



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:02 PM UTC

PDB ID : 3G5A / pdb_00003g5a
Title : Crystal Structure of Candida glabrata FMN Adenylyltransferase in complex with FMN and ATP analog AMPCPP
Authors : Huerta, C.; Zhang, H.
Deposited on : 2009-02-04
Resolution : 1.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

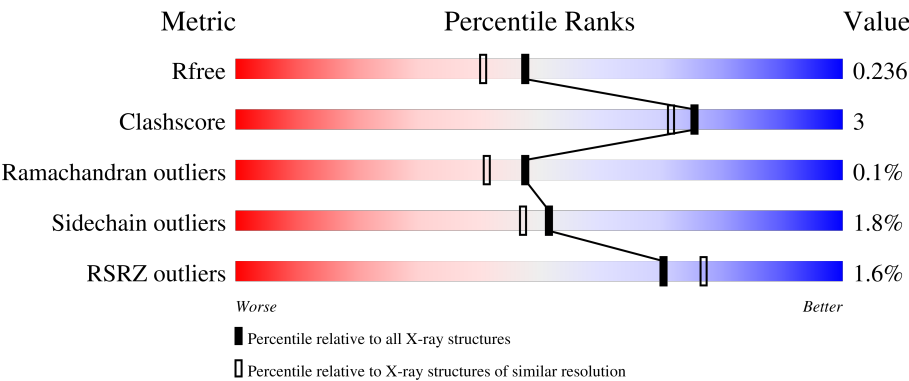
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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.



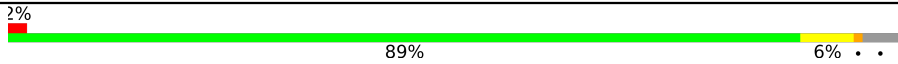
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	308	% 87%9%.
1	B	308	3% 92%7%..
1	C	308	% 87%6%6%
1	D	308	2% 91%6%.
1	E	308	% 86%7%7%

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Mol	Chain	Length	Quality of chain
1	F	308	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '2%', a large green segment labeled '89%', a small yellow segment labeled '6%', and a small grey segment at the end. There are two dots after the 6% label.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16887 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 FMN adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	4	0
			2446	1578	395	464	9			
1	B	305	Total	C	N	O	S	0	2	0
			2529	1634	411	476	8			
1	C	291	Total	C	N	O	S	0	3	0
			2414	1561	388	458	7			
1	D	301	Total	C	N	O	S	0	1	0
			2491	1608	404	472	7			
1	E	286	Total	C	N	O	S	0	2	0
			2371	1531	381	452	7			
1	F	297	Total	C	N	O	S	0	3	0
			2449	1581	395	464	9			

There are 24 discrepancies between the modelled and reference sequences:

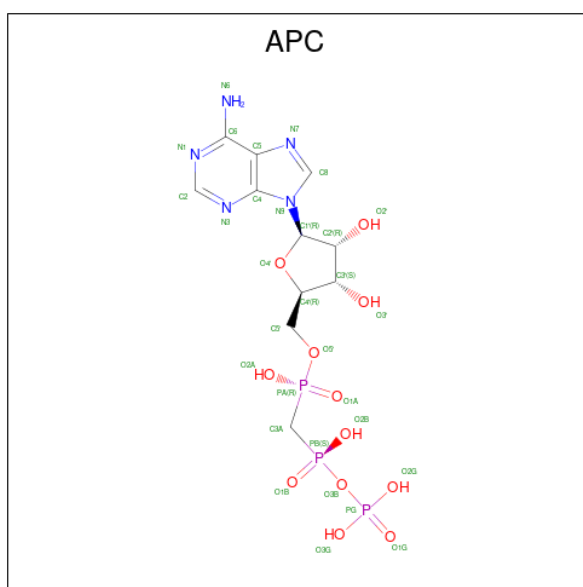
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q6FNA9
A	-2	ALA	-	expression tag	UNP Q6FNA9
A	-1	MET	-	expression tag	UNP Q6FNA9
A	0	VAL	-	expression tag	UNP Q6FNA9
B	-3	GLY	-	expression tag	UNP Q6FNA9
B	-2	ALA	-	expression tag	UNP Q6FNA9
B	-1	MET	-	expression tag	UNP Q6FNA9
B	0	VAL	-	expression tag	UNP Q6FNA9
C	-3	GLY	-	expression tag	UNP Q6FNA9
C	-2	ALA	-	expression tag	UNP Q6FNA9
C	-1	MET	-	expression tag	UNP Q6FNA9
C	0	VAL	-	expression tag	UNP Q6FNA9
D	-3	GLY	-	expression tag	UNP Q6FNA9
D	-2	ALA	-	expression tag	UNP Q6FNA9
D	-1	MET	-	expression tag	UNP Q6FNA9
D	0	VAL	-	expression tag	UNP Q6FNA9
E	-3	GLY	-	expression tag	UNP Q6FNA9

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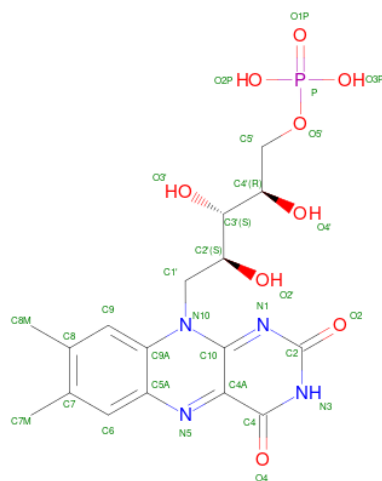
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	ALA	-	expression tag	UNP Q6FNA9
E	-1	MET	-	expression tag	UNP Q6FNA9
E	0	VAL	-	expression tag	UNP Q6FNA9
F	-3	GLY	-	expression tag	UNP Q6FNA9
F	-2	ALA	-	expression tag	UNP Q6FNA9
F	-1	MET	-	expression tag	UNP Q6FNA9
F	0	VAL	-	expression tag	UNP Q6FNA9

- Molecule 2 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			45	13	5	21	6		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	E	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

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



- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).



- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		

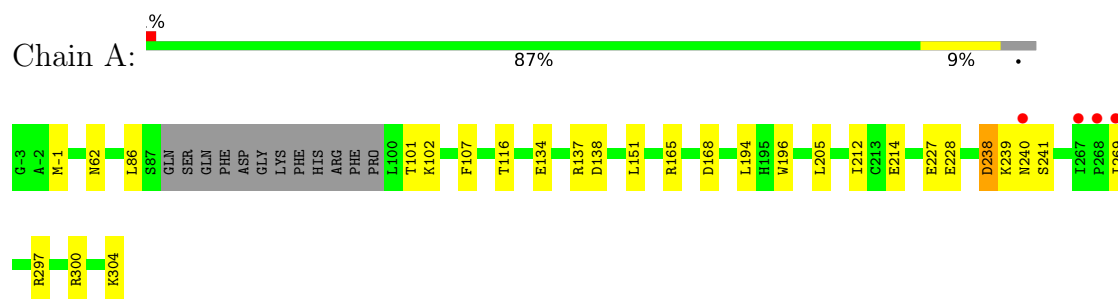
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	316	Total	O	0	0
			316	316		
6	B	311	Total	O	0	0
			311	311		
6	C	311	Total	O	0	0
			311	311		
6	D	285	Total	O	0	0
			285	285		
6	E	269	Total	O	0	0
			269	269		
6	F	298	Total	O	0	0
			298	298		

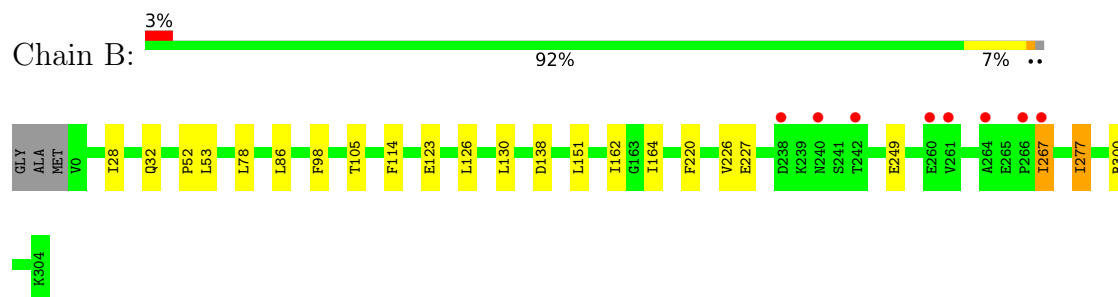
3 Residue-property plots [i](#)

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.

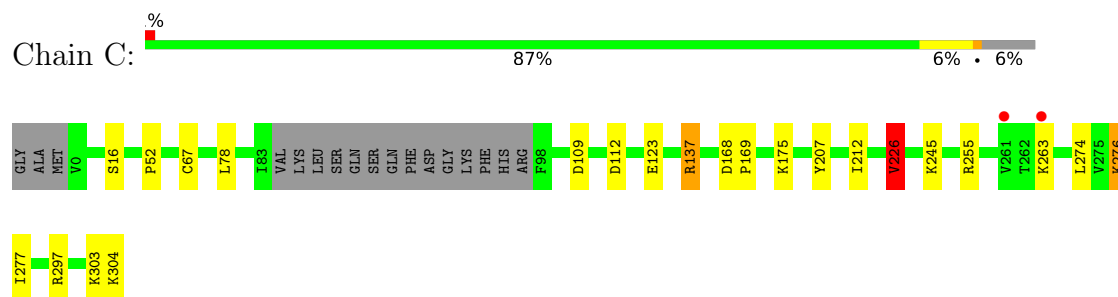
• Molecule 1: FMN adenylyltransferase



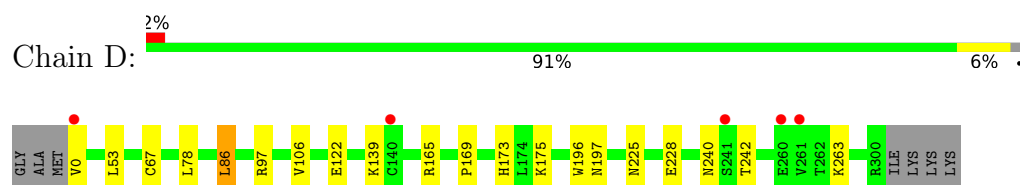
• Molecule 1: FMN adenylyltransferase



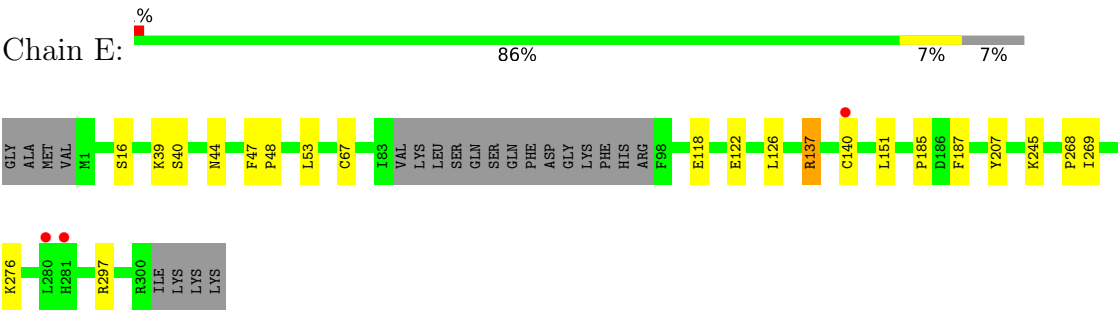
• Molecule 1: FMN adenylyltransferase



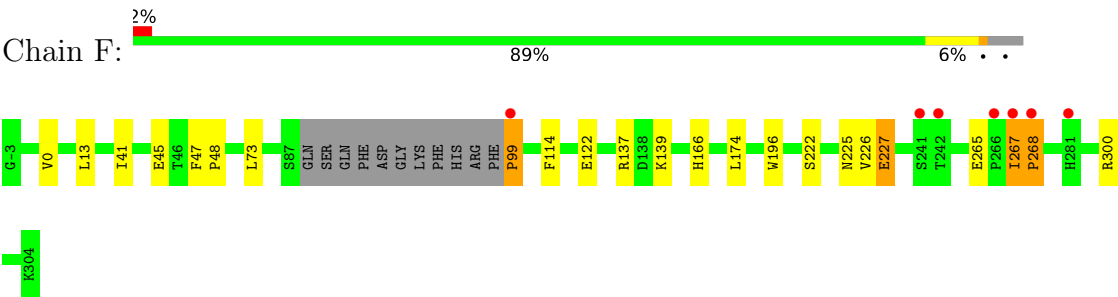
• Molecule 1: FMN adenylyltransferase



● Molecule 1: FMN adenylyltransferase



● Molecule 1: FMN adenylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.83Å 81.75Å 136.70Å 90.00° 129.67° 90.00°	Depositor
Resolution (Å)	35.07 – 1.95 35.07 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.3 (35.07-1.95) 96.2 (35.07-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.175 , 0.236 0.175 , 0.236	Depositor DCC
R_{free} test set	6202 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16887	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0079e-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, SO4, MG, APC

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	0.82	0/2524	0.90	0/3429
1	B	0.79	0/2605	0.91	5/3539 (0.1%)
1	C	0.78	0/2489	0.89	1/3384 (0.0%)
1	D	0.77	0/2564	0.88	0/3487
1	E	0.78	1/2443 (0.0%)	0.91	0/3325
1	F	0.80	0/2524	0.89	0/3429
All	All	0.79	1/15149 (0.0%)	0.90	6/20593 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	140	CYS	CB-SG	-11.64	1.42	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	ILE	CA-C-N	-6.53	113.92	120.31
1	B	267	ILE	C-N-CA	-6.53	113.92	120.31
1	B	300	ARG	N-CA-C	6.43	119.75	108.75
1	C	226	VAL	CB-CA-C	-5.87	103.06	112.16
1	B	98	PHE	CA-C-N	5.21	124.72	119.19
1	B	98	PHE	C-N-CA	5.21	124.72	119.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	267	ILE	Peptide

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	2446	0	2397	19	0
1	B	2529	0	2473	16	0
1	C	2414	0	2360	16	0
1	D	2491	0	2418	16	0
1	E	2371	0	2297	16	0
1	F	2449	0	2403	13	0
2	A	45	0	10	2	0
2	B	31	0	14	0	0
2	C	31	0	14	1	0
2	D	31	0	14	1	0
2	E	31	0	14	2	0
2	F	31	0	14	0	0
3	A	31	0	19	1	0
3	B	31	0	19	0	0
3	C	31	0	19	1	0
3	D	31	0	19	0	0
3	E	31	0	19	2	0
3	F	31	0	19	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	D	5	0	0	0	0
6	A	316	0	0	3	0
6	B	311	0	0	1	0
6	C	311	0	0	6	0
6	D	285	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	269	0	0	2	0
6	F	298	0	0	3	0
All	All	16887	0	14542	89	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (89) 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:A:304:LYS:HB3	1:C:245:LYS:HZ3	1.39	0.86
1:D:173:HIS:HB3	1:E:268:PRO:HG3	1.59	0.85
1:F:99:PRO:HB3	6:F:1685:HOH:O	1.81	0.80
1:D:53:LEU:HD11	1:D:86:LEU:HD21	1.62	0.79
1:B:227:GLU:HG2	1:D:197:ASN:ND2	1.98	0.77
1:F:225:ASN:OD1	1:F:227:GLU:HG3	1.85	0.77
1:C:263:LYS:HG2	6:C:1366:HOH:O	1.85	0.76
1:E:67:CYS:HB3	2:E:305:APC:O3'	1.94	0.68
1:C:168:ASP:OD1	1:C:297:ARG:NH2	2.26	0.68
1:E:118:GLU:OE2	1:E:137:ARG:NH2	2.23	0.67
1:A:240:ASN:HB2	6:A:436:HOH:O	2.00	0.62
3:E:306:FMN:H9	3:E:306:FMN:H2'	1.82	0.61
1:B:53:LEU:HD11	1:B:86:LEU:HD11	1.83	0.61
1:A:304:LYS:HE3	1:C:245:LYS:HD3	1.82	0.61
1:B:114:PHE:HA	1:B:226:VAL:CG1	2.31	0.60
1:B:220:PHE:HE2	1:B:277:ILE:HD11	1.66	0.58
1:D:122:GLU:HG3	6:D:1455:HOH:O	2.03	0.58
3:E:306:FMN:H2'	3:E:306:FMN:C9	2.34	0.58
1:B:227:GLU:HG2	1:D:197:ASN:CG	2.29	0.58
1:D:165:ARG:HD2	1:D:196:TRP:O	2.05	0.56
1:C:175:LYS:HE3	1:F:268:PRO:HG2	1.88	0.55
1:A:116:THR:HG21	1:A:269:ILE:HG22	1.89	0.55
1:C:123:GLU:HG2	6:C:847:HOH:O	2.08	0.53
1:B:28:ILE:O	1:B:32:GLN:HG3	2.08	0.53
1:B:220:PHE:CE2	1:B:277:ILE:HD11	2.43	0.53
1:B:114:PHE:CD1	1:B:226:VAL:HG12	2.44	0.53
1:B:162:ILE:HG22	1:B:164:ILE:HG13	1.91	0.53
1:E:297:ARG:HD2	6:E:334:HOH:O	2.08	0.52
1:A:62:ASN:OD1	2:A:305[A]:APC:H3A1	2.09	0.52
1:A:102:LYS:HE3	6:F:1003:HOH:O	2.09	0.52
1:C:109:ASP:CG	1:C:137:ARG:HB3	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1133:HOH:O	1:F:267:ILE:HG21	2.10	0.51
1:B:138:ASP:CG	1:D:169:PRO:HA	2.35	0.50
1:A:304:LYS:HB3	1:C:245:LYS:NZ	2.21	0.50
1:D:173:HIS:HB3	1:E:268:PRO:CG	2.38	0.50
1:B:249:GLU:HG2	6:B:414:HOH:O	2.11	0.49
1:D:53:LEU:CD1	1:D:86:LEU:HD21	2.36	0.49
1:A:227:GLU:HG3	6:C:352:HOH:O	2.13	0.48
1:E:39:LYS:HE3	6:E:402:HOH:O	2.13	0.47
1:B:52:PRO:HB2	1:B:78:LEU:HD21	1.96	0.47
1:E:151:LEU:HD11	1:E:187:PHE:CD1	2.48	0.47
1:A:238:ASP:OD1	1:A:241:SER:HB2	2.15	0.47
1:C:16:SER:OG	1:C:207:TYR:OH	2.30	0.47
1:C:304:LYS:HA	6:C:537:HOH:O	2.14	0.47
1:A:101:THR:O	1:A:102:LYS:HD3	2.15	0.46
1:A:168:ASP:OD1	1:A:297:ARG:NH1	2.48	0.46
1:D:0:VAL:N	6:D:449:HOH:O	2.48	0.46
1:F:222:SER:HB3	1:F:300:ARG:HH12	1.80	0.46
1:F:114:PHE:HA	1:F:226:VAL:CG1	2.45	0.46
1:D:225:ASN:ND2	1:D:228:GLU:OE1	2.42	0.46
1:D:175:LYS:HE3	1:E:269:ILE:O	2.17	0.45
1:E:151:LEU:HD11	1:E:187:PHE:HD1	1.82	0.45
1:C:52:PRO:HB2	1:C:78:LEU:HD21	1.99	0.44
1:E:151:LEU:HD12	1:E:185:PRO:HB2	1.99	0.44
1:D:67:CYS:HB3	2:D:305:APC:O3'	2.17	0.44
1:D:240:ASN:HB2	6:D:1368:HOH:O	2.17	0.44
1:A:165:ARG:HA	1:A:194:LEU:HA	1.99	0.43
1:A:205:LEU:HG	1:A:212:ILE:HG21	2.01	0.43
1:C:67:CYS:HB3	2:C:305:APC:O3'	2.19	0.43
1:C:112:ASP:O	1:C:226:VAL:HG22	2.18	0.43
1:A:138:ASP:CG	1:C:169:PRO:HA	2.42	0.43
1:A:228:GLU:O	1:A:300:ARG:HA	2.18	0.43
1:A:239:LYS:HE3	1:A:239:LYS:HB2	1.74	0.43
1:C:303:LYS:C	1:C:304:LYS:HG3	2.43	0.43
1:D:97:ARG:HD2	6:D:680:HOH:O	2.18	0.42
1:E:40:SER:O	1:E:44:ASN:HB2	2.18	0.42
1:C:276:LYS:HE2	6:C:1118:HOH:O	2.19	0.42
1:B:126:LEU:HD11	1:E:122:GLU:HG3	2.00	0.42
1:D:263:LYS:HE3	1:D:263:LYS:HB2	1.87	0.42
1:E:47:PHE:N	1:E:48:PRO:CD	2.82	0.42
1:A:165:ARG:HD2	1:A:196:TRP:O	2.20	0.42
1:F:41:ILE:O	1:F:45:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:305:APC:O1B	2:E:305:APC:H5'2	2.20	0.42
1:E:276:LYS:HE2	1:E:276:LYS:HB2	1.91	0.42
1:F:166:HIS:HE1	1:F:174:LEU:O	2.02	0.42
3:C:306:FMN:O3P	6:C:782:HOH:O	2.22	0.41
1:F:47:PHE:N	1:F:48:PRO:CD	2.84	0.41
3:A:306:FMN:H9	3:A:306:FMN:H1'1	1.80	0.41
1:B:123:GLU:HG3	1:E:122:GLU:OE2	2.21	0.41
1:F:139:LYS:HD2	6:F:1195:HOH:O	2.21	0.41
1:A:107:PHE:HD2	1:A:134:GLU:HG2	1.85	0.41
1:B:114:PHE:CG	1:B:226:VAL:HG12	2.56	0.41
1:F:227:GLU:HG3	1:F:227:GLU:H	1.73	0.41
1:F:73:LEU:HD11	1:F:196:TRP:CZ2	2.56	0.41
6:A:766:HOH:O	1:F:0:VAL:HG12	2.21	0.40
1:B:105:THR:HG21	1:B:130:LEU:HD13	2.03	0.40
1:A:214:GLU:HB3	1:A:269:ILE:CG2	2.52	0.40
1:E:16:SER:OG	1:E:207:TYR:OH	2.34	0.40

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	296/308 (96%)	290 (98%)	6 (2%)	0	100	100
1	B	305/308 (99%)	302 (99%)	3 (1%)	0	100	100
1	C	290/308 (94%)	289 (100%)	1 (0%)	0	100	100
1	D	300/308 (97%)	298 (99%)	2 (1%)	0	100	100
1	E	284/308 (92%)	277 (98%)	7 (2%)	0	100	100
1	F	296/308 (96%)	289 (98%)	6 (2%)	1 (0%)	36	28
All	All	1771/1848 (96%)	1745 (98%)	25 (1%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	268	PRO

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	274/281 (98%)	269 (98%)	5 (2%)	51	47
1	B	282/281 (100%)	279 (99%)	3 (1%)	65	64
1	C	270/281 (96%)	263 (97%)	7 (3%)	40	33
1	D	277/281 (99%)	272 (98%)	5 (2%)	51	47
1	E	264/281 (94%)	260 (98%)	4 (2%)	57	54
1	F	274/281 (98%)	268 (98%)	6 (2%)	45	40
All	All	1641/1686 (97%)	1611 (98%)	30 (2%)	51	47

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	MET
1	A	86	LEU
1	A	137	ARG
1	A	151	LEU
1	A	238	ASP
1	B	151	LEU
1	B	267	ILE
1	B	277	ILE
1	C	137	ARG
1	C	212	ILE
1	C	226	VAL
1	C	255	ARG
1	C	274	LEU
1	C	276	LYS
1	C	277	ILE
1	D	78	LEU

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Mol	Chain	Res	Type
1	D	86	LEU
1	D	106	VAL
1	D	139	LYS
1	D	242	THR
1	E	53	LEU
1	E	126	LEU
1	E	137	ARG
1	E	245	LYS
1	F	13	LEU
1	F	99	PRO
1	F	122	GLU
1	F	137	ARG
1	F	227	GLU
1	F	265	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	254	ASN
1	B	173	HIS
1	B	254	ASN
1	B	259	ASN
1	B	281	HIS
1	C	173	HIS
1	C	209	ASN
1	C	254	ASN
1	C	258	HIS
1	D	68	GLN
1	D	96	HIS
1	D	254	ASN
1	E	36	ASN
1	E	68	GLN
1	E	173	HIS
1	E	191	GLN
1	E	254	ASN
1	E	279	ASN
1	F	44	ASN
1	F	254	ASN
1	F	281	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	$\# Z > 2$
5	SO4	D	308	-	4,4,4	0.23	0	6,6,6	0.10	0
3	FMN	F	306	-	33,33,33	1.15	3 (9%)	48,50,50	1.46	10 (20%)
2	APC	A	305[A]	4	29,33,33	1.25	3 (10%)	44,52,52	1.87	11 (25%)
2	APC	D	305	4	29,33,33	1.26	3 (10%)	44,52,52	1.75	9 (20%)
3	FMN	D	306	-	33,33,33	1.04	3 (9%)	48,50,50	1.25	6 (12%)
2	APC	B	305	4	29,33,33	1.31	3 (10%)	44,52,52	1.97	10 (22%)
2	APC	F	305	4	29,33,33	1.39	3 (10%)	44,52,52	1.92	11 (25%)
3	FMN	C	306	-	33,33,33	1.14	3 (9%)	48,50,50	1.40	8 (16%)
3	FMN	A	306	-	33,33,33	1.19	2 (6%)	48,50,50	1.42	10 (20%)
2	APC	C	305	4	29,33,33	1.47	2 (6%)	44,52,52	2.08	10 (22%)
2	APC	E	305	4	29,33,33	1.39	4 (13%)	44,52,52	1.67	8 (18%)
2	APC	A	305[B]	4	29,33,33	1.24	4 (13%)	44,52,52	1.93	13 (29%)
3	FMN	B	306	-	33,33,33	1.17	3 (9%)	48,50,50	1.48	10 (20%)
3	FMN	E	306	-	33,33,33	1.08	2 (6%)	48,50,50	1.40	8 (16%)

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	FMN	F	306	-	-	6/18/18/18	0/3/3/3
2	APC	A	305[A]	4	-	3/19/38/38	0/3/3/3
2	APC	D	305	4	-	2/19/38/38	0/3/3/3
3	FMN	D	306	-	-	8/18/18/18	0/3/3/3
2	APC	B	305	4	-	1/19/38/38	0/3/3/3
2	APC	F	305	4	-	1/19/38/38	0/3/3/3
3	FMN	C	306	-	-	4/18/18/18	0/3/3/3
3	FMN	A	306	-	-	2/18/18/18	0/3/3/3
2	APC	C	305	4	-	3/19/38/38	0/3/3/3
2	APC	E	305	4	-	2/19/38/38	0/3/3/3
2	APC	A	305[B]	4	-	0/19/38/38	0/3/3/3
3	FMN	B	306	-	-	11/18/18/18	0/3/3/3
3	FMN	E	306	-	-	9/18/18/18	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	305	APC	PB-O3B	5.79	1.64	1.58
2	F	305	APC	PB-O3B	5.28	1.64	1.58
2	E	305	APC	PB-O3B	4.51	1.63	1.58
2	B	305	APC	PB-O3B	4.41	1.63	1.58
2	D	305	APC	PB-O3B	4.07	1.62	1.58
2	A	305[B]	APC	PB-O3B	3.75	1.62	1.58
3	C	306	FMN	C4A-N5	3.75	1.38	1.30
2	A	305[A]	APC	PB-O3B	3.74	1.62	1.58
3	E	306	FMN	C4A-N5	3.73	1.38	1.30
3	B	306	FMN	C4A-N5	3.71	1.38	1.30
3	F	306	FMN	C4A-N5	3.69	1.38	1.30
3	A	306	FMN	C4A-N5	3.49	1.38	1.30
3	B	306	FMN	C10-N1	3.10	1.39	1.33
3	E	306	FMN	C10-N1	2.94	1.39	1.33
3	A	306	FMN	C10-N1	2.94	1.39	1.33
3	D	306	FMN	C4A-N5	2.89	1.37	1.30
2	B	305	APC	C8-N7	2.73	1.36	1.31
3	C	306	FMN	C10-N1	2.68	1.38	1.33
2	C	305	APC	PA-O2A	-2.63	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	306	FMN	C10-N1	2.62	1.38	1.33
2	F	305	APC	PB-O2B	-2.60	1.50	1.56
2	E	305	APC	PB-O2B	-2.60	1.50	1.56
3	F	306	FMN	C10-N1	2.60	1.38	1.33
2	D	305	APC	C8-N7	2.44	1.36	1.31
2	B	305	APC	C5-N7	-2.33	1.34	1.39
3	B	306	FMN	C1'-N10	2.31	1.53	1.47
2	E	305	APC	C8-N7	2.31	1.36	1.31
2	A	305[B]	APC	PA-O2A	-2.27	1.50	1.56
2	A	305[B]	APC	PB-O2B	-2.21	1.51	1.56
2	F	305	APC	PA-O2A	-2.15	1.51	1.56
2	A	305[A]	APC	PB-O2B	-2.15	1.51	1.56
2	A	305[A]	APC	C5-N7	-2.08	1.35	1.39
2	A	305[B]	APC	C5-N7	-2.08	1.35	1.39
2	D	305	APC	PB-O2B	-2.08	1.51	1.56
3	F	306	FMN	C5'-C4'	2.07	1.54	1.51
3	D	306	FMN	C1'-N10	2.06	1.52	1.47
3	C	306	FMN	C1'-N10	2.06	1.52	1.47
2	E	305	APC	C4-N9	-2.01	1.33	1.37

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	305	APC	C5-C4-N3	-5.91	118.57	126.72
2	D	305	APC	C5-C4-N3	-5.73	118.83	126.72
2	B	305	APC	N3-C2-N1	-5.63	120.07	128.58
2	A	305[A]	APC	N3-C2-N1	-5.27	120.60	128.58
2	A	305[B]	APC	N3-C2-N1	-5.27	120.60	128.58
2	E	305	APC	N3-C2-N1	-5.23	120.66	128.58
2	C	305	APC	N3-C2-N1	-5.23	120.67	128.58
2	F	305	APC	C5-C4-N3	-5.14	119.64	126.72
2	F	305	APC	N3-C2-N1	-5.04	120.95	128.58
2	A	305[A]	APC	C5-C4-N3	-4.93	119.93	126.72
2	A	305[B]	APC	C5-C4-N3	-4.93	119.93	126.72
2	B	305	APC	C5-C4-N3	-4.87	120.00	126.72
2	E	305	APC	C5-C4-N3	-4.76	120.16	126.72
2	B	305	APC	N9-C8-N7	-4.49	107.56	113.94
2	D	305	APC	N3-C2-N1	-4.41	121.91	128.58
2	C	305	APC	N3-C4-N9	4.20	134.32	127.17
2	F	305	APC	C4-C5-N7	-4.11	105.88	110.58
2	C	305	APC	N9-C8-N7	-4.04	108.20	113.94
2	D	305	APC	N3-C4-N9	3.85	133.72	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	305	APC	C2-N3-C4	3.80	121.11	111.83
2	A	305[A]	APC	C5'-C4'-C3'	-3.76	101.69	115.21
2	C	305	APC	C5-N7-C8	3.68	109.23	103.45
2	F	305	APC	C2-N3-C4	3.59	120.61	111.83
2	D	305	APC	C2-N3-C4	3.58	120.58	111.83
2	F	305	APC	N9-C8-N7	-3.57	108.87	113.94
3	E	306	FMN	C4'-C3'-C2'	-3.53	107.69	113.57
2	B	305	APC	C2-N3-C4	3.53	120.44	111.83
2	A	305[A]	APC	N3-C4-N9	3.45	133.04	127.17
2	A	305[B]	APC	N3-C4-N9	3.45	133.04	127.17
2	A	305[A]	APC	C2-N3-C4	3.45	120.26	111.83
2	A	305[B]	APC	C2-N3-C4	3.45	120.26	111.83
2	B	305	APC	O3G-PG-O2G	3.44	120.68	107.80
3	B	306	FMN	C4A-C10-N10	3.40	121.35	116.48
2	A	305[A]	APC	N9-C8-N7	-3.39	109.12	113.94
2	A	305[B]	APC	N9-C8-N7	-3.39	109.12	113.94
2	A	305[B]	APC	PB-O3B-PG	-3.38	120.33	132.45
3	D	306	FMN	C4A-C10-N10	3.37	121.31	116.48
2	E	305	APC	C2-N3-C4	3.29	119.88	111.83
2	F	305	APC	C5-N7-C8	3.28	108.60	103.45
2	B	305	APC	N3-C4-N9	3.27	132.73	127.17
3	C	306	FMN	C4A-C10-N10	3.26	121.15	116.48
2	B	305	APC	C5-N7-C8	3.24	108.54	103.45
3	F	306	FMN	C4A-C10-N10	3.23	121.11	116.48
3	F	306	FMN	C5'-C4'-C3'	3.22	118.29	112.22
3	B	306	FMN	C4-N3-C2	-3.19	119.98	125.64
2	B	305	APC	C4-N9-C8	3.09	108.99	105.74
2	D	305	APC	N9-C8-N7	-3.01	109.66	113.94
3	A	306	FMN	C1'-C2'-C3'	3.01	117.81	109.66
2	C	305	APC	C4-C5-N7	-2.97	107.19	110.58
2	E	305	APC	N3-C4-N9	2.96	132.21	127.17
3	F	306	FMN	C4-N3-C2	-2.92	120.45	125.64
2	A	305[A]	APC	C5-N7-C8	2.90	108.01	103.45
2	A	305[B]	APC	C5-N7-C8	2.90	108.01	103.45
3	A	306	FMN	C4A-C10-N10	2.88	120.60	116.48
3	C	306	FMN	C4-N3-C2	-2.85	120.59	125.64
2	F	305	APC	N3-C4-N9	2.83	131.98	127.17
2	C	305	APC	O2A-PA-O1A	2.83	119.16	109.95
3	E	306	FMN	C4A-C10-N10	2.82	120.52	116.48
2	B	305	APC	O2A-PA-O1A	2.82	119.12	109.95
2	A	305[A]	APC	C4-C5-N7	-2.80	107.38	110.58
2	A	305[B]	APC	C4-C5-N7	-2.80	107.38	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	306	FMN	C4A-C4-N3	2.79	120.36	113.25
3	F	306	FMN	O3P-P-O5'	2.76	113.87	106.67
3	C	306	FMN	C5A-C9A-N10	2.72	120.42	117.97
2	C	305	APC	O2B-PB-O1B	2.62	118.49	109.95
3	A	306	FMN	C5A-C9A-N10	2.60	120.32	117.97
2	A	305[A]	APC	C4-N9-C8	2.58	108.45	105.74
2	A	305[B]	APC	C4-N9-C8	2.58	108.45	105.74
3	D	306	FMN	C5'-C4'-C3'	2.58	117.08	112.22
3	C	306	FMN	C10-C4A-N5	-2.57	119.55	124.81
2	B	305	APC	C4-C5-N7	-2.57	107.64	110.58
3	C	306	FMN	C4A-C4-N3	2.55	119.75	113.25
3	F	306	FMN	C4A-C4-N3	2.55	119.73	113.25
3	B	306	FMN	C10-C4A-N5	-2.54	119.63	124.81
3	E	306	FMN	C10-C4A-N5	-2.52	119.65	124.81
3	E	306	FMN	O3'-C3'-C4'	2.52	114.65	108.93
3	B	306	FMN	C5A-C9A-N10	2.47	120.20	117.97
3	A	306	FMN	C10-C4A-N5	-2.44	119.82	124.81
2	C	305	APC	C4-N9-C8	2.42	108.28	105.74
3	E	306	FMN	C4-N3-C2	-2.42	121.35	125.64
2	F	305	APC	C4-N9-C8	2.40	108.26	105.74
3	B	306	FMN	O2P-P-O5'	2.40	112.93	106.67
2	F	305	APC	O2A-PA-O1A	2.39	117.74	109.95
3	A	306	FMN	C4A-C4-N3	2.39	119.34	113.25
2	A	305[B]	APC	O2A-PA-O1A	2.38	117.71	109.95
3	B	306	FMN	C5'-C4'-C3'	2.37	116.69	112.22
3	A	306	FMN	C9A-C5A-N5	-2.37	119.94	122.45
2	E	305	APC	N9-C8-N7	-2.37	110.58	113.94
3	D	306	FMN	C10-C4A-N5	-2.36	119.98	124.81
3	F	306	FMN	C10-C4A-N5	-2.36	119.98	124.81
2	F	305	APC	C5-C4-N9	2.36	108.38	105.81
3	E	306	FMN	O4-C4-C4A	-2.34	120.36	126.53
3	F	306	FMN	O4-C4-C4A	-2.33	120.39	126.53
2	F	305	APC	PB-O3B-PG	-2.33	124.11	132.45
3	D	306	FMN	C4-N3-C2	-2.32	121.53	125.64
3	A	306	FMN	C10-N1-C2	2.31	121.86	116.85
2	D	305	APC	C4-C5-N7	-2.30	107.96	110.58
3	D	306	FMN	O2P-P-O5'	2.30	112.66	106.67
3	A	306	FMN	C5'-C4'-C3'	2.29	116.55	112.22
3	A	306	FMN	C4A-C10-N1	-2.28	118.99	124.59
3	A	306	FMN	O3P-P-O5'	2.28	112.61	106.67
3	E	306	FMN	C4A-C4-N3	2.27	119.04	113.25
2	A	305[B]	APC	O2B-PB-O1B	2.26	117.30	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	306	FMN	C1'-C2'-C3'	2.24	115.73	109.66
3	E	306	FMN	C4-C4A-N5	2.24	121.30	118.21
3	B	306	FMN	C4A-C10-N1	-2.23	119.13	124.59
2	A	305[A]	APC	O2B-PB-O1B	2.23	117.19	109.95
2	D	305	APC	C5-N7-C8	2.19	106.90	103.45
2	D	305	APC	C4-N9-C8	2.18	108.03	105.74
3	F	306	FMN	C5A-C9A-N10	2.17	119.93	117.97
3	C	306	FMN	O5'-P-O1P	2.17	112.29	106.44
2	A	305[B]	APC	O2G-PG-O1G	2.10	119.03	110.83
2	E	305	APC	O3B-PG-O1G	-2.08	100.12	111.04
3	F	306	FMN	O2-C2-N1	-2.07	118.36	121.80
2	A	305[A]	APC	C2-N1-C6	2.07	122.13	118.73
2	A	305[B]	APC	C2-N1-C6	2.07	122.13	118.73
2	E	305	APC	O2B-PB-O1B	2.06	116.66	109.95
3	C	306	FMN	C1'-C2'-C3'	2.05	115.22	109.66
2	E	305	APC	C4-C5-N7	-2.05	108.24	110.58
3	F	306	FMN	C4-C4A-N5	2.05	121.04	118.21
3	D	306	FMN	C4A-C4-N3	2.04	118.43	113.25
3	B	306	FMN	C4-C4A-N5	2.02	121.00	118.21
3	C	306	FMN	C4A-C10-N1	-2.01	119.67	124.59
2	D	305	APC	C5-C6-N6	-2.00	118.32	123.29

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	305[A]	APC	PA-C3A-PB-O1B
2	A	305[A]	APC	PA-C3A-PB-O2B
2	A	305[A]	APC	PA-C3A-PB-O3B
2	C	305	APC	PA-C3A-PB-O1B
2	C	305	APC	PA-C3A-PB-O2B
2	C	305	APC	PA-C3A-PB-O3B
2	D	305	APC	PA-C3A-PB-O1B
2	D	305	APC	PA-C3A-PB-O2B
2	E	305	APC	PA-C3A-PB-O1B
3	B	306	FMN	C2'-C3'-C4'-O4'
3	B	306	FMN	C2'-C3'-C4'-C5'
3	B	306	FMN	O3'-C3'-C4'-O4'
3	B	306	FMN	C3'-C4'-C5'-O5'
3	B	306	FMN	O4'-C4'-C5'-O5'
3	B	306	FMN	C5'-O5'-P-O2P
3	B	306	FMN	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
3	C	306	FMN	C5'-O5'-P-O2P
3	C	306	FMN	C5'-O5'-P-O3P
3	D	306	FMN	C3'-C4'-C5'-O5'
3	D	306	FMN	O4'-C4'-C5'-O5'
3	E	306	FMN	C1'-C2'-C3'-O3'
3	E	306	FMN	C1'-C2'-C3'-C4'
3	E	306	FMN	O2'-C2'-C3'-O3'
3	E	306	FMN	O2'-C2'-C3'-C4'
3	E	306	FMN	C3'-C4'-C5'-O5'
3	E	306	FMN	C5'-O5'-P-O2P
3	E	306	FMN	C5'-O5'-P-O3P
3	F	306	FMN	O4'-C4'-C5'-O5'
3	F	306	FMN	C5'-O5'-P-O1P
3	F	306	FMN	C5'-O5'-P-O2P
3	F	306	FMN	C5'-O5'-P-O3P
3	D	306	FMN	C2'-C3'-C4'-O4'
3	B	306	FMN	O3'-C3'-C4'-C5'
3	D	306	FMN	C2'-C3'-C4'-C5'
3	E	306	FMN	O4'-C4'-C5'-O5'
3	D	306	FMN	O3'-C3'-C4'-O4'
3	A	306	FMN	C3'-C4'-C5'-O5'
3	E	306	FMN	C2'-C1'-N10-C9A
3	F	306	FMN	C2'-C3'-C4'-C5'
3	C	306	FMN	C5'-O5'-P-O1P
3	D	306	FMN	O3'-C3'-C4'-C5'
2	B	305	APC	PB-C3A-PA-O2A
2	E	305	APC	PA-C3A-PB-O2B
2	F	305	APC	PB-C3A-PA-O2A
3	B	306	FMN	C5'-O5'-P-O1P
3	F	306	FMN	O3'-C3'-C4'-C5'
3	D	306	FMN	O2'-C2'-C3'-O3'
3	A	306	FMN	O4'-C4'-C5'-O5'
3	B	306	FMN	C1'-C2'-C3'-O3'
3	D	306	FMN	C1'-C2'-C3'-O3'
3	B	306	FMN	O2'-C2'-C3'-O3'
3	C	306	FMN	C2'-C3'-C4'-C5'

There are no ring outliers.

7 monomers are involved in 10 short contacts:

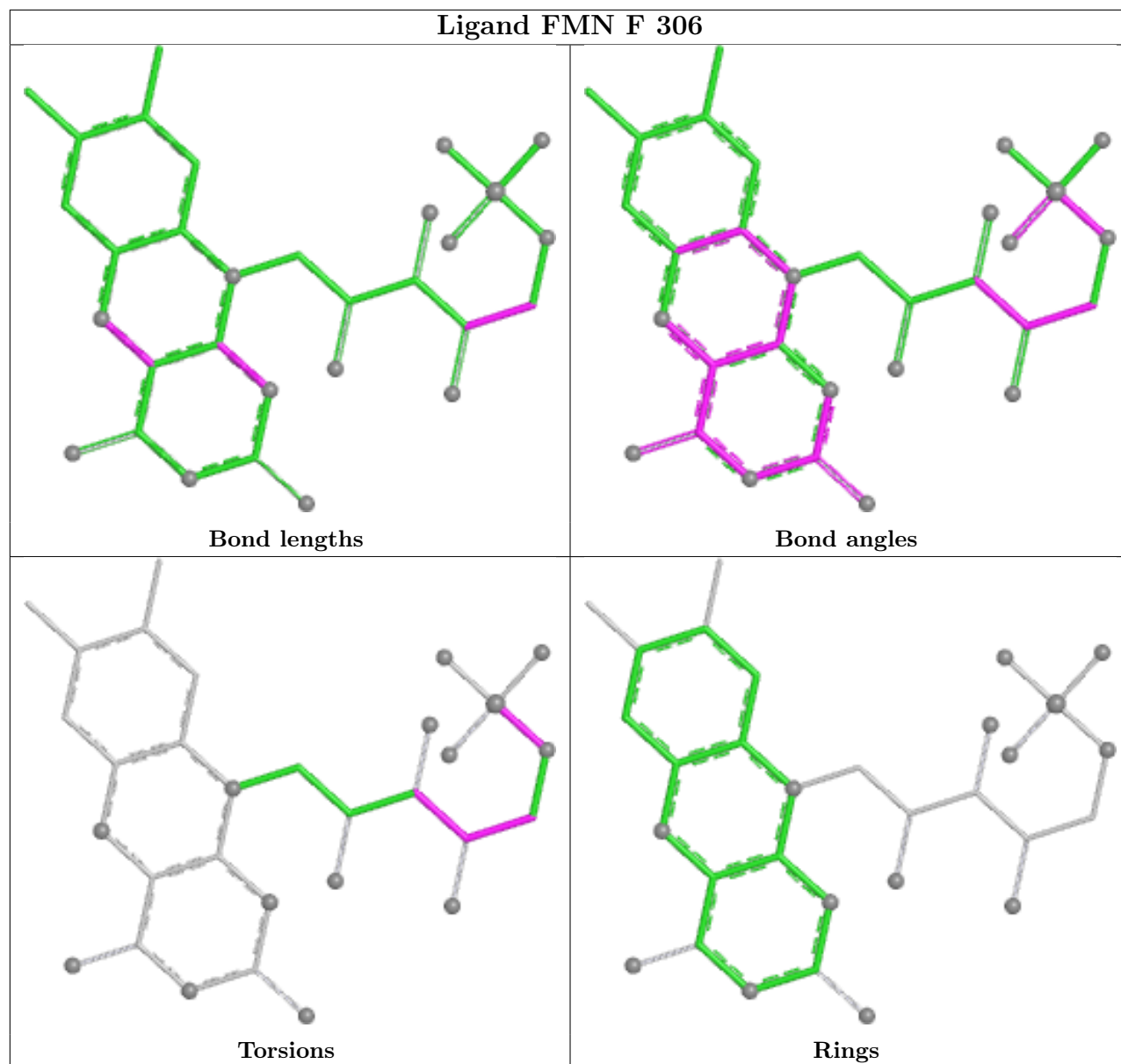
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	305[A]	APC	2	0

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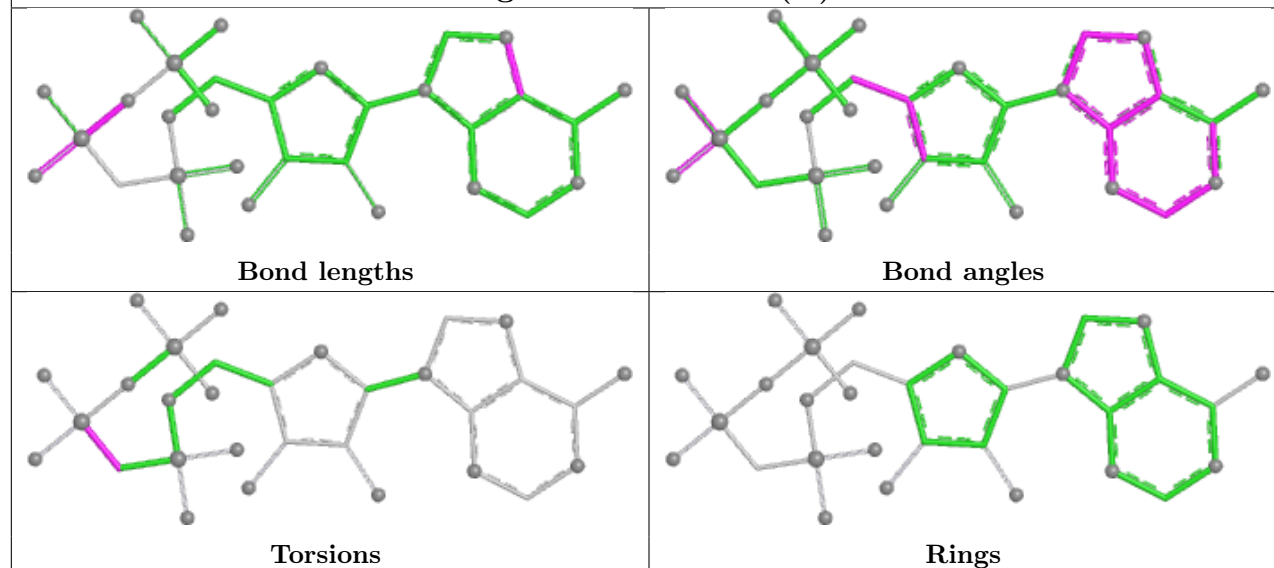
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	305	APC	1	0
3	C	306	FMN	1	0
3	A	306	FMN	1	0
2	C	305	APC	1	0
2	E	305	APC	2	0
3	E	306	FMN	2	0

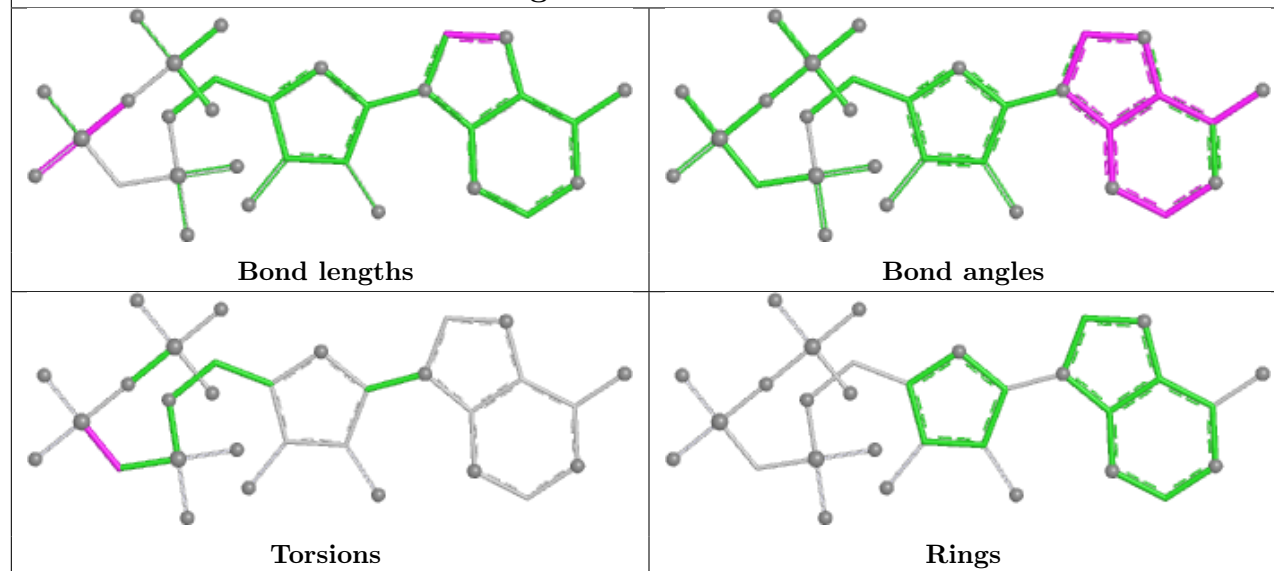
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

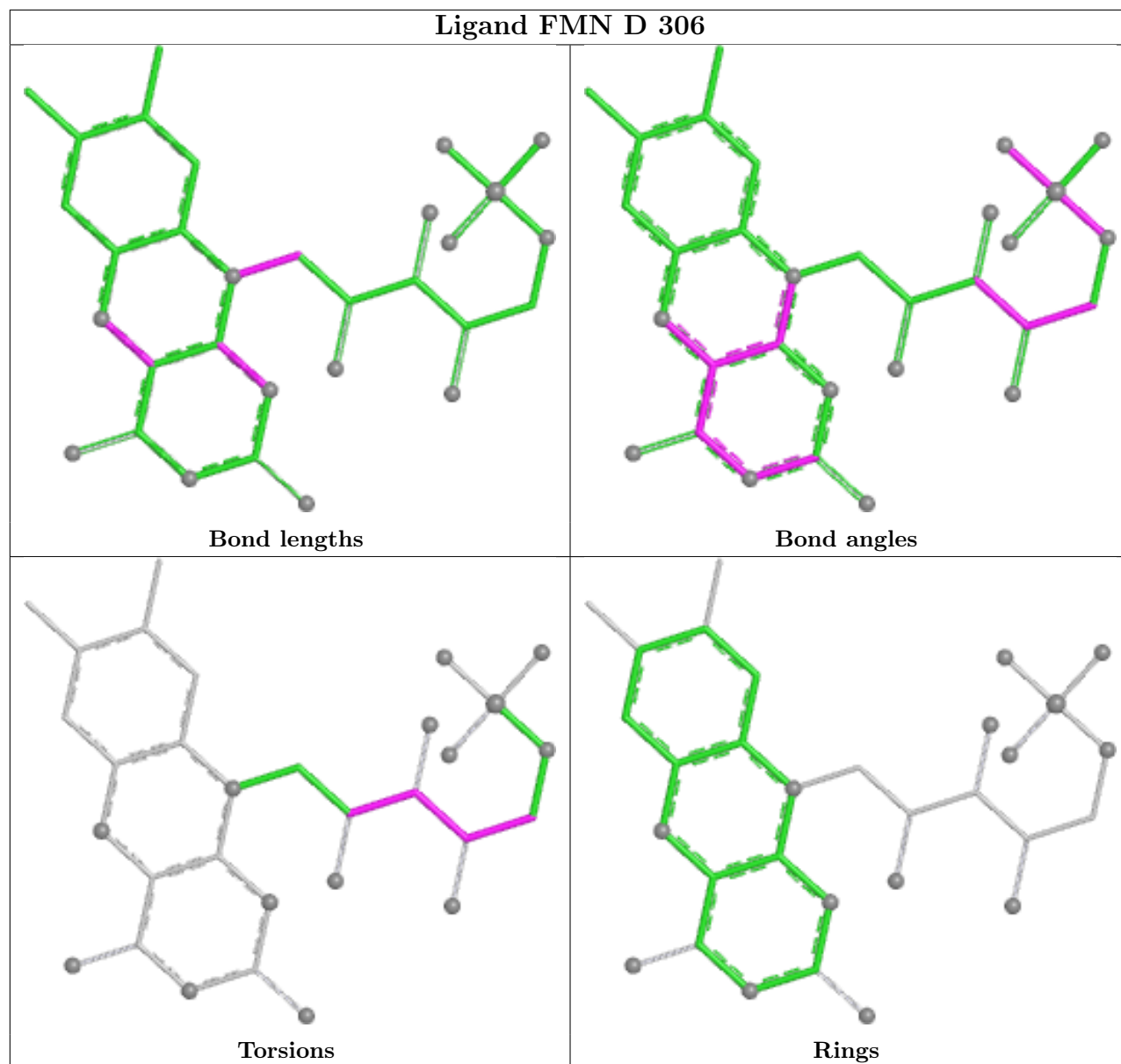


Ligand APC A 305 (A)

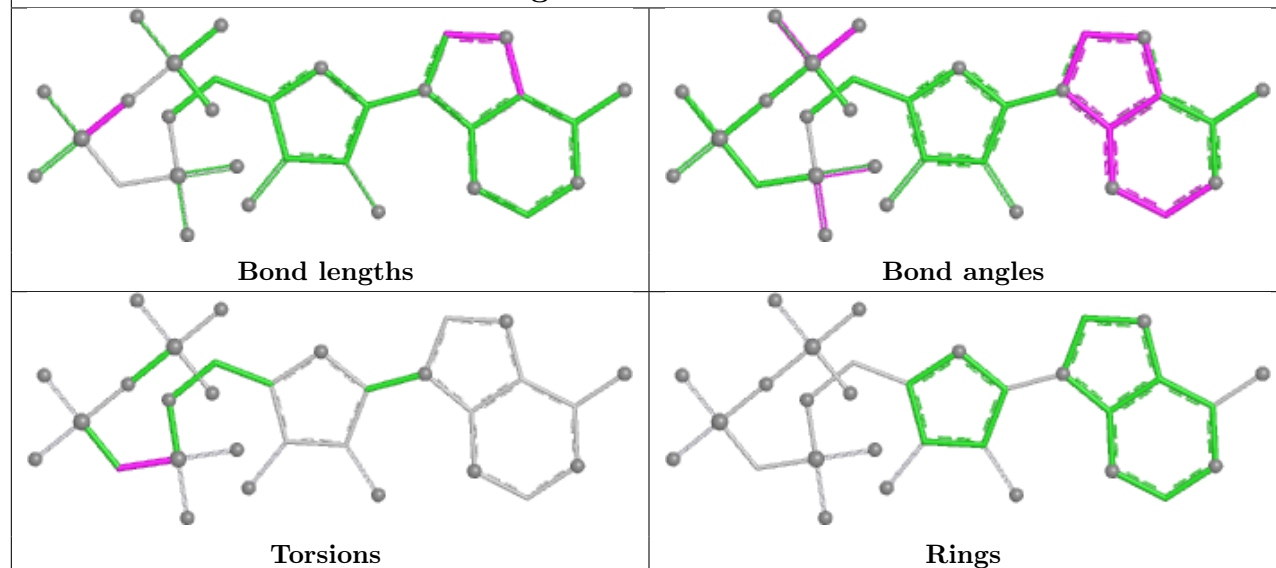


Ligand APC D 305

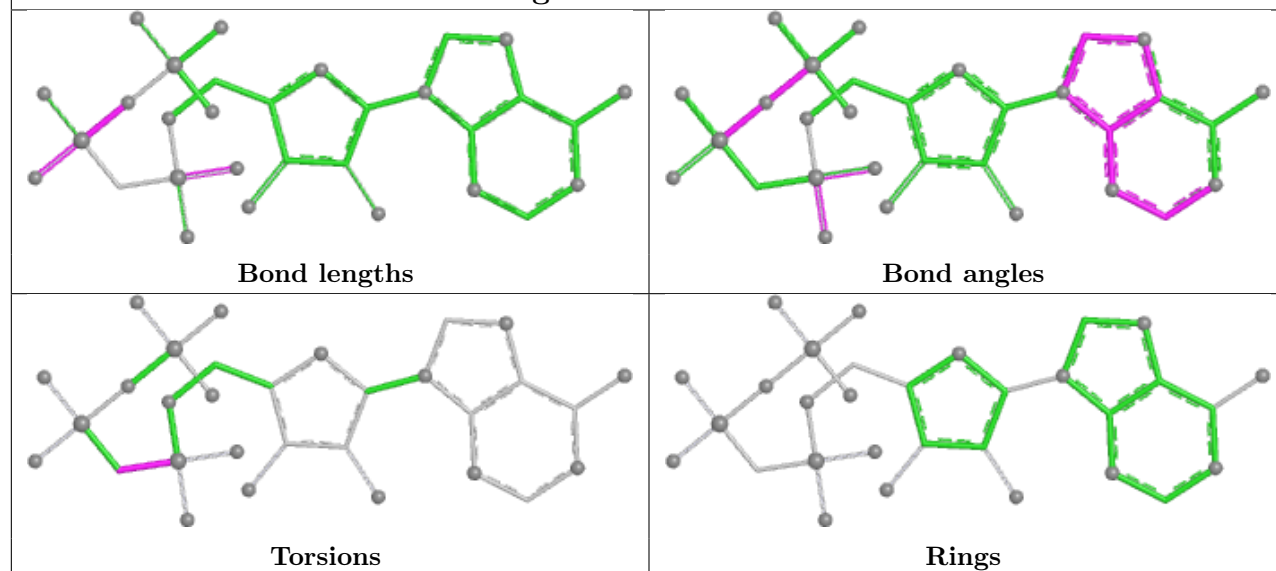


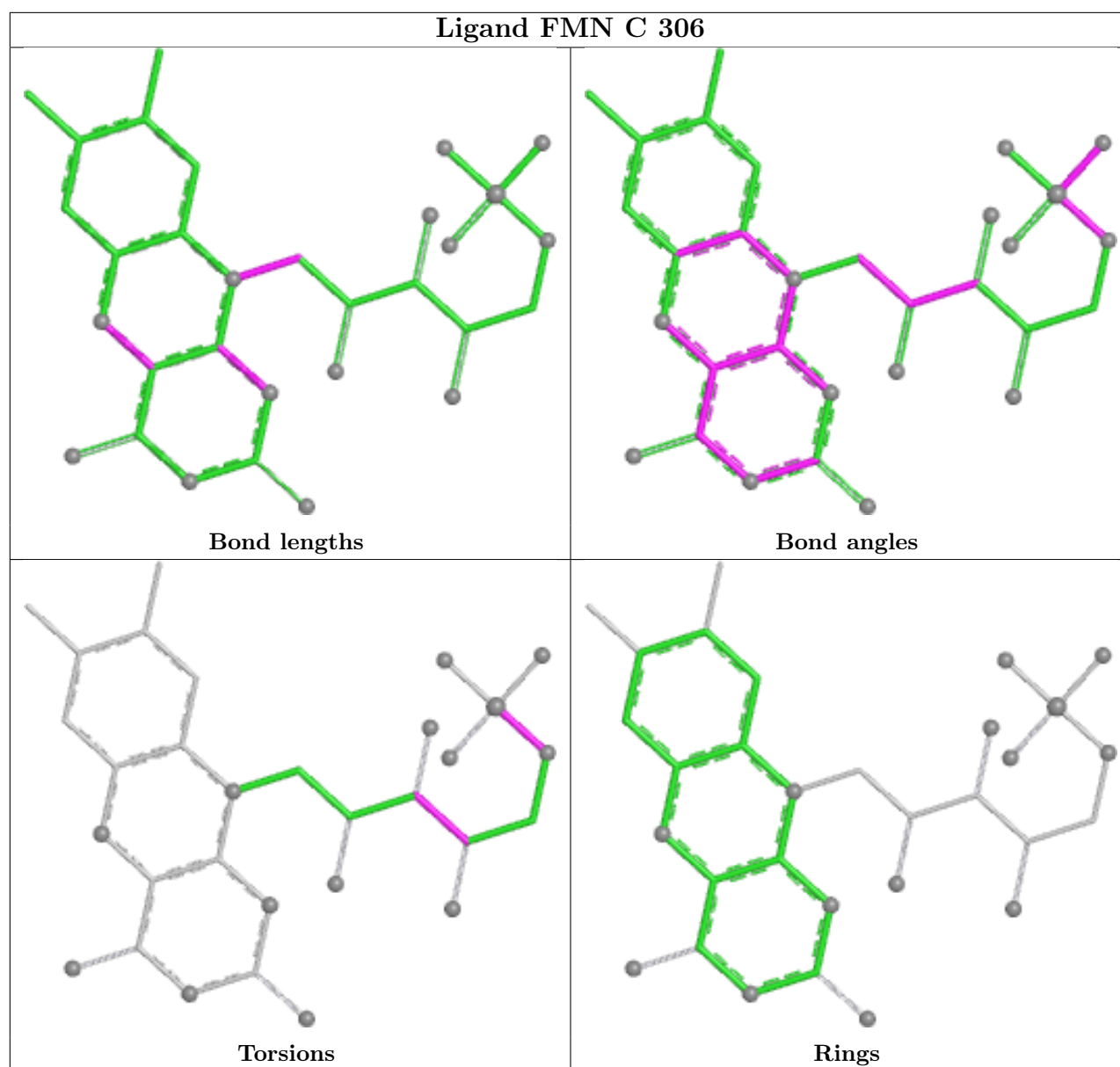


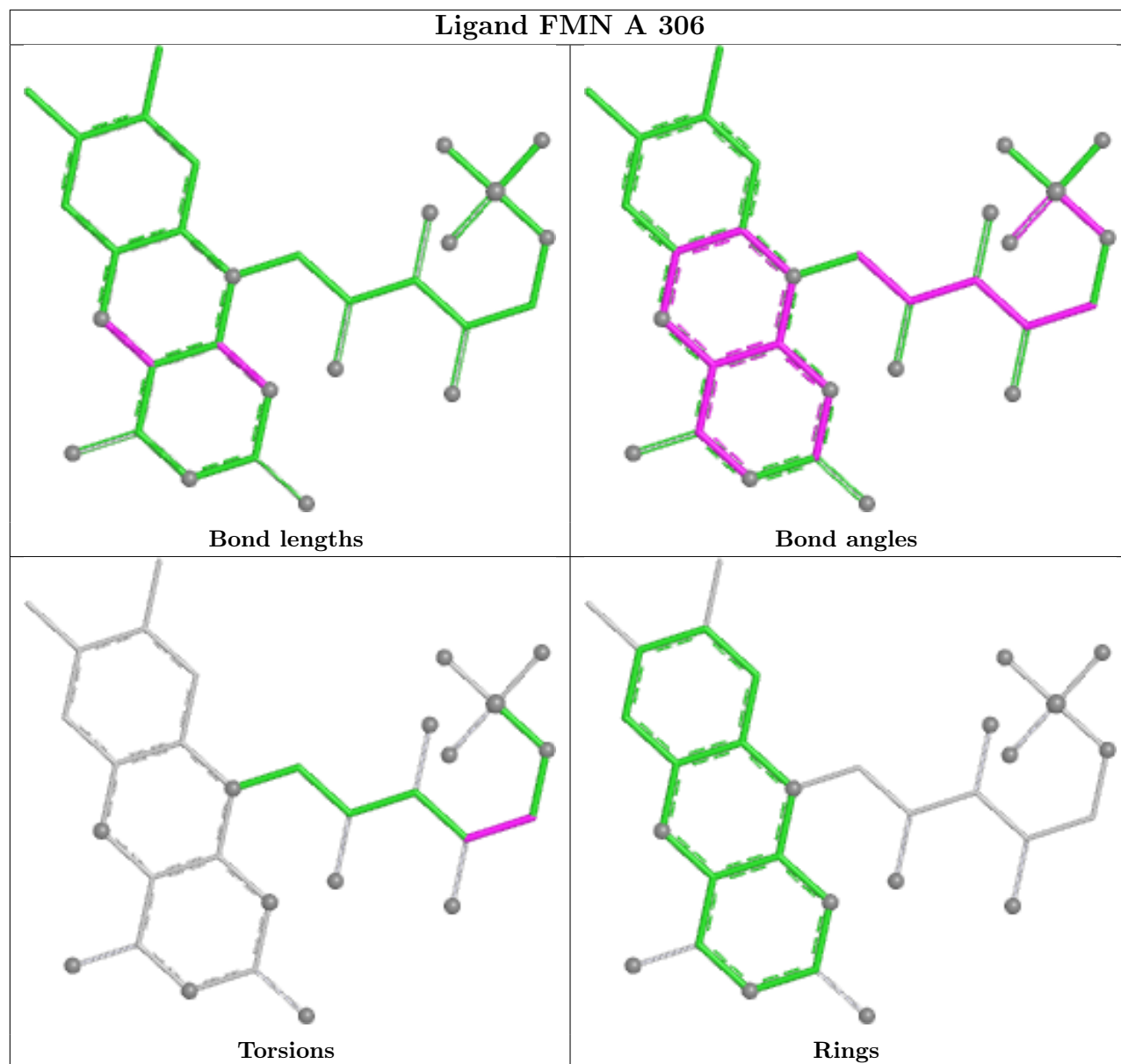
Ligand APC B 305



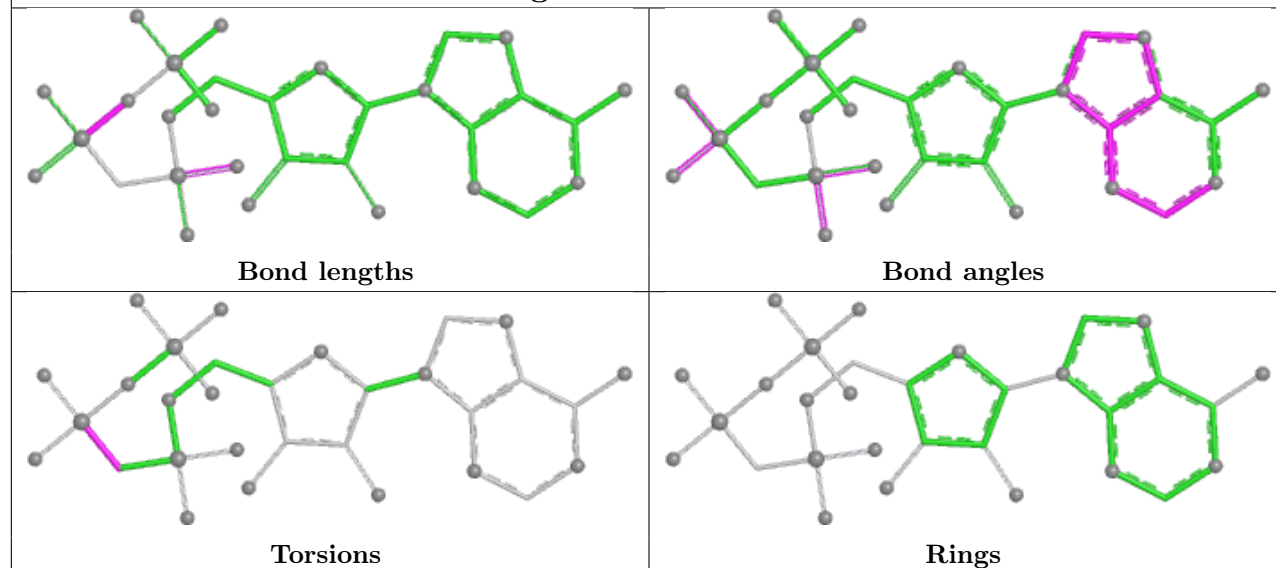
Ligand APC F 305



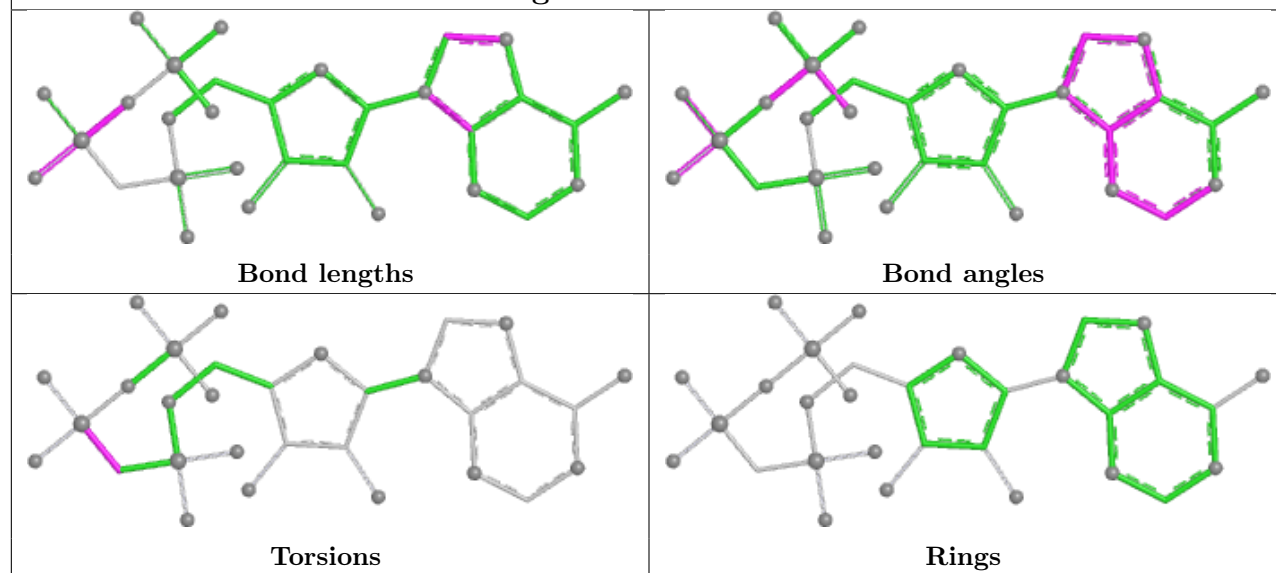


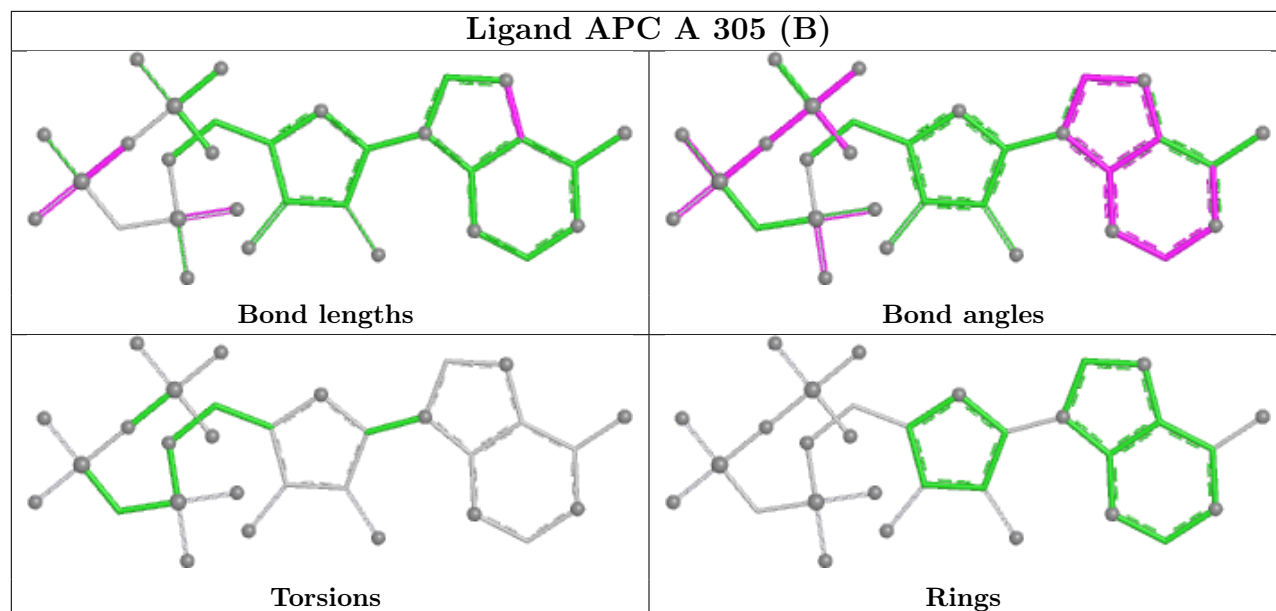


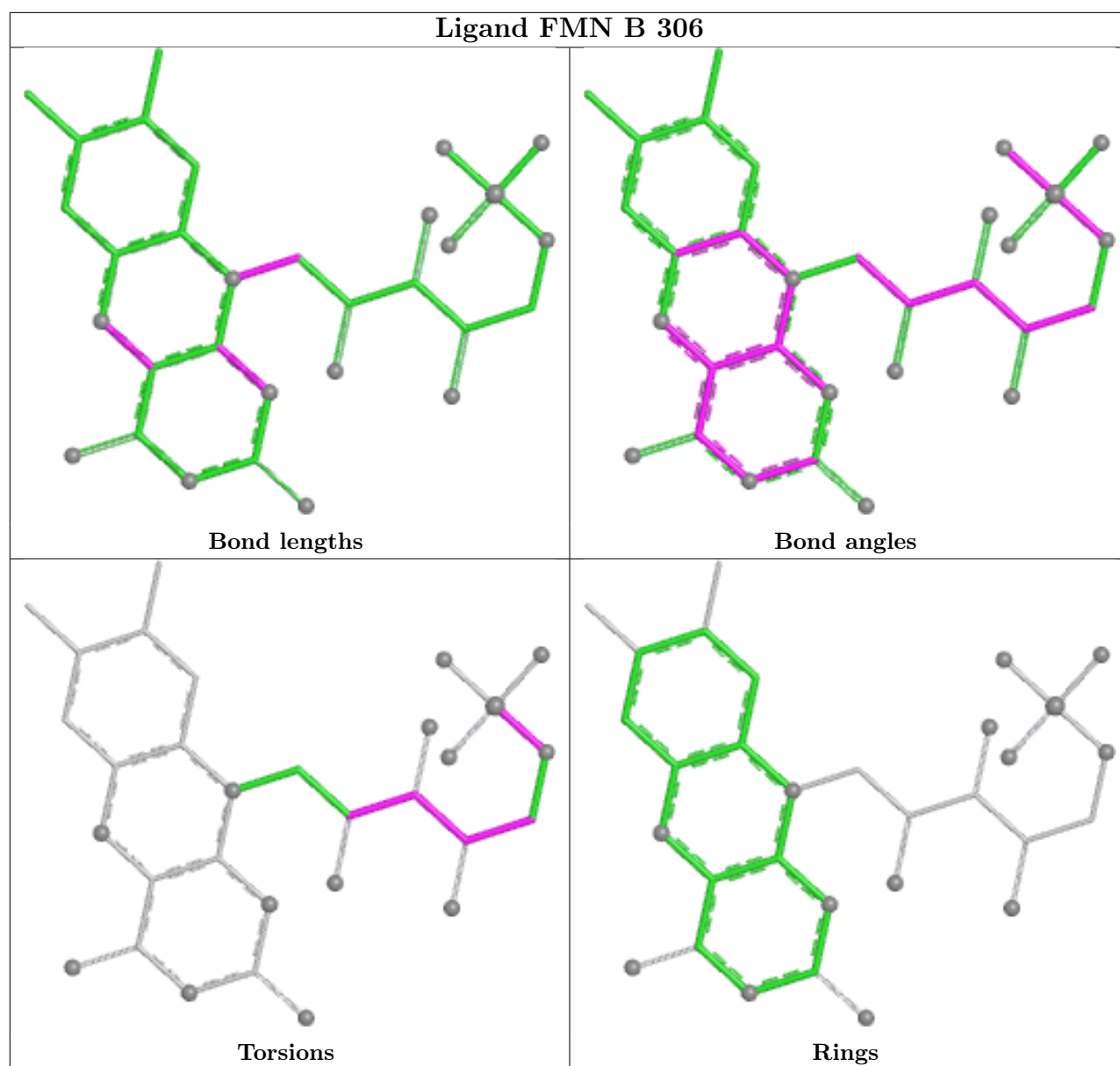
Ligand APC C 305

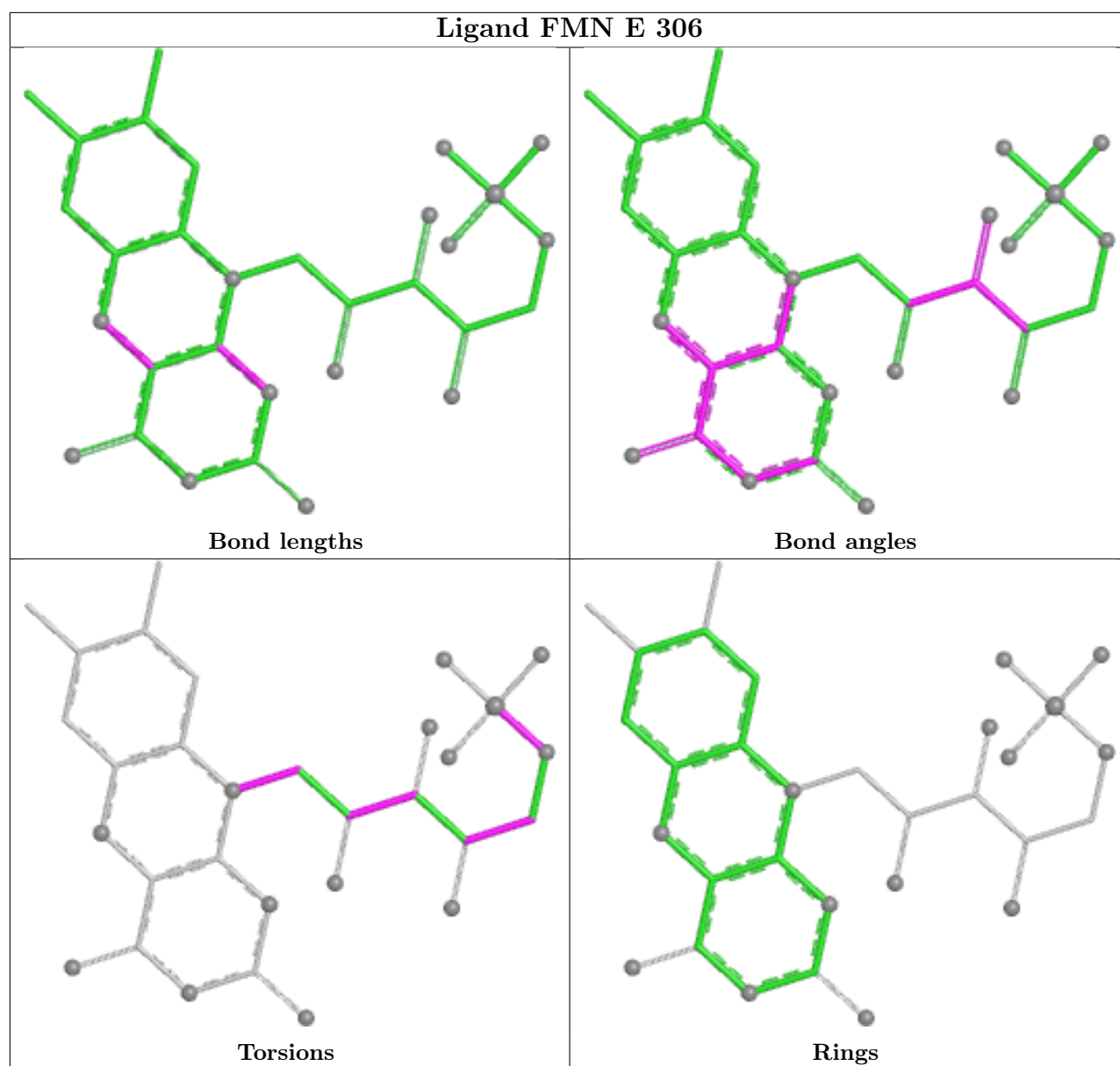


Ligand APC E 305









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	296/308 (96%)	-0.30	4 (1%)	73 79	6, 14, 29, 40	4 (1%)
1	B	305/308 (99%)	-0.13	8 (2%)	57 64	8, 16, 35, 54	2 (0%)
1	C	291/308 (94%)	-0.29	2 (0%)	84 88	8, 16, 30, 42	3 (1%)
1	D	301/308 (97%)	-0.18	5 (1%)	69 76	8, 16, 33, 43	1 (0%)
1	E	286/308 (92%)	-0.10	3 (1%)	79 84	8, 19, 33, 49	2 (0%)
1	F	297/308 (96%)	-0.21	7 (2%)	59 66	6, 16, 31, 50	3 (1%)
All	All	1776/1848 (96%)	-0.20	29 (1%)	70 77	6, 16, 32, 54	15 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	ILE	5.3
1	B	261	VAL	4.0
1	F	267	ILE	3.8
1	B	240	ASN	3.5
1	C	261	VAL	3.4
1	B	242	THR	3.0
1	B	267	ILE	3.0
1	D	261	VAL	2.9
1	A	268	PRO	2.9
1	F	268	PRO	2.8
1	E	140	CYS	2.7
1	A	269	ILE	2.7
1	F	99	PRO	2.6
1	D	260	GLU	2.5
1	B	264	ALA	2.4
1	F	242	THR	2.4
1	A	240	ASN	2.4
1	B	266	PRO	2.4
1	D	140	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	263	LYS	2.2
1	B	238	ASP	2.2
1	D	241	SER	2.2
1	E	280	LEU	2.2
1	F	266	PRO	2.1
1	E	281	HIS	2.1
1	F	281	HIS	2.1
1	B	260	GLU	2.0
1	F	241	SER	2.0
1	D	0	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FMN	E	306	31/31	0.81	0.13	22,24,35,36	6
3	FMN	D	306	31/31	0.86	0.12	19,21,32,32	8
3	FMN	B	306	31/31	0.88	0.11	15,19,34,34	8
3	FMN	C	306	31/31	0.90	0.10	13,17,27,29	8
3	FMN	F	306	31/31	0.90	0.10	14,17,23,24	8
3	FMN	A	306	31/31	0.92	0.09	13,15,25,25	8
5	SO4	D	308	5/5	0.92	0.10	39,39,40,40	5
2	APC	C	305	31/31	0.95	0.06	10,13,19,20	0
2	APC	A	305[A]	31/31	0.97	0.05	7,9,10,11	14
2	APC	A	305[B]	31/31	0.97	0.05	7,9,10,11	14
2	APC	E	305	31/31	0.98	0.04	10,13,15,16	0
4	MG	C	307	1/1	0.98	0.03	16,16,16,16	0
2	APC	B	305	31/31	0.98	0.04	10,11,15,16	0

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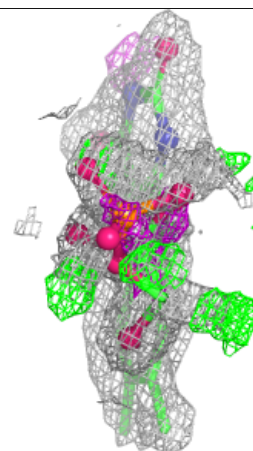
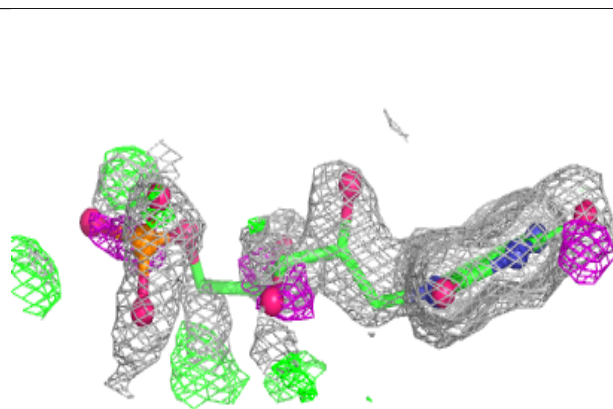
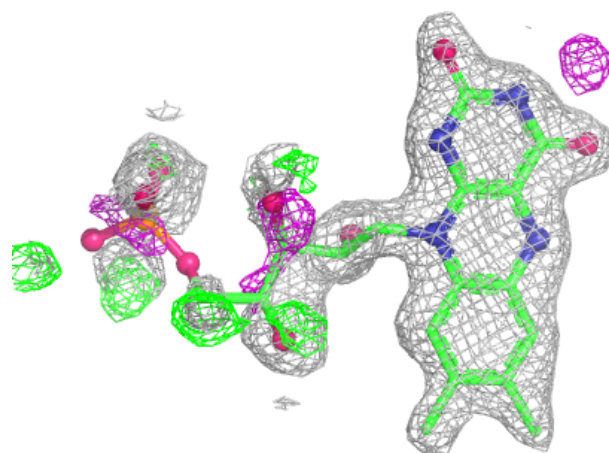
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	307	1/1	0.99	0.03	15,15,15,15	0
4	MG	B	307	1/1	0.99	0.03	13,13,13,13	0
2	APC	D	305	31/31	0.99	0.03	8,12,13,14	0
4	MG	D	307	1/1	0.99	0.03	13,13,13,13	0
4	MG	E	307	1/1	0.99	0.02	17,17,17,17	0
4	MG	F	307	1/1	0.99	0.03	11,11,11,11	0
2	APC	F	305	31/31	0.99	0.04	8,10,12,13	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.

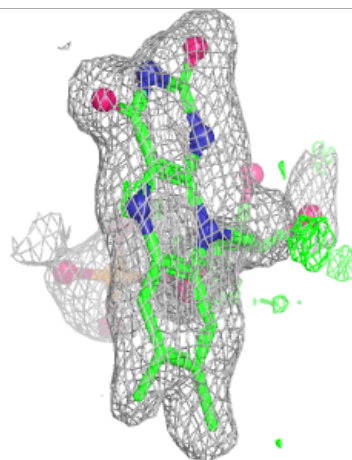
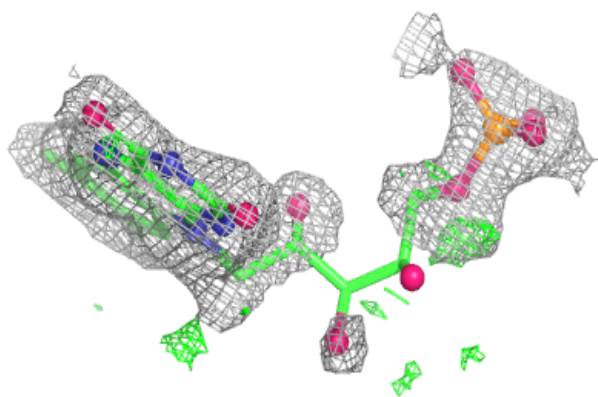
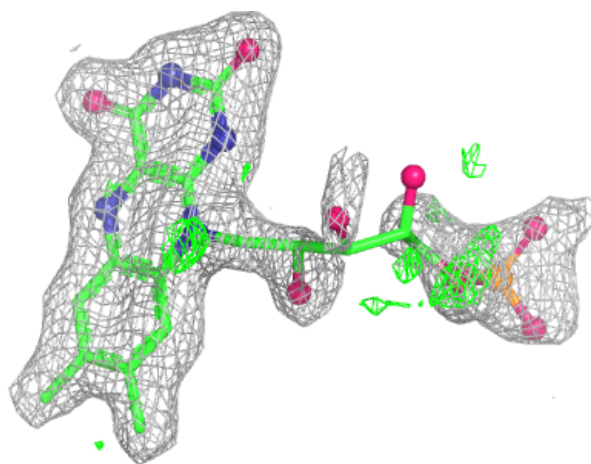
Electron density around FMN E 306:

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



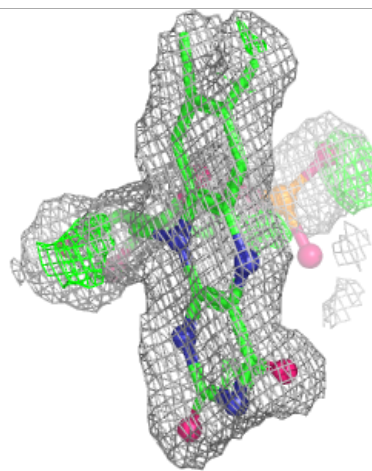
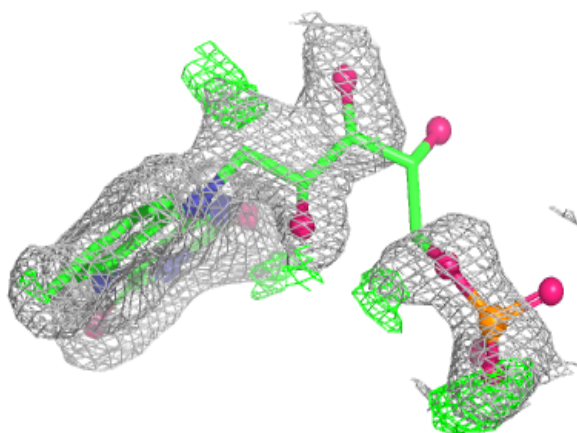
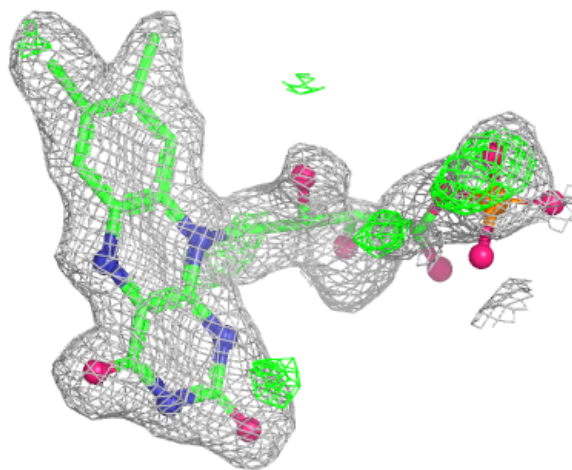
Electron density around FMN D 306:

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



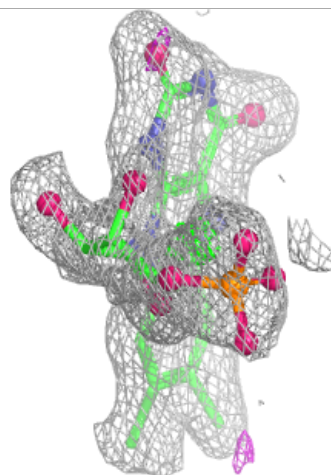
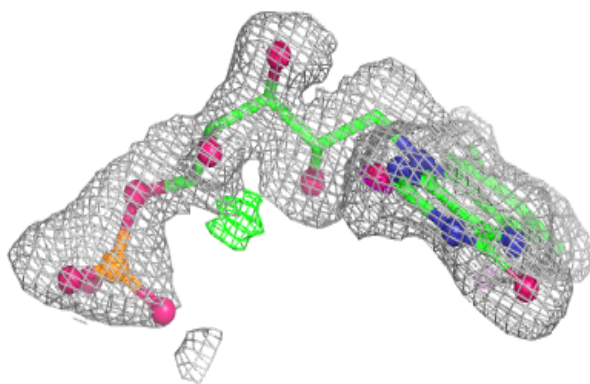
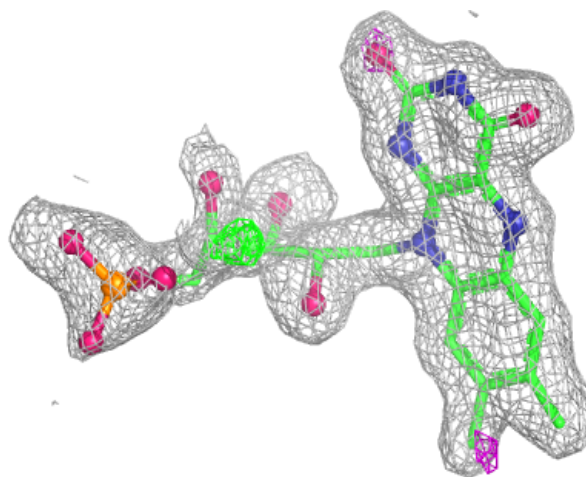
Electron density around FMN B 306:

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



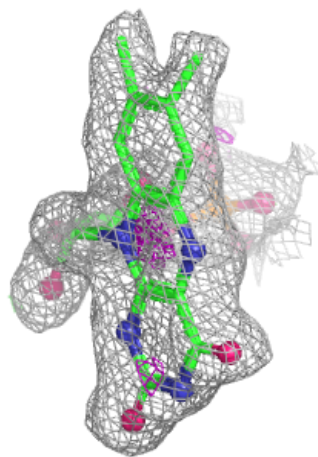
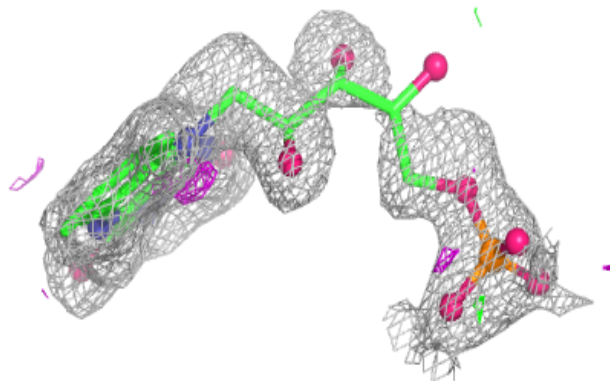
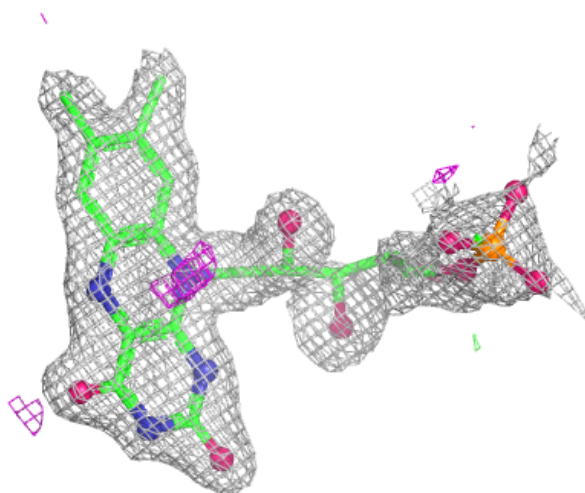
Electron density around FMN C 306:

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



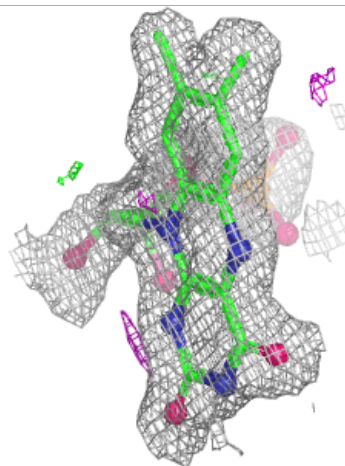
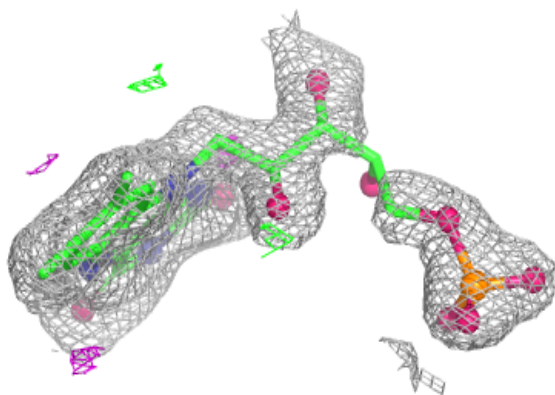
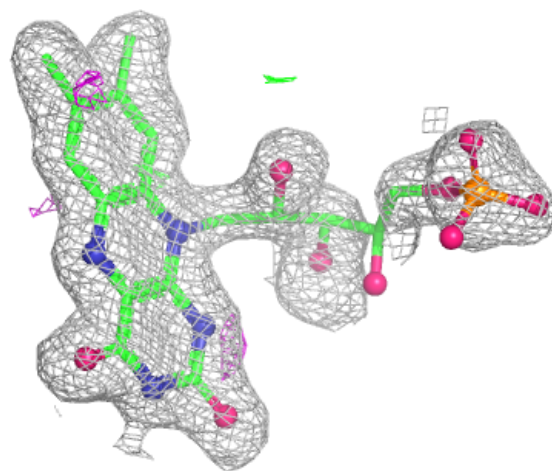
Electron density around FMN F 306:

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



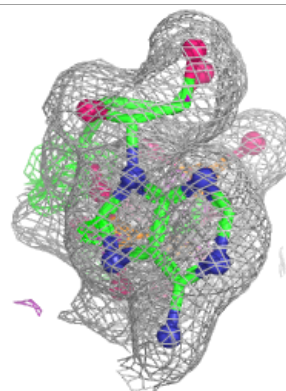
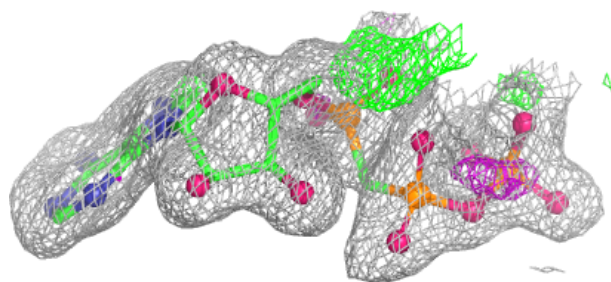
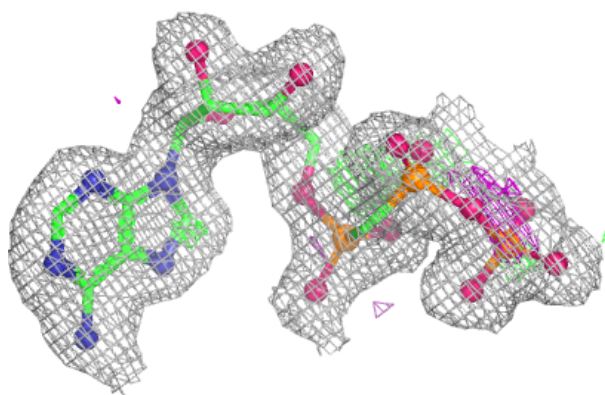
Electron density around FMN A 306:

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and green (positive)

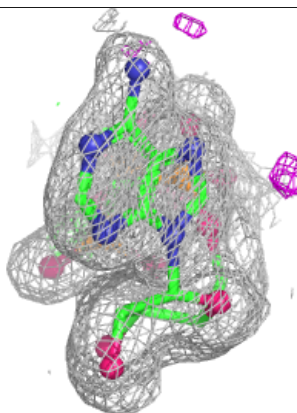
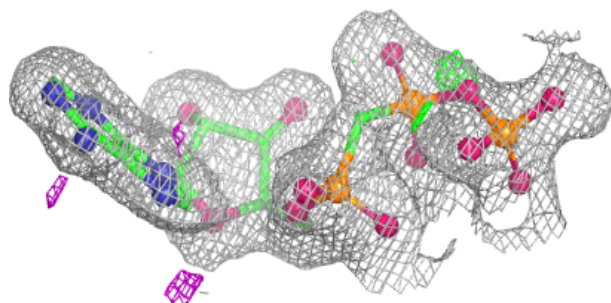
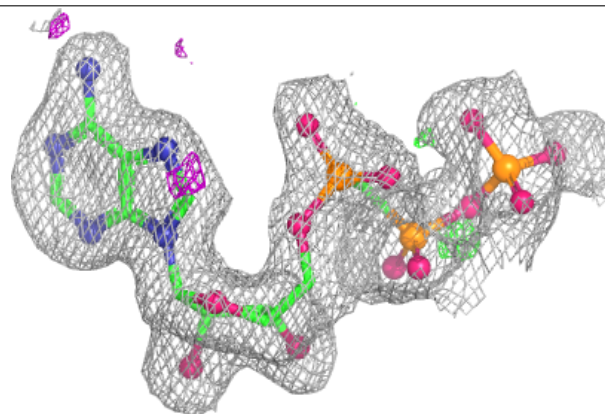


Electron density around APC C 305:

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and green (positive)

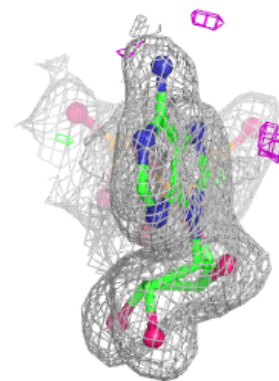
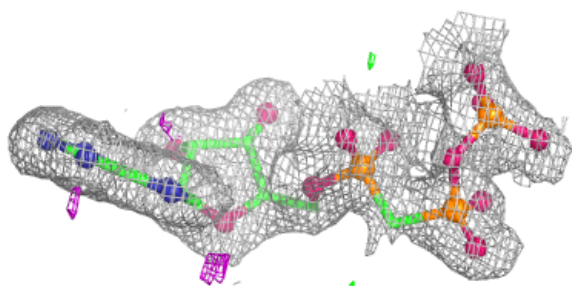
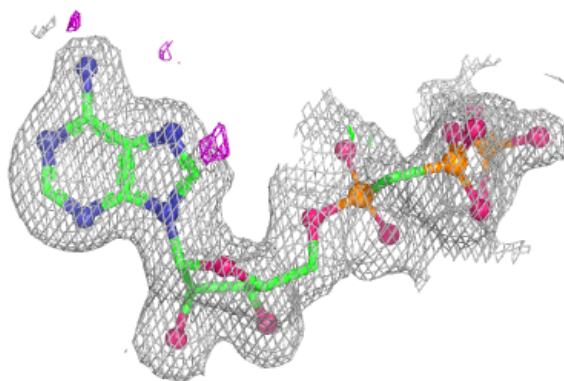
**Electron density around APC A 305 (A):**

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

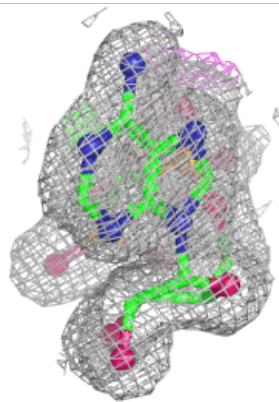
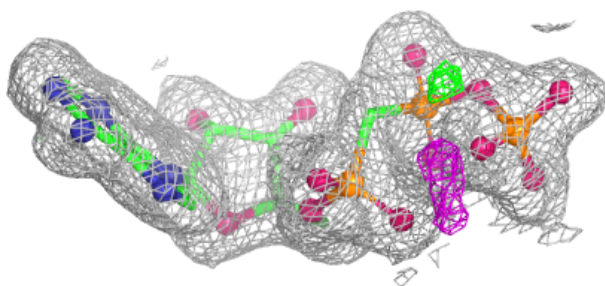
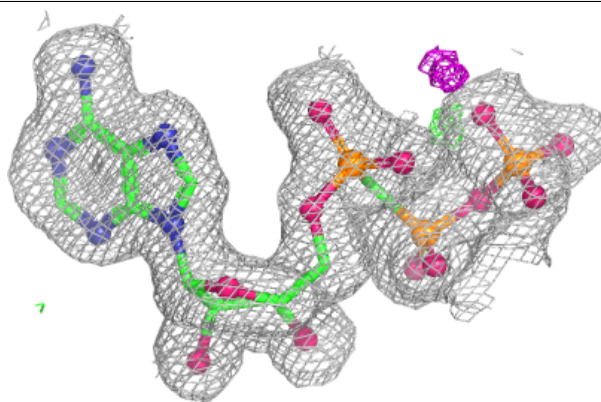


Electron density around APC A 305 (B):

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

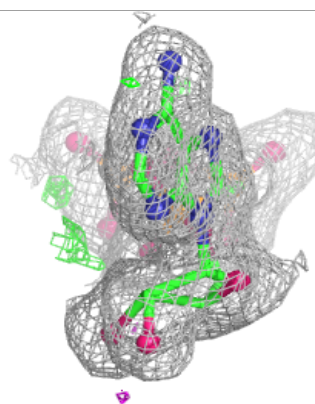
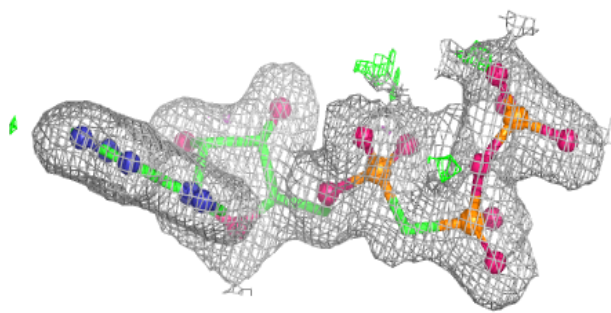
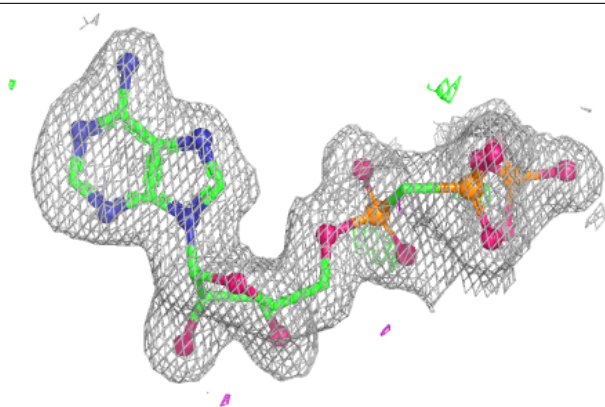
**Electron density around APC E 305:**

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

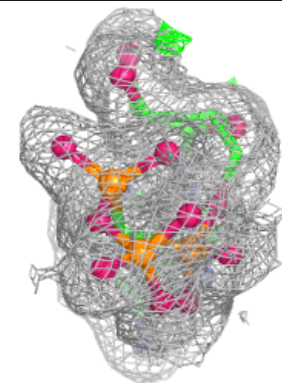
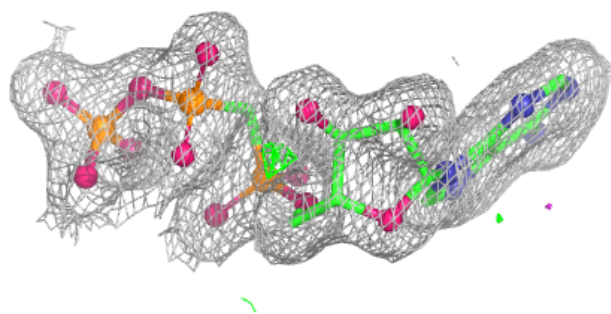
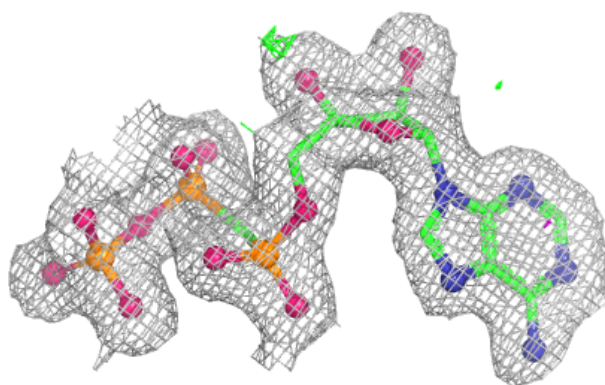


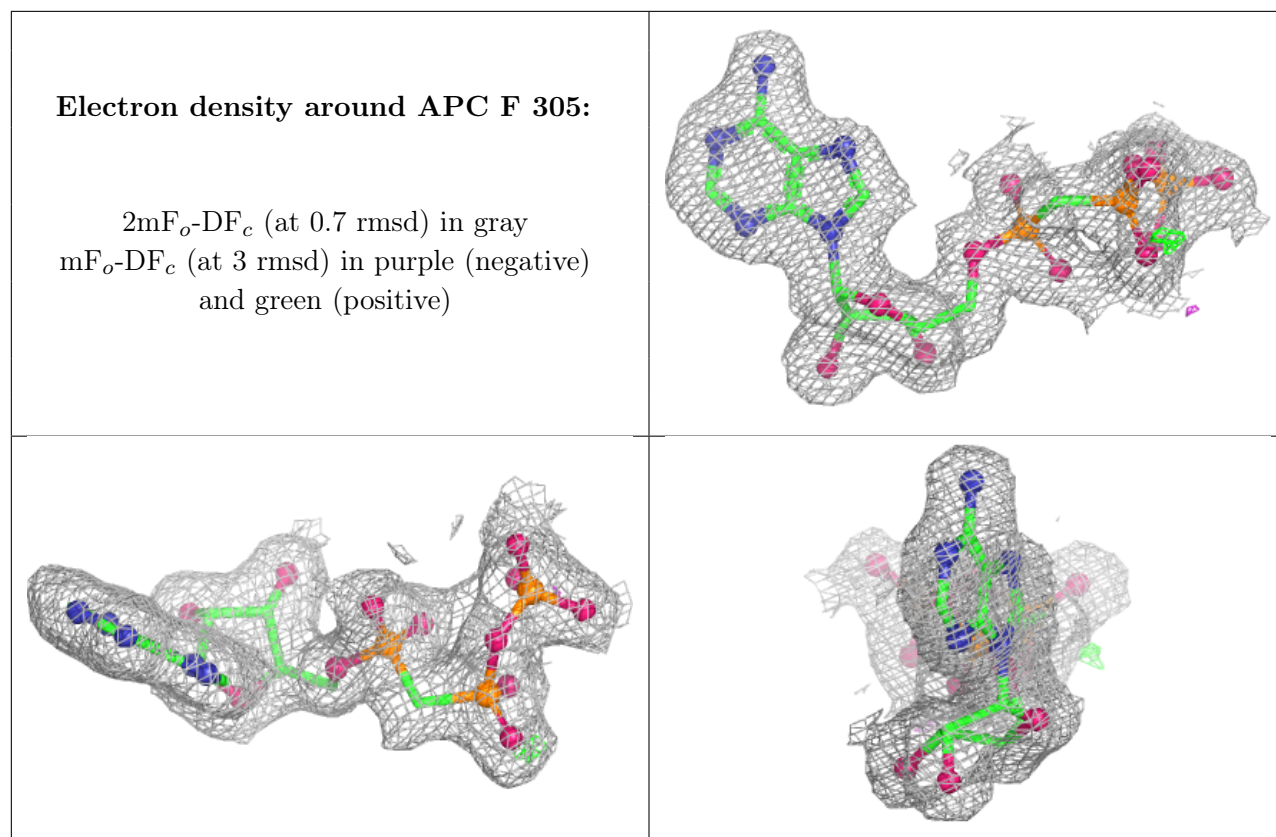
Electron density around APC B 305:

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

**Electron density around APC D 305:**

$2mF_o-DF_c$ (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.