THR	5.3
1	A	2	GLY	5.2
1	G	144[A]	ASN	4.7
1	I	144	ASN	4.5

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 carbohydrates in this entry.

6.4 Ligands [i](#)

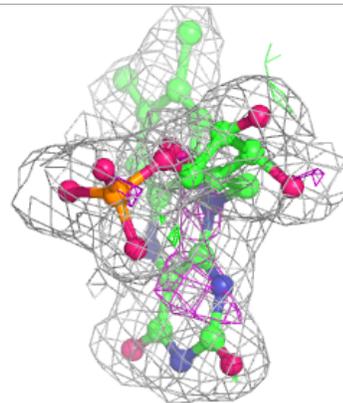
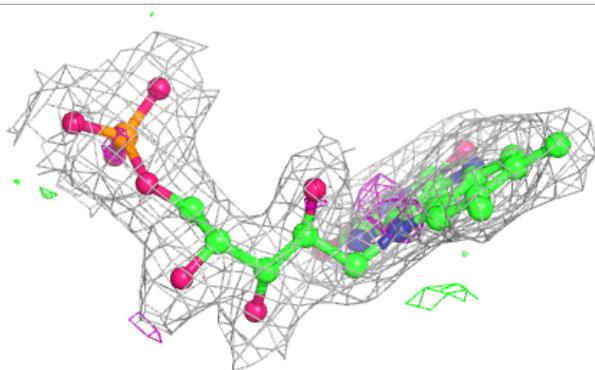
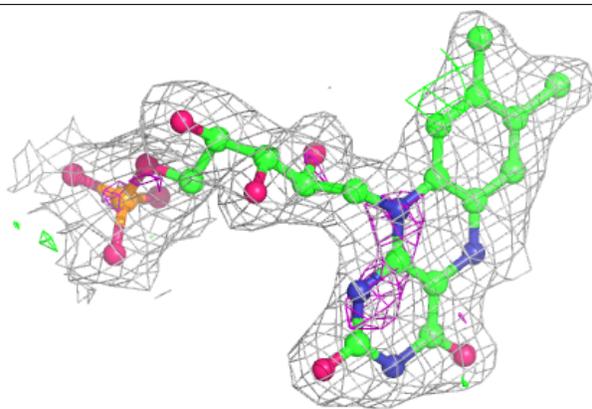
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FMN	E	501	31/31	0.95	0.12	23,27,30,35	0
2	FMN	C	501	31/31	0.95	0.12	14,21,23,25	0
2	FMN	L	501	31/31	0.95	0.11	19,26,30,31	0
2	FMN	F	501	31/31	0.95	0.10	21,25,28,28	0
2	FMN	K	501	31/31	0.95	0.13	19,25,27,28	0
2	FMN	I	501	31/31	0.95	0.12	20,23,26,28	0
2	FMN	J	501	31/31	0.96	0.12	19,25,29,29	0
3	CL	D	702	1/1	0.96	0.07	31,31,31,31	0
2	FMN	D	501	31/31	0.96	0.11	17,22,26,28	0
2	FMN	B	501	31/31	0.96	0.14	12,18,22,23	0
2	FMN	A	501	31/31	0.96	0.13	13,18,21,22	0
2	FMN	G	501	31/31	0.96	0.12	18,24,28,28	0
2	FMN	H	501	31/31	0.97	0.12	17,22,25,26	0
3	CL	J	704	1/1	0.98	0.08	30,30,30,30	0
3	CL	D	706	1/1	0.98	0.08	33,33,33,33	0
3	CL	J	703	1/1	0.98	0.07	29,29,29,29	0
3	CL	A	701	1/1	0.99	0.07	23,23,23,23	0
3	CL	A	705	1/1	0.99	0.10	32,32,32,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

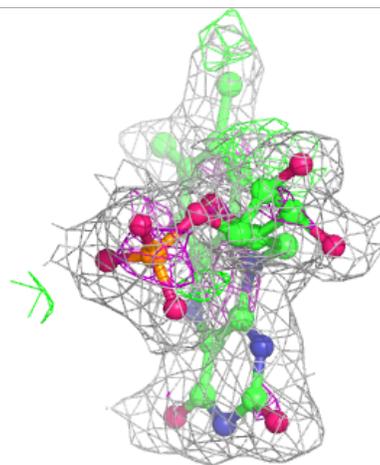
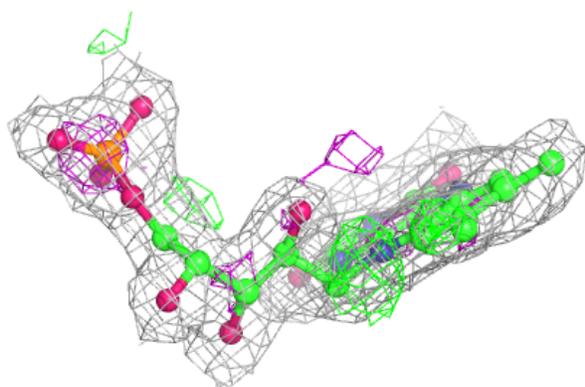
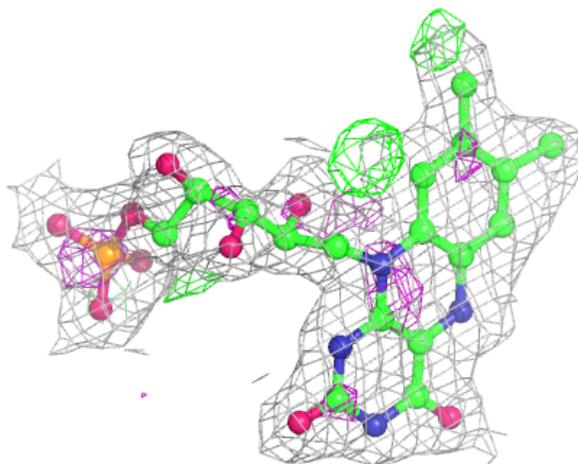
Electron density around FMN E 501:

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



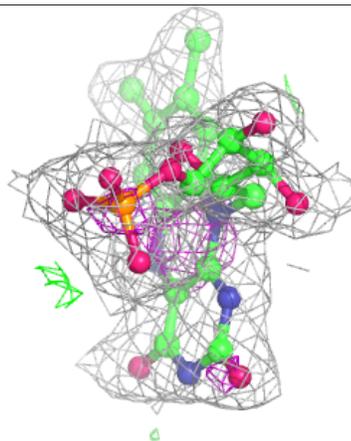
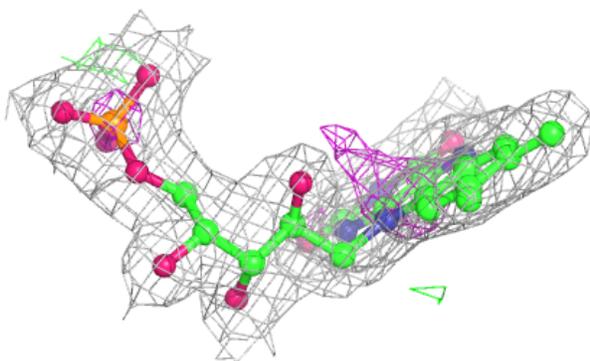
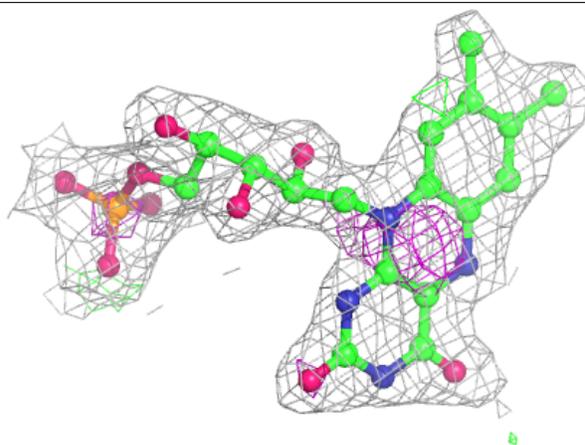
Electron density around FMN C 501:

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



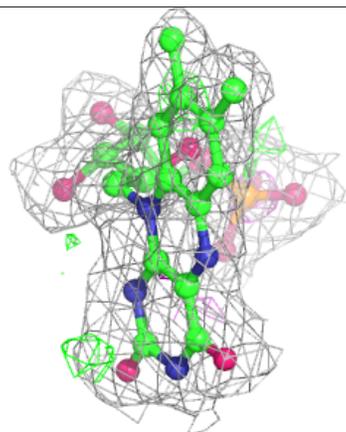
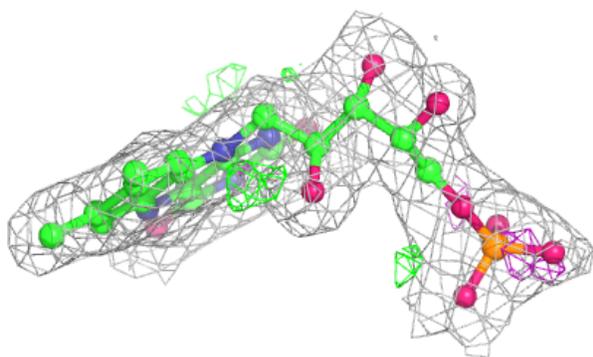
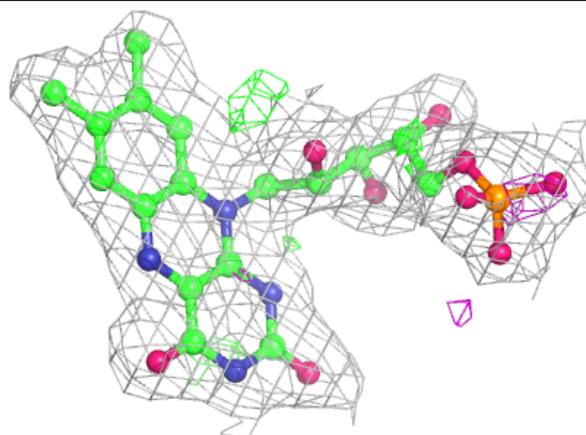
Electron density around FMN L 501:

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and green (positive)

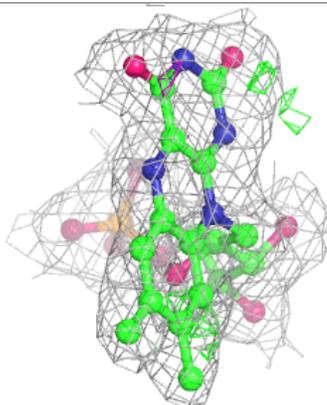
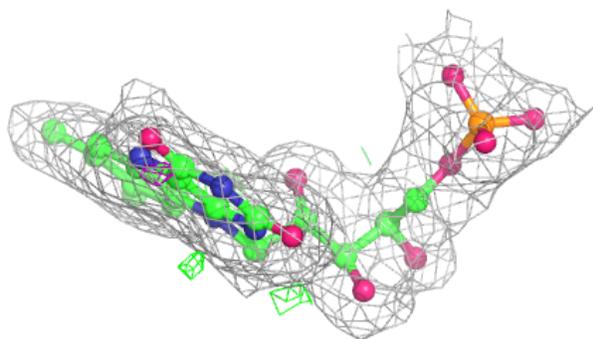
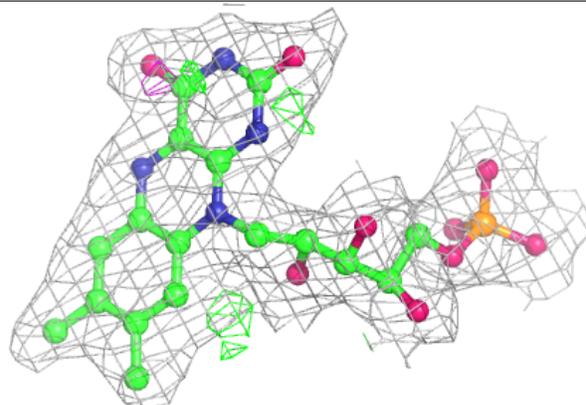


Electron density around FMN F 501:

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and green (positive)

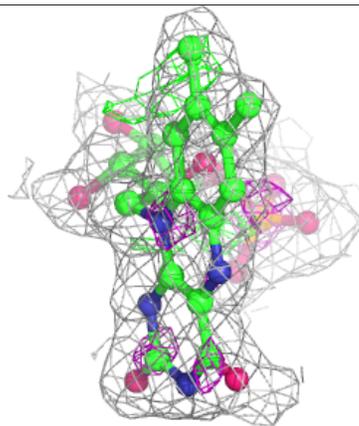
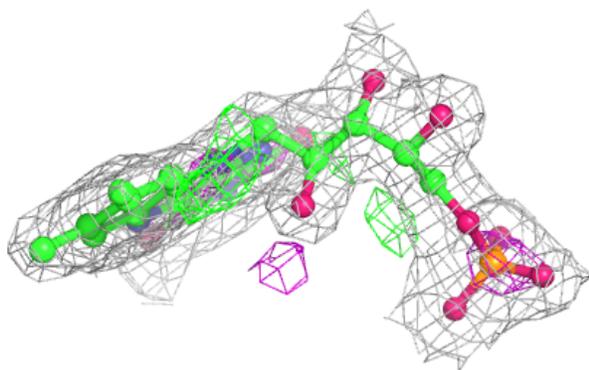
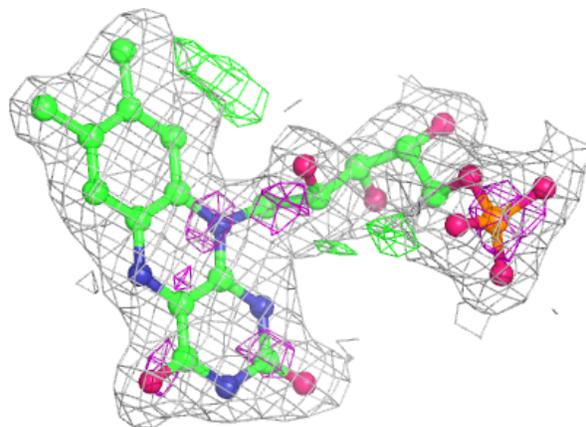
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and green (positive)

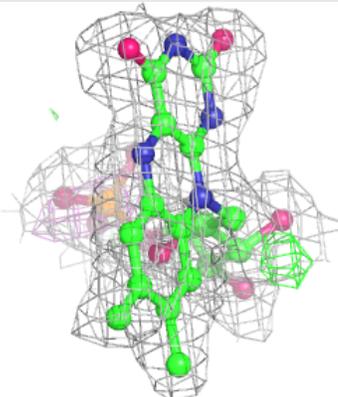
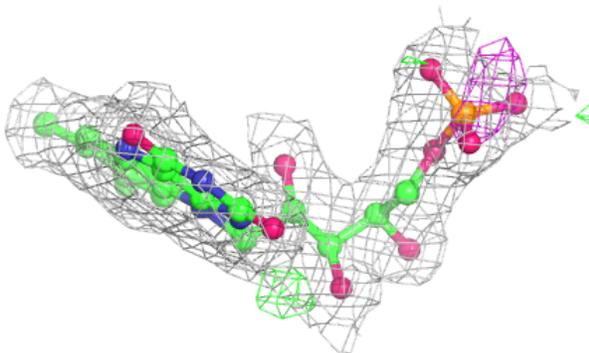
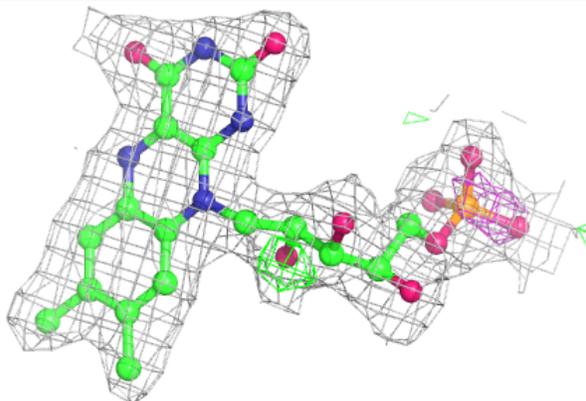


Electron density around FMN I 501:

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and green (positive)

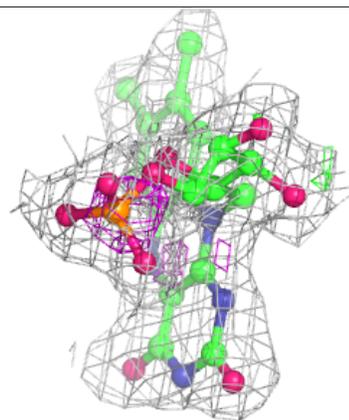
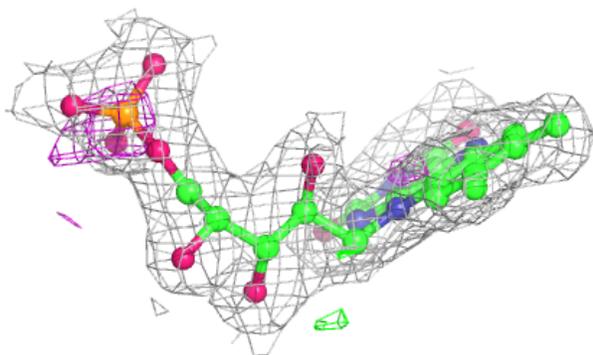
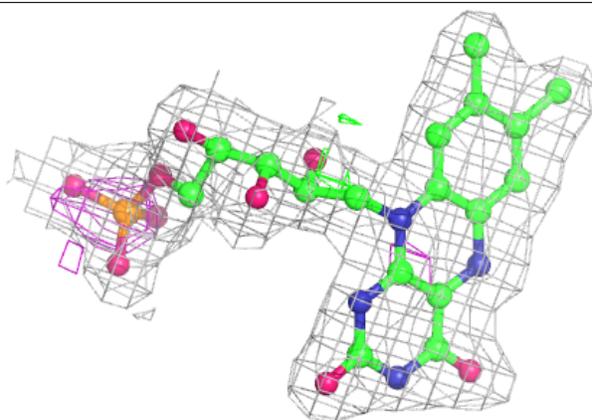
**Electron density around FMN J 501:**

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and green (positive)



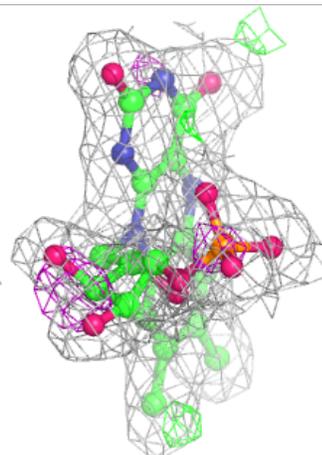
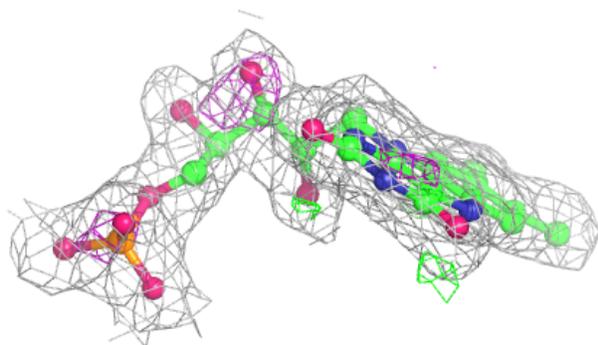
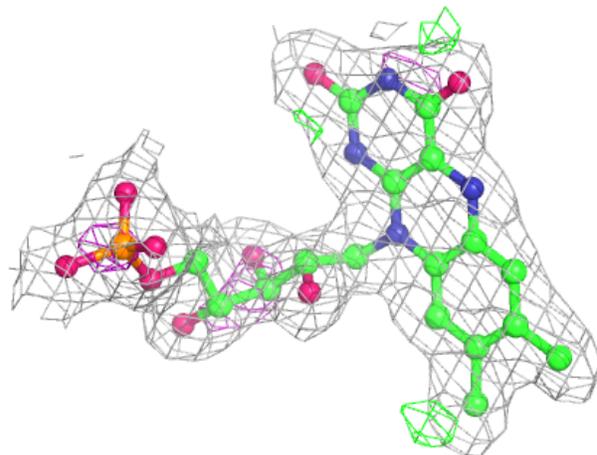
Electron density around FMN D 501:

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



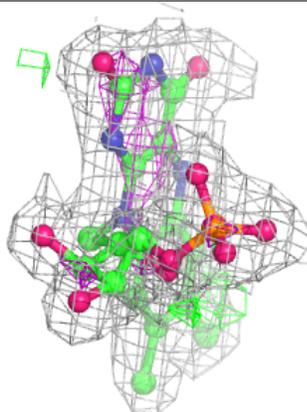
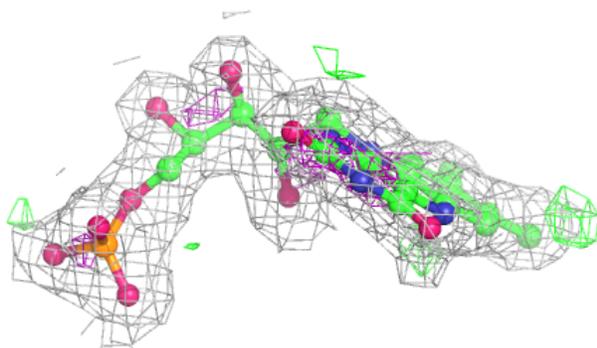
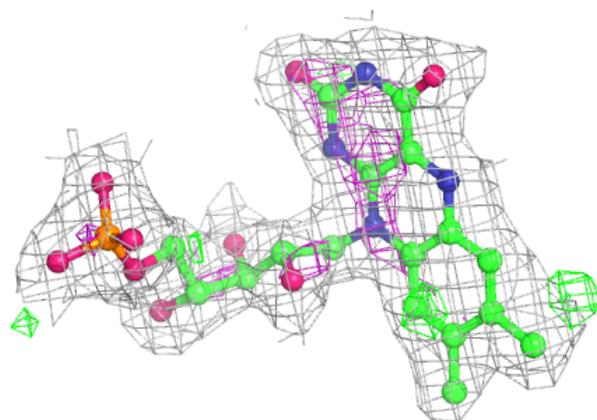
Electron density around FMN B 501:

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



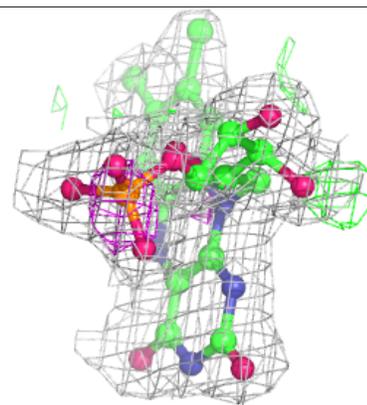
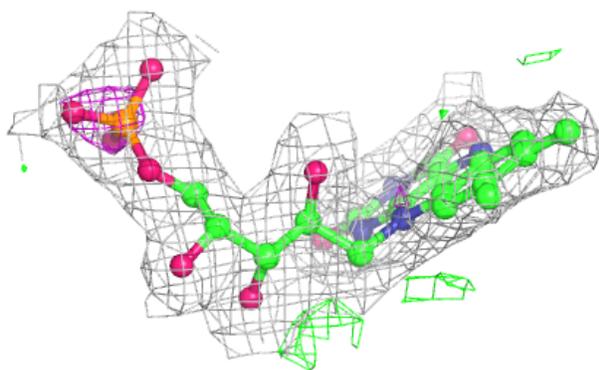
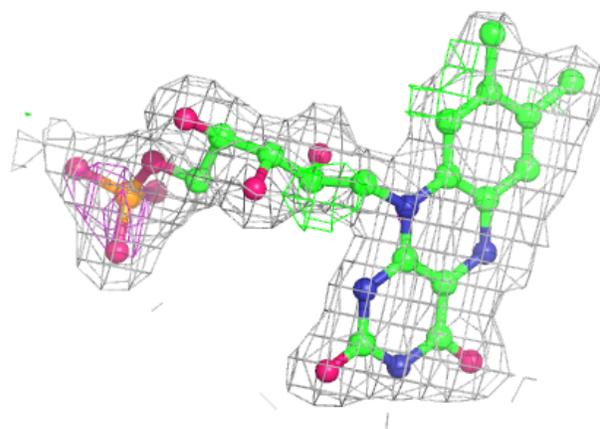
Electron density around FMN A 501:

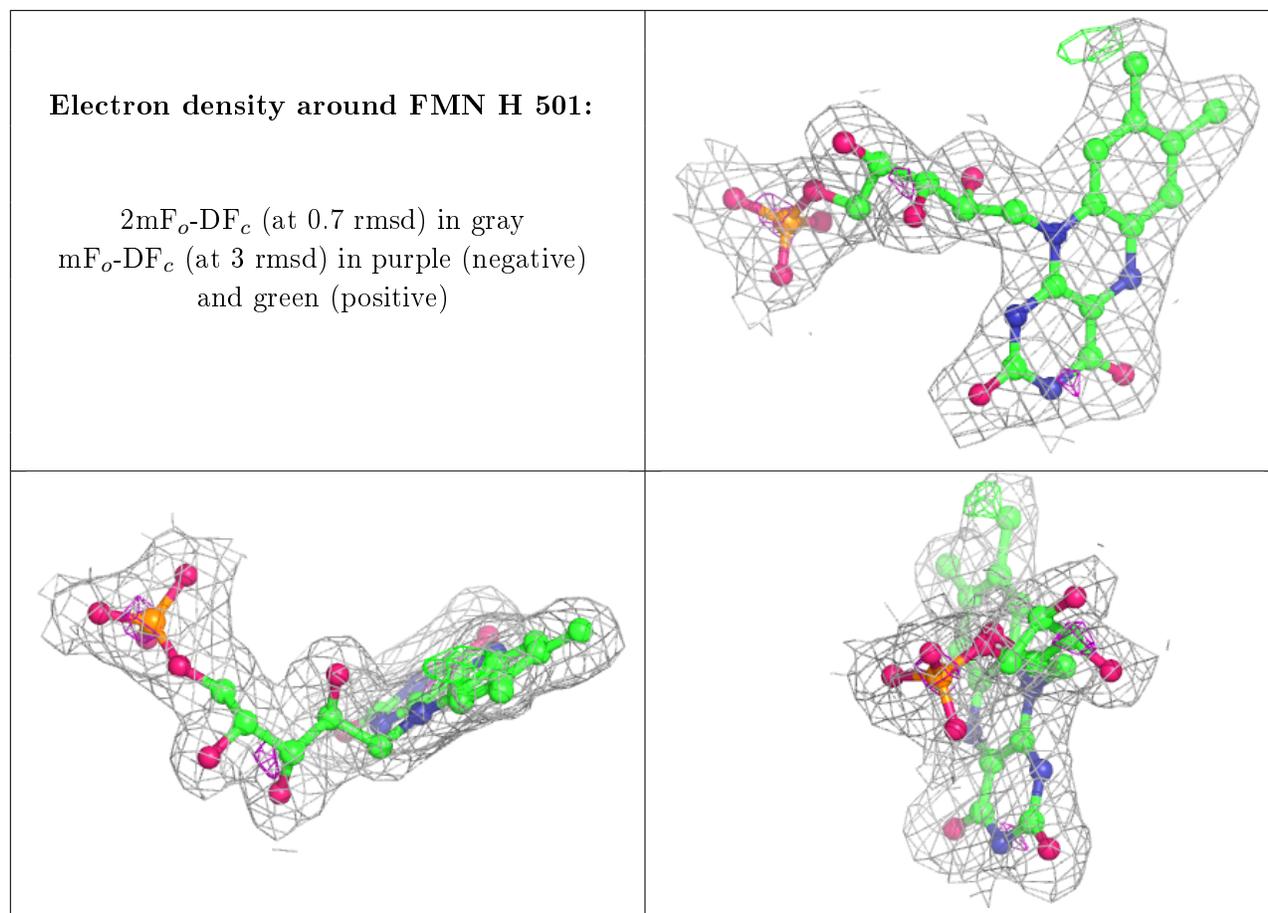
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN G 501:

$2mF_o-DF_c$ (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.