



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 01:53 PM EDT

PDB ID : 3G4A  
Title : Crystal structure of flavine dependant thymidylate synthase S88A mutant from *Thermotoga maritima* at 1.95 angstrom resolution  
Authors : Mathews, I.I.; Lesley, S.A.; Kohen, A.  
Deposited on : 2009-02-03  
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](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 : 2.23.2  
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) : 2.23.2

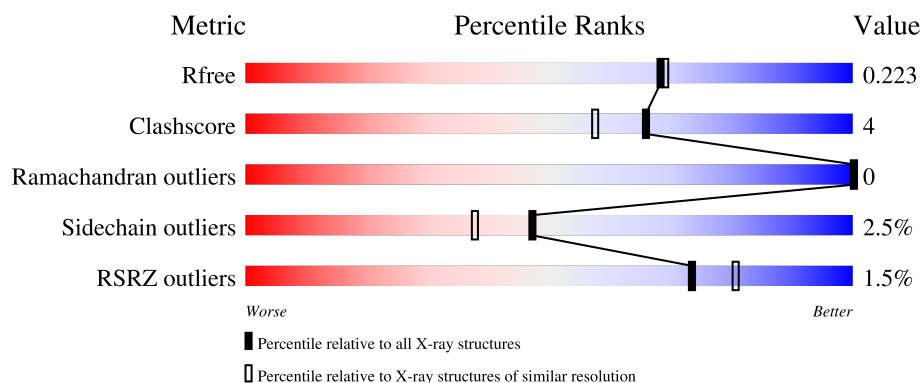
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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  $\geq 3$ , 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	232	<div> <div>85%</div> <div>8%</div> <div>6%</div> </div>
1	B	232	<div> <div>%</div> <div>79%</div> <div>15%</div> <div>5%</div> </div>
1	C	232	<div> <div>%</div> <div>86%</div> <div>5%</div> <div>8%</div> </div>
1	D	232	<div> <div>3%</div> <div>82%</div> <div>9%</div> <div>9%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7493 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 Thymidylate synthase thyX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1767	1159	295	307	6			
1	B	220	Total	C	N	O	S	0	0	0
			1786	1177	300	303	6			
1	C	214	Total	C	N	O	S	0	0	0
			1743	1147	292	299	5			
1	D	212	Total	C	N	O	S	0	0	0
			1746	1142	300	299	5			

There are 52 discrepancies between the modelled and reference sequences:

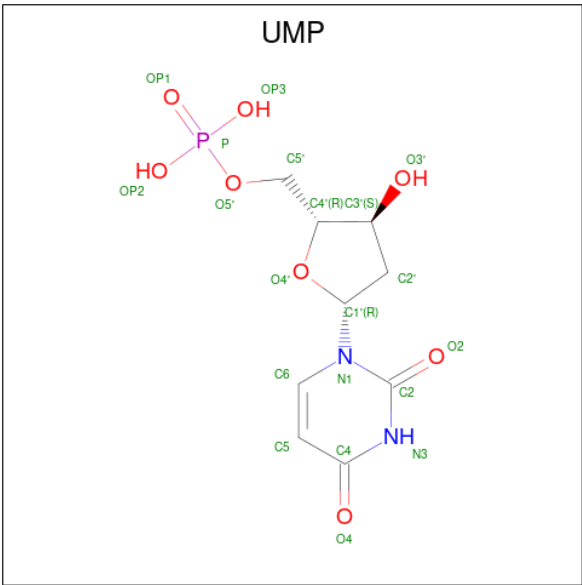
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	LEADER SEQUENCE	UNP Q9WYT0
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYT0
A	-9	SER	-	LEADER SEQUENCE	UNP Q9WYT0
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYT0
A	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYT0
A	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYT0
A	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
A	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
A	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
A	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
A	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
A	0	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
A	88	ALA	SER	engineered mutation	UNP Q9WYT0
B	-11	MET	-	LEADER SEQUENCE	UNP Q9WYT0
B	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYT0
B	-9	SER	-	LEADER SEQUENCE	UNP Q9WYT0
B	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYT0
B	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYT0
B	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYT0

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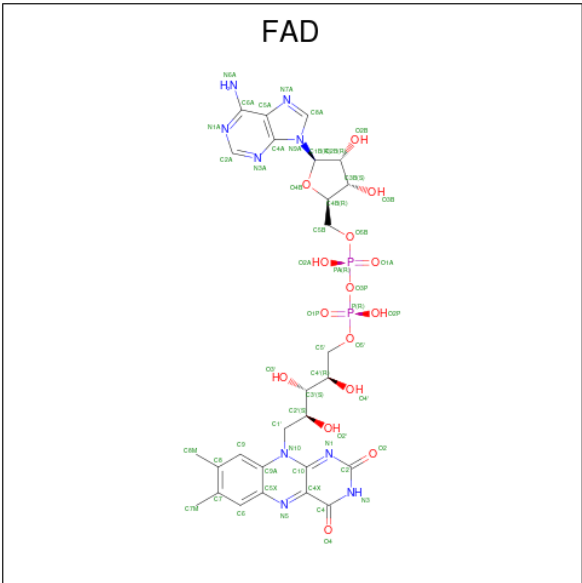
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	0	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	88	ALA	SER	engineered mutation	UNP Q9WYT0
C	-11	MET	-	LEADER SEQUENCE	UNP Q9WYT0
C	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYT0
C	-9	SER	-	LEADER SEQUENCE	UNP Q9WYT0
C	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYT0
C	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYT0
C	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	0	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	88	ALA	SER	engineered mutation	UNP Q9WYT0
D	-11	MET	-	LEADER SEQUENCE	UNP Q9WYT0
D	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYT0
D	-9	SER	-	LEADER SEQUENCE	UNP Q9WYT0
D	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYT0
D	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYT0
D	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	0	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	88	ALA	SER	engineered mutation	UNP Q9WYT0

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula:  $C_9H_{13}N_2O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		


- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	40	Total	O	0	0
			40	40		
4	C	44	Total	O	0	0
			44	44		
4	D	32	Total	O	0	0
			32	32		

### 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.

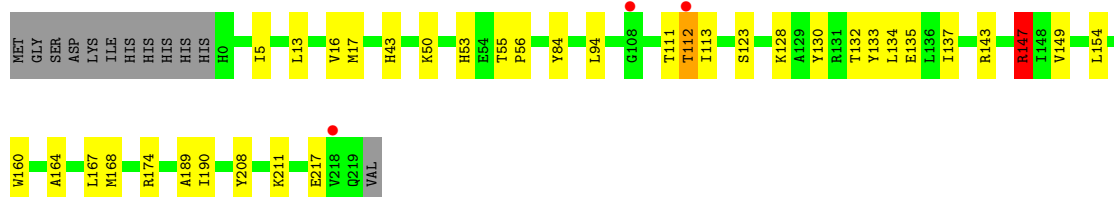
- Molecule 1: Thymidylate synthase thyX

Chain A: 




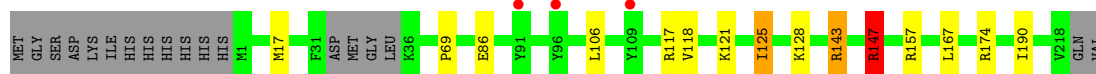
- Molecule 1: Thymidylate synthase thyX

Chain B: 




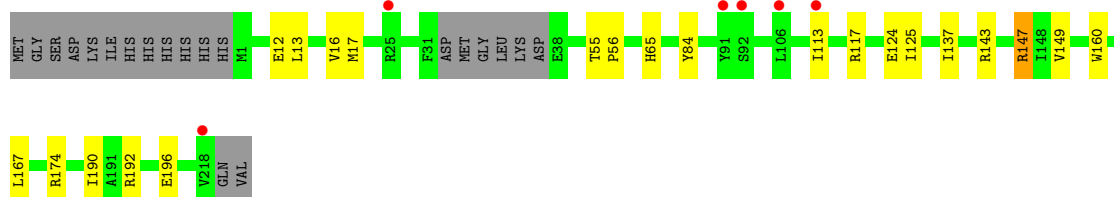
- Molecule 1: Thymidylate synthase thyX

Chain C: 



- Molecule 1: Thymidylate synthase thyX

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.95Å 116.22Å 140.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.40 – 1.95 70.36 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (89.40-1.95) 99.5 (70.36-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.186 , 0.222 0.193 , 0.223	Depositor DCC
$R_{free}$ test set	3288 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7493	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.66	0/1816	0.68	0/2461
1	B	0.64	0/1836	0.70	1/2487 (0.0%)
1	C	0.68	0/1790	0.75	1/2425 (0.0%)
1	D	0.67	0/1793	0.71	0/2427
All	All	0.66	0/7235	0.71	2/9800 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	C	147	ARG	NE-CZ-NH2	-5.07	117.77	120.30

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	1767	0	1726	13	0
1	B	1786	0	1756	25	0
1	C	1743	0	1715	14	0
1	D	1746	0	1730	19	0
2	A	20	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	11	1	0
2	C	20	0	11	2	0
2	D	20	0	11	1	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
3	C	53	0	31	0	0
3	D	53	0	31	0	0
4	A	43	0	0	1	0
4	B	40	0	0	0	0
4	C	44	0	0	0	0
4	D	32	0	0	0	0
All	All	7493	0	7095	57	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 4.

All (57) 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:174:ARG:HH12	2:D:318:UMP:HN3	1.19	0.91
1:B:174:ARG:HH12	2:C:313:UMP:HN3	1.13	0.90
1:B:111:THR:HG22	1:B:113:ILE:O	1.73	0.89
2:B:308:UMP:HN3	1:C:174:ARG:HH12	1.20	0.89
2:A:303:UMP:HN3	1:D:174:ARG:HH12	1.19	0.88
1:D:167:LEU:HD11	1:D:190:ILE:CG2	2.03	0.87
1:D:167:LEU:HD11	1:D:190:ILE:HG21	1.59	0.84
1:B:132:THR:HG21	1:C:125:ILE:HD13	1.62	0.81
1:C:167:LEU:HD11	1:C:190:ILE:CG2	2.11	0.81
1:A:128:LYS:NZ	1:D:124:GLU:OE2	2.17	0.77
1:A:17:MET:HB2	1:B:17:MET:HB2	1.70	0.74
1:B:132:THR:HG21	1:C:125:ILE:CD1	2.20	0.71
1:C:167:LEU:HD11	1:C:190:ILE:HG21	1.72	0.71
1:C:17:MET:HB2	1:D:17:MET:HB2	1.73	0.70
1:B:167:LEU:HD11	1:B:190:ILE:CG2	2.21	0.69
1:B:111:THR:CG2	1:B:113:ILE:O	2.41	0.68
1:B:149:VAL:HG11	1:C:125:ILE:HD11	1.75	0.68
1:B:5:ILE:HD11	1:B:189:ALA:HB2	1.79	0.65
1:B:167:LEU:HD11	1:B:190:ILE:HG21	1.79	0.64
1:B:135:GLU:OE1	1:C:121:LYS:NZ	2.32	0.61
1:D:137:ILE:HD13	1:D:143:ARG:HH11	1.67	0.59
1:A:128:LYS:HG3	1:D:125:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:LEU:CD1	1:C:118:VAL:HG11	2.37	0.55
1:B:149:VAL:HB	1:C:125:ILE:HD12	1.88	0.55
1:B:94:LEU:HD13	1:B:154:LEU:HD21	1.90	0.53
1:B:164:ALA:O	1:B:168:MET:HG3	2.08	0.53
1:D:13:LEU:HD11	1:D:16:VAL:CG2	2.40	0.52
1:A:26:ALA:O	1:A:29:VAL:HG12	2.09	0.52
1:A:143:ARG:O	1:A:147:ARG:HG3	2.10	0.52
1:A:5:ILE:HD11	1:A:189:ALA:HB2	1.92	0.50
1:B:84:TYR:CE2	1:B:160:TRP:CD1	3.00	0.50
1:D:143:ARG:O	1:D:147:ARG:HG3	2.12	0.50
1:A:149:VAL:HB	1:D:125:ILE:HG21	1.94	0.50
1:D:113:ILE:HG22	1:D:117:ARG:HB3	1.95	0.49
1:B:13:LEU:HD21	1:B:16:VAL:CG2	2.42	0.49
1:B:130:TYR:CE2	1:B:134:LEU:HD11	2.49	0.48
1:D:84:TYR:CE2	1:D:160:TRP:CD1	3.02	0.47
1:C:143:ARG:O	1:C:147:ARG:HG3	2.15	0.46
1:B:112:THR:HG22	1:B:113:ILE:HG23	2.00	0.44
1:D:12:GLU:HG2	1:D:65:HIS:HB3	1.98	0.43
1:A:128:LYS:HG3	1:D:125:ILE:CD1	2.48	0.43
1:A:-1:HIS:N	4:A:256:HOH:O	2.36	0.42
1:B:43:HIS:O	1:B:43:HIS:ND1	2.52	0.42
1:A:125:ILE:HG21	1:D:149:VAL:HB	2.02	0.42
1:B:55:THR:N	1:B:56:PRO:CD	2.82	0.42
1:D:192:ARG:HH12	1:D:196:GLU:HG2	1.83	0.42
1:D:55:THR:N	1:D:56:PRO:CD	2.83	0.41
1:B:128:LYS:HZ2	1:C:128:LYS:HD3	1.84	0.41
1:B:132:THR:CG2	1:C:125:ILE:HD13	2.41	0.41
1:D:192:ARG:NH1	1:D:196:GLU:HG2	2.35	0.41
1:B:143:ARG:O	1:B:147:ARG:HG3	2.20	0.41
1:C:86:GLU:HB3	2:C:313:UMP:H4'	2.03	0.41
1:A:55:THR:N	1:A:56:PRO:CD	2.84	0.41
1:B:50:LYS:HB3	1:B:208:TYR:CD1	2.55	0.41
1:B:133:TYR:CZ	1:B:137:ILE:HD11	2.56	0.41
1:D:113:ILE:HG23	1:D:117:ARG:HG2	2.04	0.40
1:A:127:ASP:O	1:A:131:ARG:HG3	2.22	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	216/232 (93%)	210 (97%)	6 (3%)	0	100	100
1	B	218/232 (94%)	211 (97%)	7 (3%)	0	100	100
1	C	210/232 (90%)	203 (97%)	7 (3%)	0	100	100
1	D	208/232 (90%)	203 (98%)	5 (2%)	0	100	100
All	All	852/928 (92%)	827 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	178/206 (86%)	173 (97%)	5 (3%)	43	33
1	B	177/206 (86%)	171 (97%)	6 (3%)	37	25
1	C	174/206 (84%)	168 (97%)	6 (3%)	37	25
1	D	178/206 (86%)	177 (99%)	1 (1%)	86	85
All	All	707/824 (86%)	689 (98%)	18 (2%)	47	38

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	96	TYR

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Mol	Chain	Res	Type
1	A	106	LEU
1	A	147	ARG
1	A	197	LYS
1	B	53	HIS
1	B	112	THR
1	B	123	SER
1	B	147	ARG
1	B	211	LYS
1	B	217	GLU
1	C	69	PRO
1	C	117	ARG
1	C	125	ILE
1	C	143	ARG
1	C	147	ARG
1	C	157	ARG
1	D	147	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	51	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	UMP	A	303	-	18,21,21	2.72	4 (22%)	21,31,31	1.31	3 (14%)
3	FAD	D	300	-	51,58,58	3.16	21 (41%)	60,89,89	1.90	10 (16%)
2	UMP	D	318	-	18,21,21	2.70	3 (16%)	21,31,31	1.14	2 (9%)
2	UMP	B	308	-	18,21,21	2.98	5 (27%)	21,31,31	1.34	3 (14%)
3	FAD	C	305	-	51,58,58	3.23	19 (37%)	60,89,89	1.92	13 (21%)
3	FAD	B	310	-	51,58,58	3.08	18 (35%)	60,89,89	2.06	10 (16%)
2	UMP	C	313	-	18,21,21	2.94	4 (22%)	21,31,31	1.13	2 (9%)
3	FAD	A	315	-	51,58,58	3.25	18 (35%)	60,89,89	2.08	13 (21%)

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	UMP	A	303	-	-	0/7/22/22	0/2/2/2
3	FAD	D	300	-	-	1/30/50/50	0/6/6/6
2	UMP	D	318	-	-	0/7/22/22	0/2/2/2
2	UMP	B	308	-	-	0/7/22/22	0/2/2/2
3	FAD	C	305	-	-	1/30/50/50	0/6/6/6
3	FAD	B	310	-	-	1/30/50/50	0/6/6/6
2	UMP	C	313	-	-	0/7/22/22	0/2/2/2
3	FAD	A	315	-	-	1/30/50/50	0/6/6/6

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	315	FAD	C4X-C10	13.91	1.52	1.38
3	C	305	FAD	C4X-C10	13.72	1.52	1.38
3	B	310	FAD	C4X-C10	13.05	1.51	1.38
3	D	300	FAD	C4X-C10	13.02	1.51	1.38
2	C	313	UMP	C6-N1	9.21	1.47	1.35
2	B	308	UMP	C6-N1	9.00	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	318	UMP	C6-N1	8.11	1.45	1.35
2	A	303	UMP	C6-N1	7.71	1.45	1.35
2	A	303	UMP	C6-C5	-6.71	1.23	1.38
2	C	313	UMP	C6-C5	-6.43	1.23	1.38
3	C	305	FAD	C6-C5X	6.09	1.51	1.41
3	D	300	FAD	C6-C5X	6.01	1.51	1.41
3	D	300	FAD	C5X-N5	5.96	1.45	1.35
3	A	315	FAD	C4-N3	5.91	1.43	1.33
3	A	315	FAD	C5X-N5	5.90	1.45	1.35
3	C	305	FAD	C4-N3	5.87	1.43	1.33
2	D	318	UMP	C6-C5	-5.85	1.25	1.38
3	B	310	FAD	C6-C5X	5.76	1.50	1.41
2	B	308	UMP	C6-C5	-5.69	1.25	1.38
3	A	315	FAD	C6-C5X	5.64	1.50	1.41
3	C	305	FAD	C5X-N5	5.57	1.44	1.35
3	D	300	FAD	C4-N3	5.54	1.42	1.33
3	B	310	FAD	C6-C7	5.43	1.51	1.37
2	B	308	UMP	C4-N3	5.40	1.42	1.33
3	C	305	FAD	C9-C8	5.39	1.51	1.37
3	C	305	FAD	C9A-N10	5.15	1.45	1.38
3	D	300	FAD	C6-C7	5.12	1.50	1.37
3	A	315	FAD	C6-C7	5.11	1.50	1.37
3	B	310	FAD	C5X-N5	5.09	1.43	1.35
3	A	315	FAD	C9-C8	5.00	1.50	1.37
3	D	300	FAD	C9-C8	4.99	1.50	1.37
3	B	310	FAD	C4-N3	4.91	1.41	1.33
3	B	310	FAD	C9-C8	4.80	1.50	1.37
3	A	315	FAD	C8-C7	4.77	1.52	1.40
3	B	310	FAD	C9A-N10	4.70	1.44	1.38
3	C	305	FAD	C6-C7	4.69	1.49	1.37
3	D	300	FAD	C9A-N10	4.68	1.44	1.38
3	B	310	FAD	C9-C9A	4.66	1.50	1.40
2	D	318	UMP	C4-N3	4.59	1.41	1.33
3	A	315	FAD	C9A-C5X	4.50	1.51	1.42
3	A	315	FAD	C4-C4X	4.47	1.49	1.41
3	C	305	FAD	C8-C7	4.46	1.52	1.40
3	D	300	FAD	C9-C9A	4.42	1.49	1.40
3	A	315	FAD	C9-C9A	4.40	1.49	1.40
3	A	315	FAD	C2A-N3A	4.35	1.39	1.32
2	A	303	UMP	C4-N3	4.19	1.40	1.33
3	D	300	FAD	C8-C7	4.18	1.51	1.40
3	D	300	FAD	C9A-C5X	4.14	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	315	FAD	C9A-N10	4.10	1.44	1.38
3	B	310	FAD	C8-C7	4.06	1.51	1.40
3	C	305	FAD	C2A-N3A	3.99	1.38	1.32
3	B	310	FAD	C4-C4X	3.98	1.48	1.41
3	C	305	FAD	C9-C9A	3.93	1.48	1.40
2	C	313	UMP	C4-N3	3.93	1.39	1.33
3	A	315	FAD	C6A-N6A	3.91	1.48	1.34
3	B	310	FAD	C9A-C5X	3.91	1.50	1.42
3	C	305	FAD	C4-C4X	3.87	1.48	1.41
3	C	305	FAD	C9A-C5X	3.80	1.50	1.42
3	D	300	FAD	C2B-C1B	-3.64	1.48	1.53
3	D	300	FAD	C2A-N3A	3.61	1.37	1.32
3	B	310	FAD	C2A-N3A	3.56	1.37	1.32
3	D	300	FAD	C4-C4X	3.48	1.47	1.41
3	C	305	FAD	C6A-N6A	3.36	1.46	1.34
3	B	310	FAD	C2-N1	3.24	1.44	1.38
3	B	310	FAD	C6A-N6A	3.23	1.45	1.34
3	C	305	FAD	C2-N1	3.13	1.44	1.38
3	D	300	FAD	C6A-N6A	3.05	1.45	1.34
3	C	305	FAD	C2-N3	2.94	1.44	1.38
3	D	300	FAD	C2-N1	2.78	1.43	1.38
3	D	300	FAD	C2-N3	2.77	1.43	1.38
3	D	300	FAD	C1'-N10	-2.76	1.45	1.48
3	C	305	FAD	O4B-C1B	2.67	1.44	1.41
3	A	315	FAD	C2A-N1A	2.62	1.38	1.33
3	A	315	FAD	C2-N1	2.61	1.43	1.38
3	B	310	FAD	C2A-N1A	2.60	1.38	1.33
3	A	315	FAD	C2-N3	2.60	1.43	1.38
3	D	300	FAD	C4A-N3A	2.58	1.39	1.35
3	B	310	FAD	C2-N3	2.55	1.43	1.38
3	C	305	FAD	C2A-N1A	2.53	1.38	1.33
3	C	305	FAD	C4A-N3A	2.50	1.39	1.35
3	B	310	FAD	C1'-N10	-2.49	1.45	1.48
3	D	300	FAD	C2A-N1A	2.48	1.38	1.33
3	A	315	FAD	C2B-C1B	-2.46	1.50	1.53
2	C	313	UMP	C2-N3	2.38	1.42	1.38
3	B	310	FAD	C4A-N3A	2.33	1.38	1.35
2	B	308	UMP	O4-C4	2.22	1.30	1.24
2	B	308	UMP	C2-N3	2.18	1.42	1.38
3	C	305	FAD	C2B-C1B	-2.14	1.50	1.53
3	D	300	FAD	O4B-C1B	2.12	1.44	1.41
2	A	303	UMP	C2-N3	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	315	FAD	C8M-C8	2.04	1.55	1.51
3	D	300	FAD	C5A-N7A	2.01	1.47	1.39

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	310	FAD	C4-N3-C2	8.58	122.39	115.14
3	A	315	FAD	C4-N3-C2	8.18	122.05	115.14
3	B	310	FAD	C1'-N10-C9A	7.06	123.85	118.29
3	D	300	FAD	C4-N3-C2	7.05	121.09	115.14
3	C	305	FAD	C4-N3-C2	6.74	120.83	115.14
3	A	315	FAD	C1'-N10-C9A	6.62	123.50	118.29
3	D	300	FAD	N3A-C2A-N1A	-5.70	119.77	128.68
3	B	310	FAD	N3A-C2A-N1A	-5.45	120.16	128.68
3	C	305	FAD	N3A-C2A-N1A	-5.27	120.45	128.68
3	A	315	FAD	N3A-C2A-N1A	-5.23	120.51	128.68
3	D	300	FAD	C1'-N10-C9A	4.64	121.94	118.29
3	A	315	FAD	C4X-C4-N3	-4.62	117.11	123.43
3	B	310	FAD	C4X-C4-N3	-4.29	117.56	123.43
3	D	300	FAD	C4X-C4-N3	-3.98	117.98	123.43
2	B	308	UMP	C5-C4-N3	-3.94	114.64	123.31
3	C	305	FAD	C5X-C9A-N10	3.77	120.44	117.72
3	C	305	FAD	C1'-N10-C9A	3.76	121.25	118.29
3	D	300	FAD	C4X-N5-C5X	3.68	120.45	116.77
3	B	310	FAD	C4X-N5-C5X	3.62	120.39	116.77
3	C	305	FAD	C4X-N5-C5X	3.51	120.27	116.77
2	A	303	UMP	C2'-C1'-N1	-3.43	106.36	114.27
3	A	315	FAD	C4-C4X-C10	-3.40	117.70	119.95
2	C	313	UMP	C5-C4-N3	-3.37	115.89	123.31
3	D	300	FAD	C1B-N9A-C4A	-3.31	120.83	126.64
3	C	305	FAD	C4X-C4-N3	-3.25	118.99	123.43
3	C	305	FAD	C4-C4X-C10	-3.23	117.81	119.95
3	C	305	FAD	C2A-N1A-C6A	3.16	124.16	118.75
3	A	315	FAD	C4X-N5-C5X	3.11	119.88	116.77
2	B	308	UMP	C2'-C1'-N1	-3.04	107.25	114.27
2	D	318	UMP	C2'-C1'-N1	-3.00	107.34	114.27
3	A	315	FAD	C9A-N10-C10	-2.99	117.99	121.91
3	C	305	FAD	C9A-N10-C10	-2.95	118.04	121.91
2	D	318	UMP	C5-C4-N3	-2.93	116.85	123.31
3	A	315	FAD	C5X-C9A-N10	2.82	119.76	117.72
3	B	310	FAD	C9A-N10-C10	-2.79	118.26	121.91
3	C	305	FAD	C1'-N10-C10	2.57	120.71	118.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	310	FAD	C1B-N9A-C4A	-2.56	122.14	126.64
3	A	315	FAD	P-O3P-PA	-2.52	124.17	132.83
2	A	303	UMP	C5-C4-N3	-2.47	117.88	123.31
3	B	310	FAD	P-O3P-PA	-2.46	124.38	132.83
3	D	300	FAD	P-O3P-PA	-2.46	124.38	132.83
3	B	310	FAD	C2A-N1A-C6A	2.42	122.89	118.75
3	D	300	FAD	C5X-C9A-N10	2.42	119.47	117.72
3	C	305	FAD	P-O3P-PA	-2.37	124.69	132.83
3	D	300	FAD	C9A-N10-C10	-2.36	118.82	121.91
3	D	300	FAD	C4-C4X-C10	-2.36	118.39	119.95
2	C	313	UMP	C2'-C1'-N1	-2.33	108.89	114.27
3	B	310	FAD	C4-C4X-C10	-2.31	118.42	119.95
3	C	305	FAD	C6-C5X-C9A	2.21	121.95	119.05
3	A	315	FAD	O2A-PA-O1A	2.19	123.06	112.24
3	C	305	FAD	O2A-PA-O1A	2.13	122.77	112.24
3	A	315	FAD	C1B-N9A-C4A	-2.08	122.99	126.64
2	A	303	UMP	OP3-P-OP1	2.05	118.69	110.68
2	B	308	UMP	OP3-P-OP1	2.02	118.61	110.68
3	A	315	FAD	C2A-N1A-C6A	2.02	122.20	118.75
3	A	315	FAD	C5A-C6A-N6A	2.01	123.41	120.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	305	FAD	C5'-O5'-P-O1P
3	D	300	FAD	O4'-C4'-C5'-O5'
3	A	315	FAD	PA-O3P-P-O2P
3	B	310	FAD	C5'-O5'-P-O1P

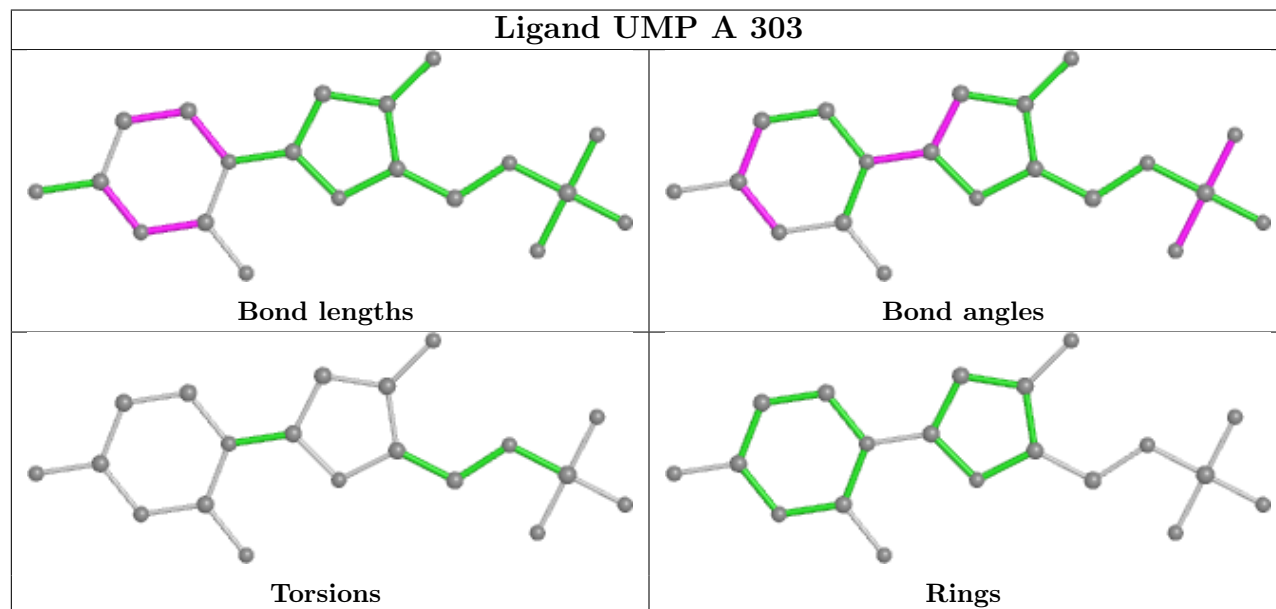
There are no ring outliers.

4 monomers are involved in 5 short contacts:

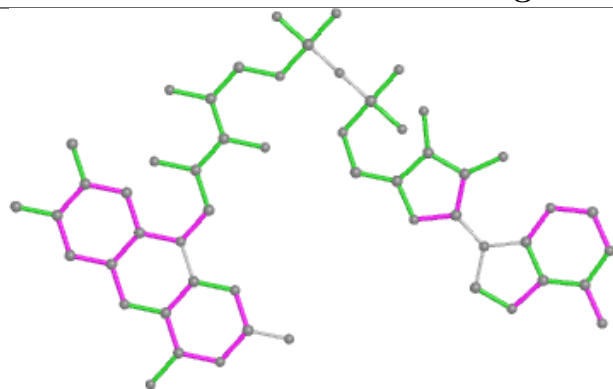
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	303	UMP	1	0
2	D	318	UMP	1	0
2	B	308	UMP	1	0
2	C	313	UMP	2	0

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

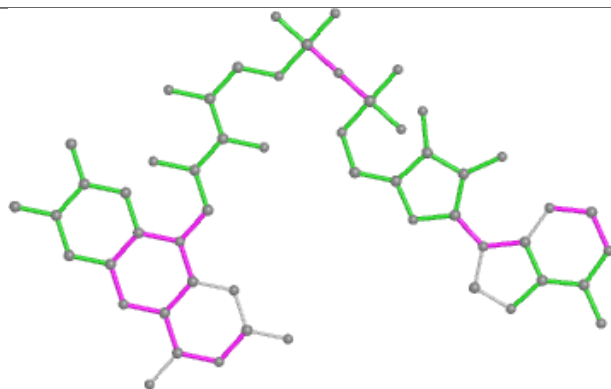
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



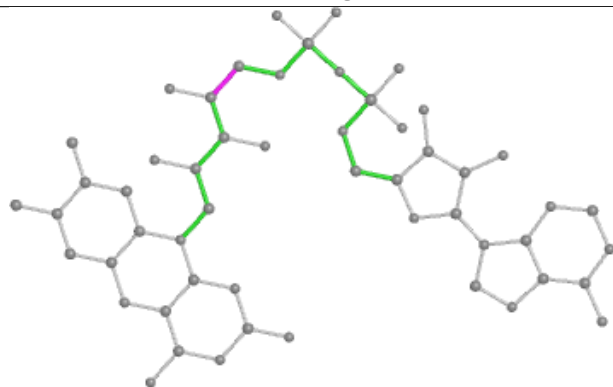
## Ligand FAD D 300



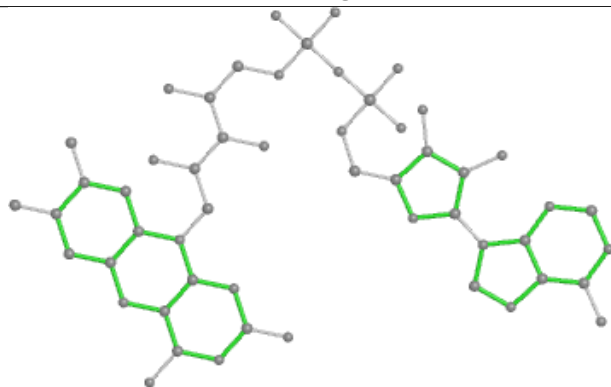
Bond lengths



Bond angles

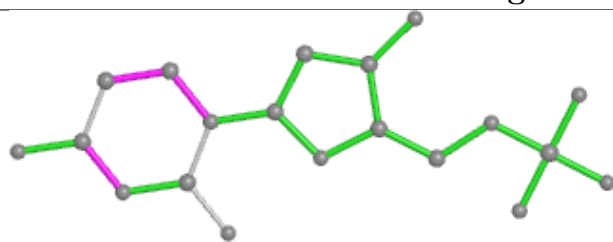


Torsions

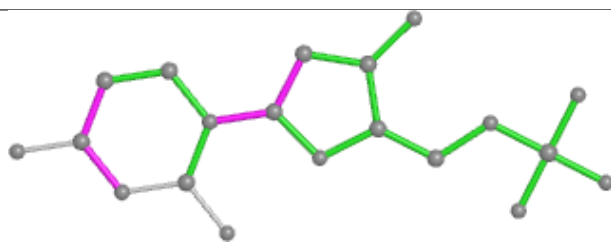


Rings

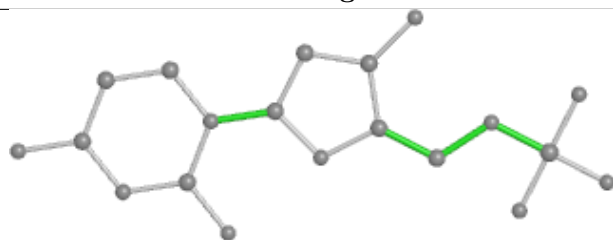
## Ligand UMP D 318



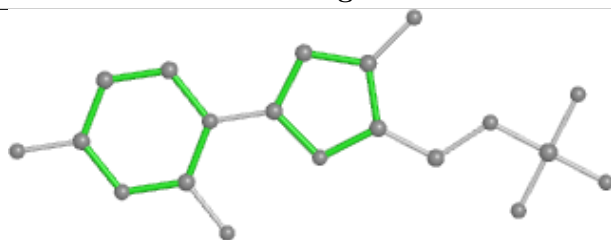
Bond lengths



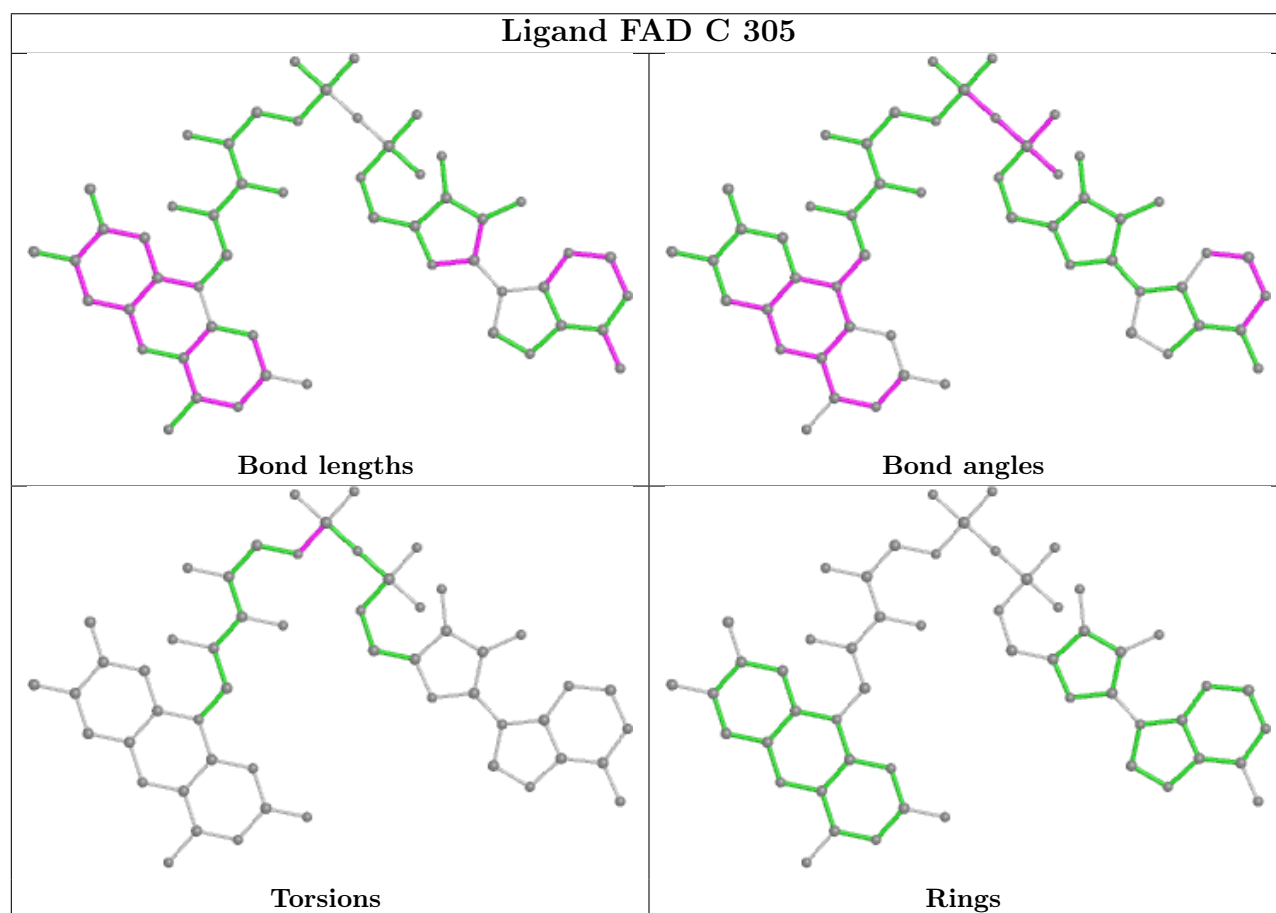
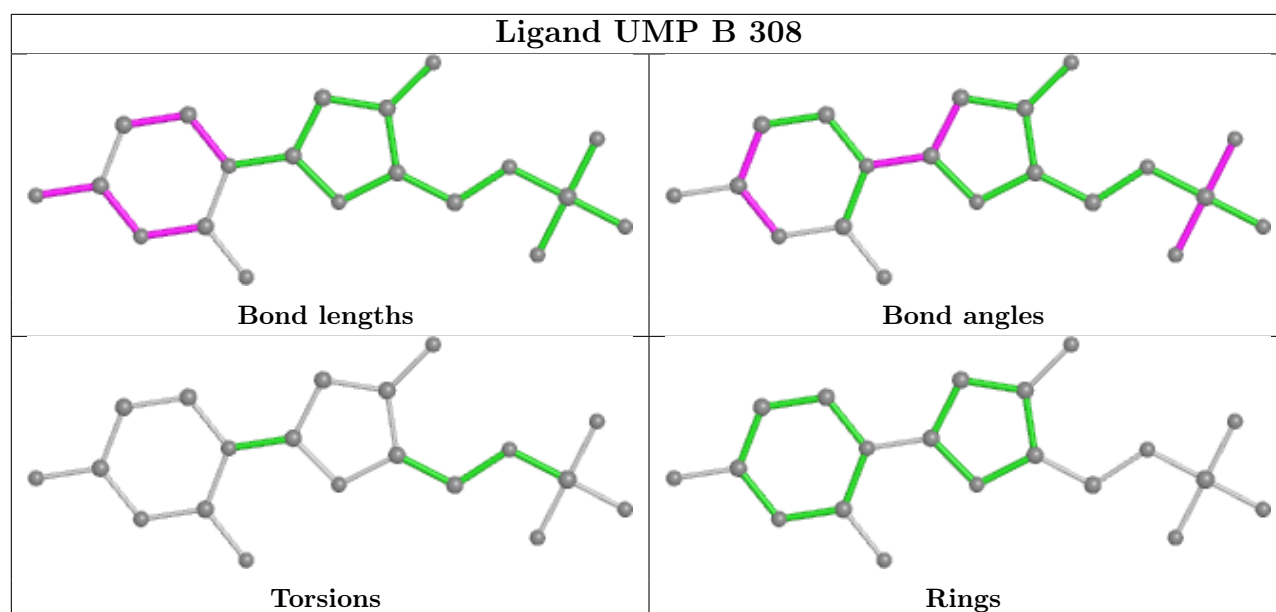
Bond angles



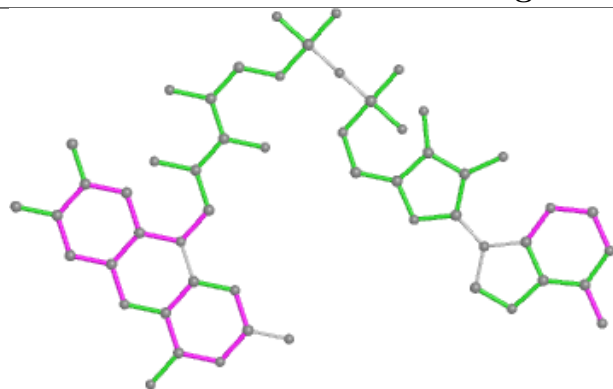
Torsions



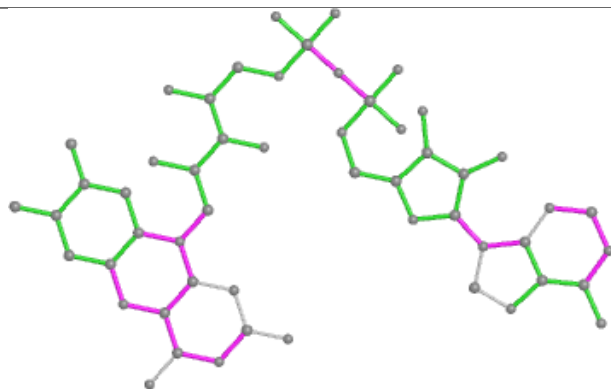
Rings



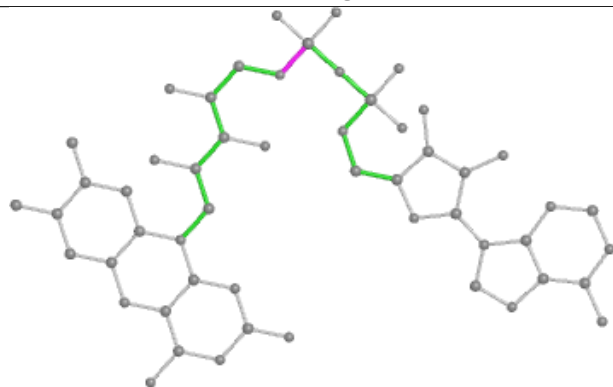
## Ligand FAD B 310



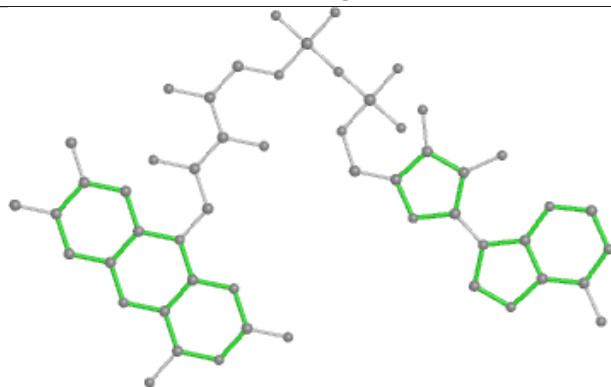
Bond lengths



Bond angles

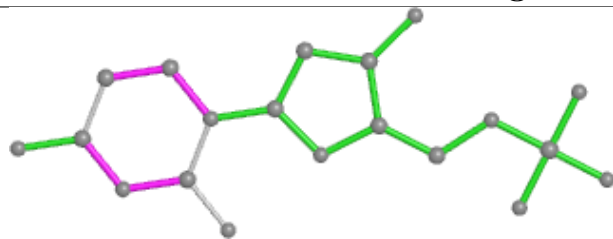


Torsions

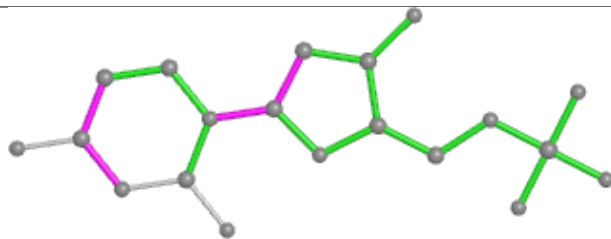


Rings

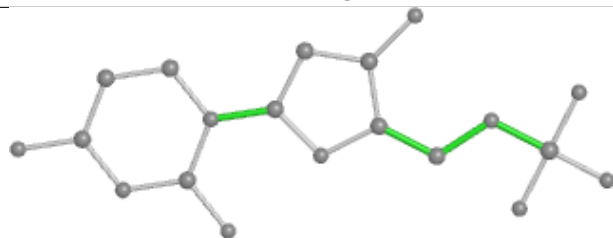
## Ligand UMP C 313



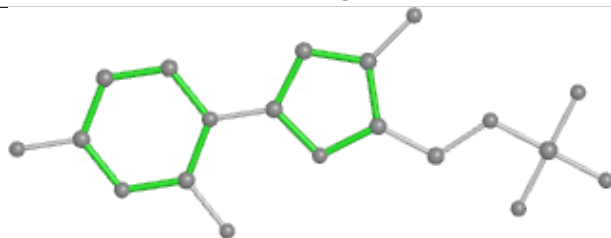
Bond lengths



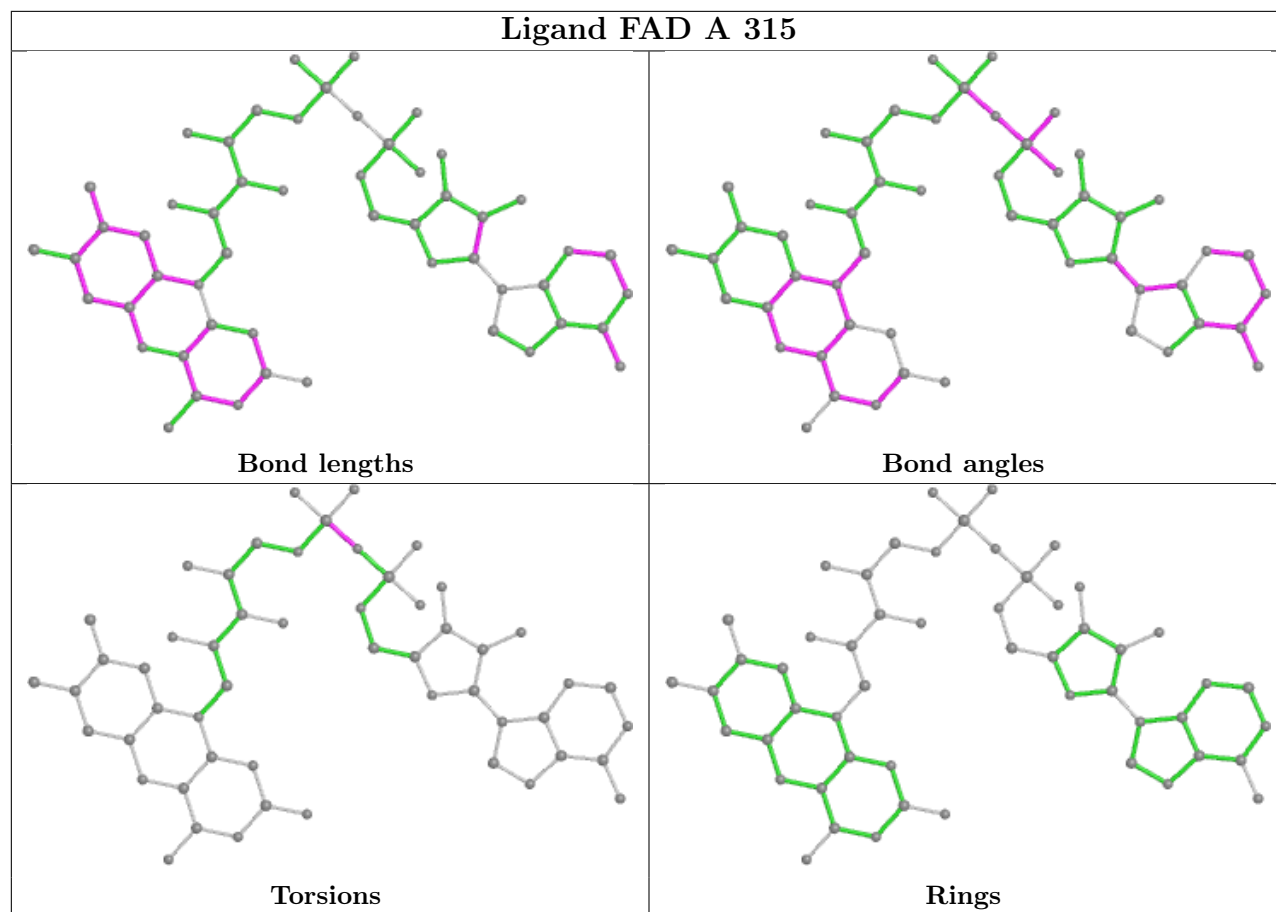
Bond angles



Torsions



Rings



## 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, 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	218/232 (93%)	0.01	1 (0%) 91 94	29, 35, 48, 54	0
1	B	220/232 (94%)	0.03	3 (1%) 75 82	29, 35, 50, 52	0
1	C	214/232 (92%)	0.07	3 (1%) 75 82	29, 35, 47, 53	0
1	D	212/232 (91%)	0.21	6 (2%) 53 62	29, 35, 48, 51	0
All	All	864/928 (93%)	0.08	13 (1%) 73 81	29, 35, 48, 54	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	91	TYR	4.8
1	D	92	SER	3.6
1	D	218	VAL	3.4
1	C	109	TYR	3.3
1	B	108	GLY	3.0
1	D	113	ILE	2.8
1	B	218	VAL	2.6
1	C	96	TYR	2.6
1	B	112	THR	2.5
1	C	91	TYR	2.4
1	D	106	LEU	2.2
1	A	47	TYR	2.2
1	D	25	ARG	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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 [i](#)

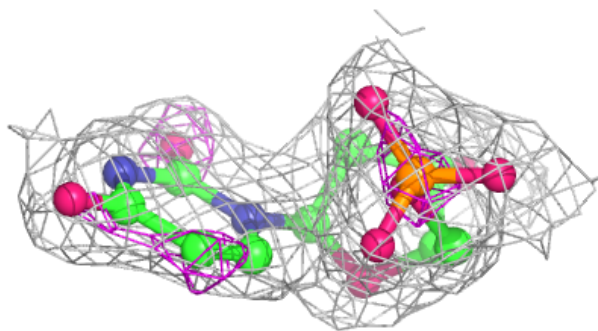
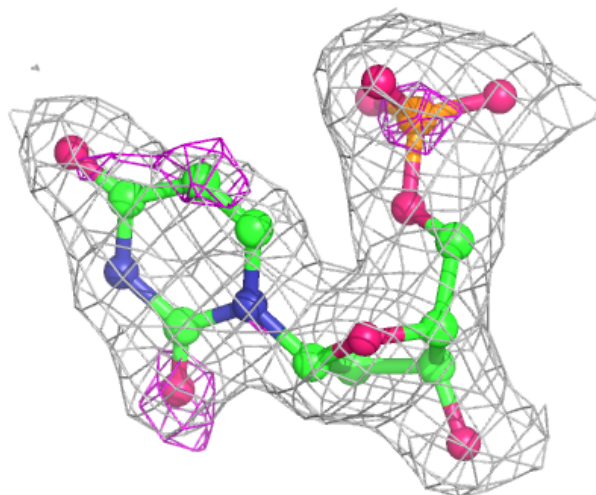
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	UMP	C	313	20/20	0.95	0.12	30,33,38,40	0
2	UMP	D	318	20/20	0.96	0.10	34,37,38,39	0
3	FAD	A	315	53/53	0.96	0.11	31,36,39,42	0
3	FAD	B	310	53/53	0.96	0.11	32,37,40,42	0
3	FAD	C	305	53/53	0.96	0.12	25,34,36,37	0
3	FAD	D	300	53/53	0.96	0.10	27,37,38,40	0
2	UMP	A	303	20/20	0.98	0.08	27,30,32,33	0
2	UMP	B	308	20/20	0.98	0.06	27,30,32,32	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.

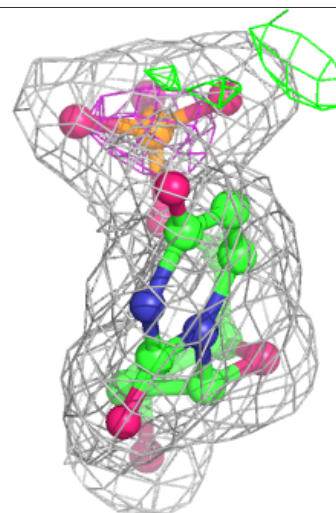
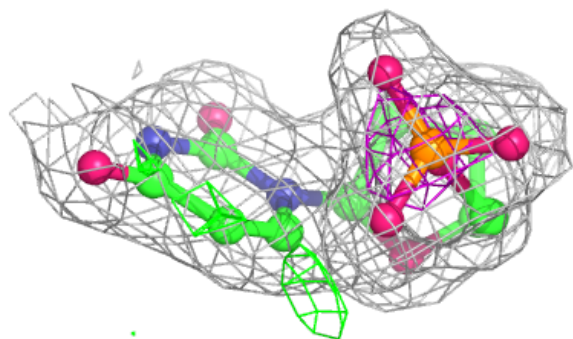
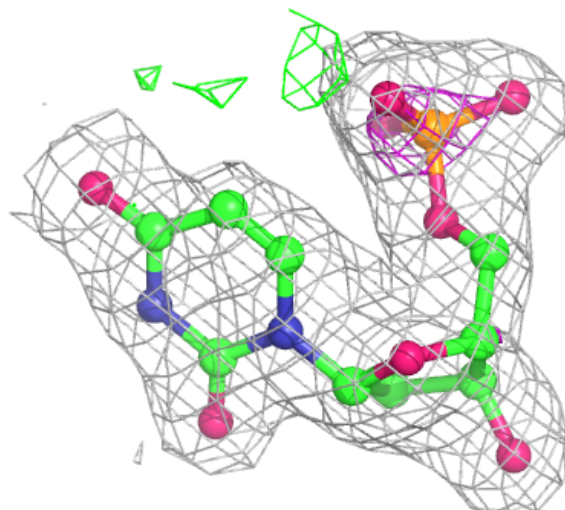
**Electron density around UMP C 313:**

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



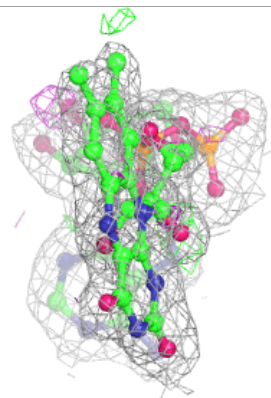
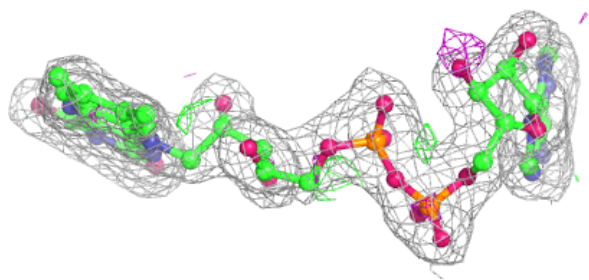
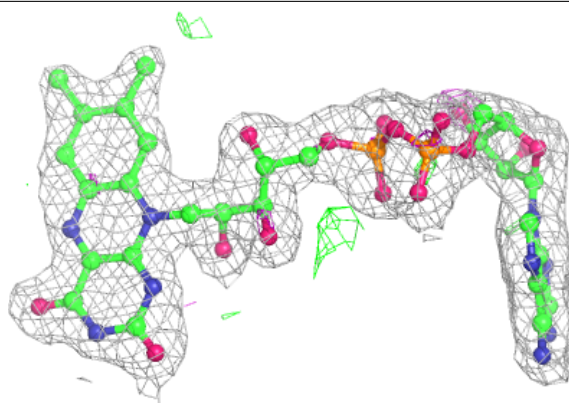
**Electron density around UMP D 318:**

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

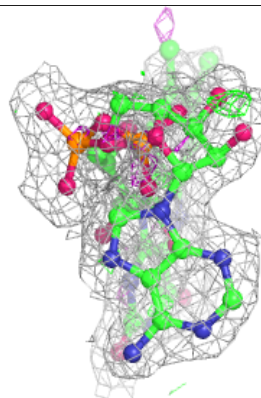
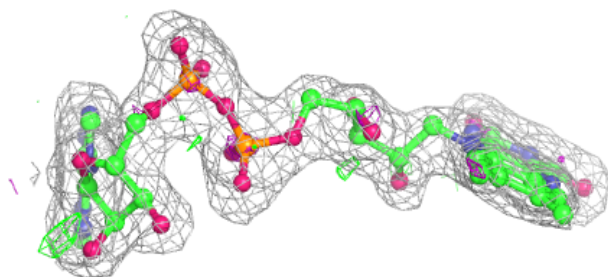
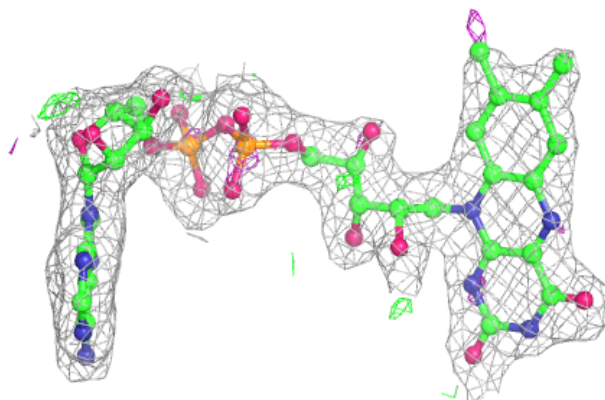


**Electron density around FAD A 315:**

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

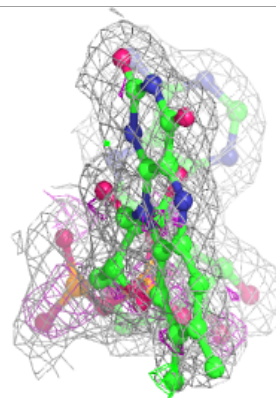
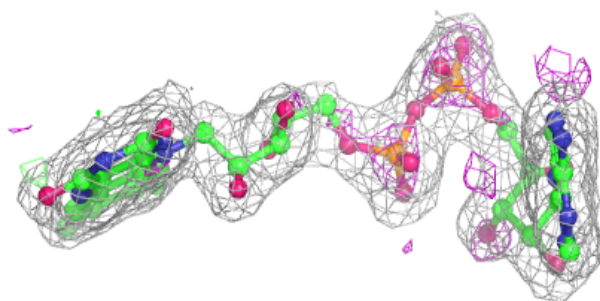
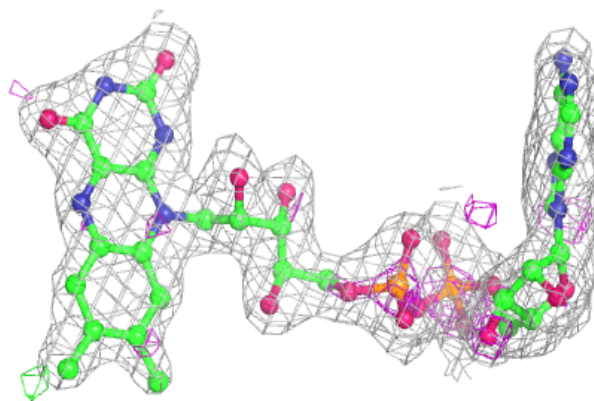
**Electron density around FAD B 310:**

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

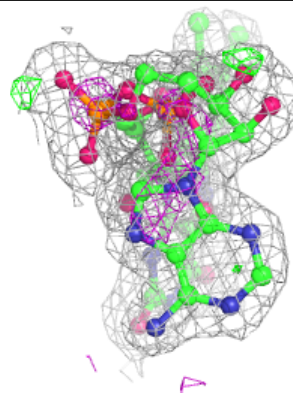
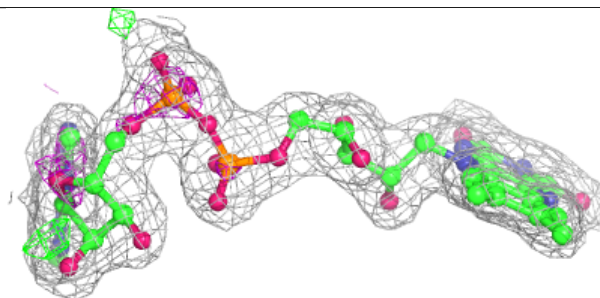
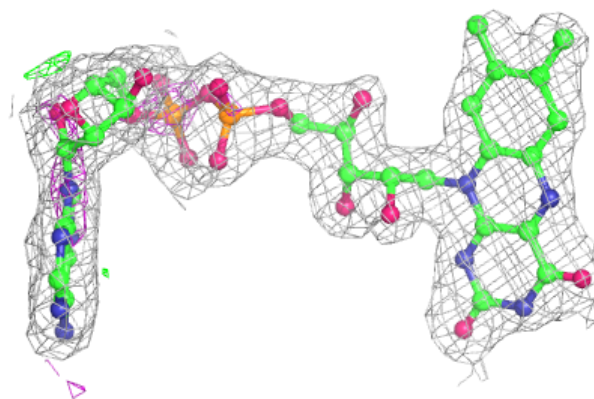


**Electron density around FAD C 305:**

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

**Electron density around FAD D 300:**

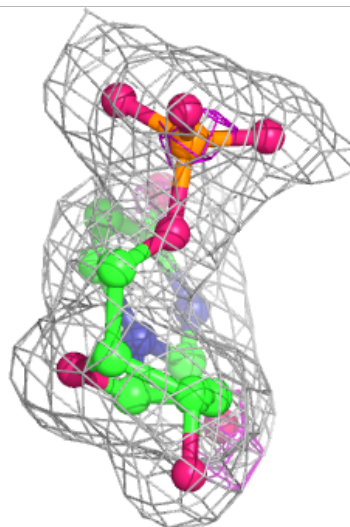
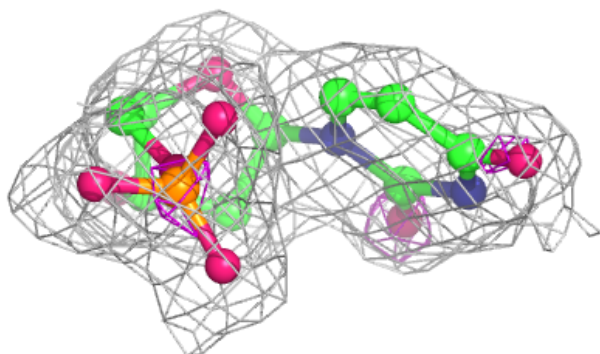
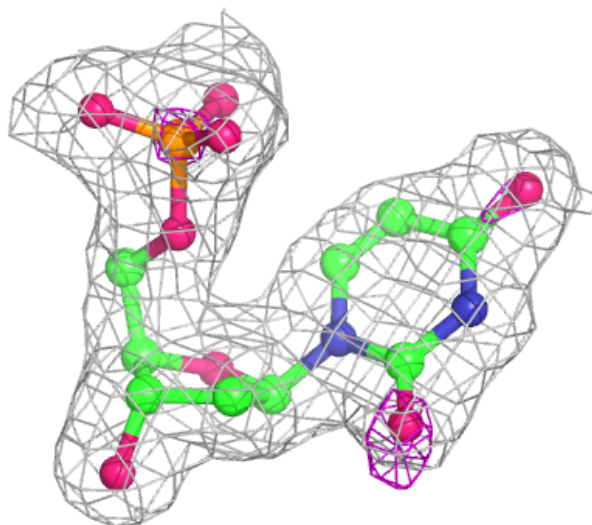
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





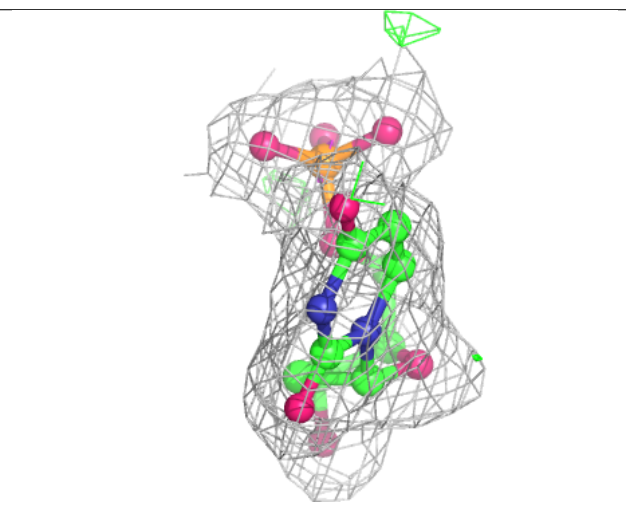
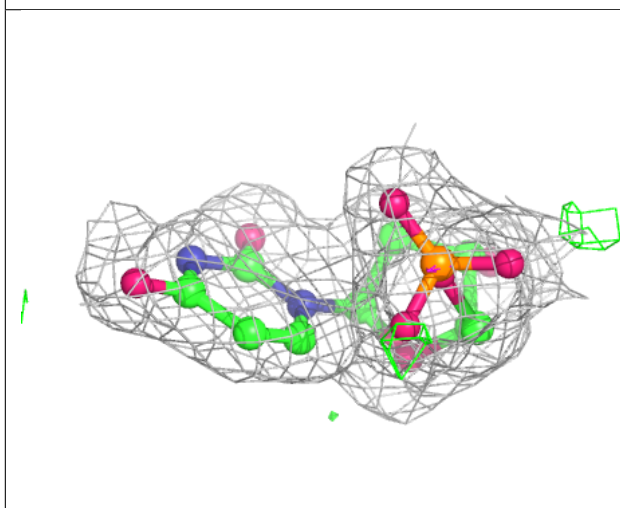
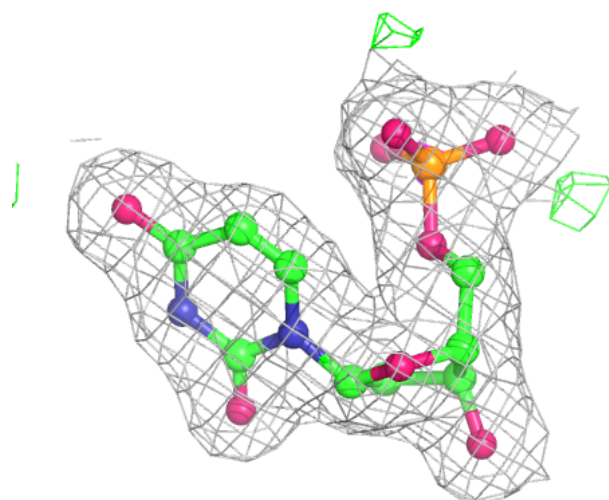
**Electron density around UMP A 303:**

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



**Electron density around UMP B 308:**

$2mF_o-DF_c$  (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.