



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2020 – 02:10 am BST

PDB ID : 3HE3
Title : Crystal Structure of UDP-galactopyranose mutase in complex with UDP
Authors : Partha, S.K.; van Straaten, K.E.; Sanders, D.A.R.
Deposited on : 2009-05-07
Resolution : 2.40 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

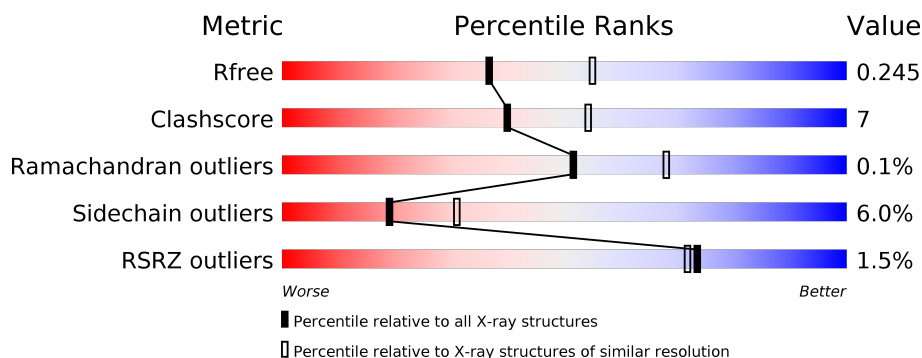
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	397	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 16%, green 75%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 75% 16% • 8% </div> </div>
1	B	397	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 16%, green 75%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 75% 16% • 8% </div> </div>
1	C	397	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 75%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 75% 15% • 9% </div> </div>
1	D	397	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 17%, green 72%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 72% 17% • 9% </div> </div>
1	E	397	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 20%, green 69%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 69% 20% • 8% </div> </div>
1	F	397	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 15%, green 76%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 76% 15% • 9% </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	397	<div><div><div>%</div><div><div></div><div>72%</div><div>18%</div><div>•</div><div>9%</div></div></div></div>
1	H	397	<div><div><div>%</div><div><div></div><div>71%</div><div>19%</div><div>•</div><div>9%</div></div></div></div>
1	I	397	<div><div><div>%</div><div><div></div><div>76%</div><div>13%</div><div>•</div><div>8%</div></div></div></div>
1	J	397	<div><div><div>2%</div><div><div></div><div>72%</div><div>17%</div><div>••</div><div>9%</div></div></div></div>

2 Entry composition

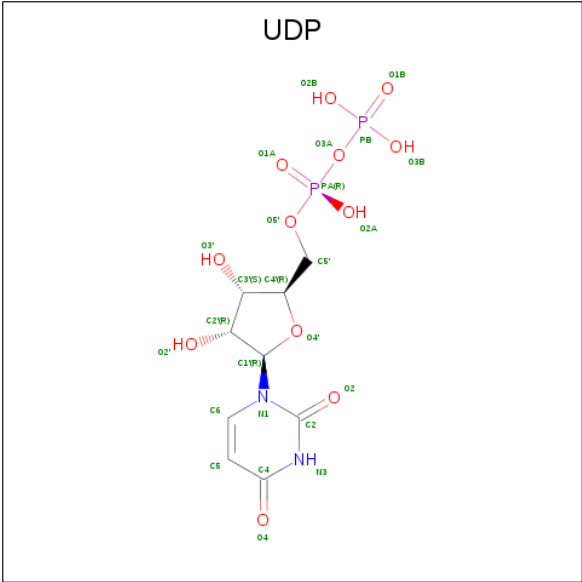
There are 4 unique types of molecules in this entry. The entry contains 31550 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-galactopyranose mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2993	1909	520	556	8			
1	B	364	Total	C	N	O	S	1	0	0
			2971	1896	516	551	8			
1	C	362	Total	C	N	O	S	1	0	0
			2950	1885	511	546	8			
1	D	362	Total	C	N	O	S	1	0	0
			2960	1891	514	547	8			
1	E	364	Total	C	N	O	S	0	0	0
			2975	1899	516	552	8			
1	F	363	Total	C	N	O	S	1	0	0
			2969	1896	516	549	8			
1	G	363	Total	C	N	O	S	0	0	0
			2965	1894	515	548	8			
1	H	363	Total	C	N	O	S	0	0	0
			2969	1896	516	549	8			
1	I	364	Total	C	N	O	S	0	0	0
			2975	1899	517	551	8			
1	J	361	Total	C	N	O	S	0	0	0
			2951	1885	512	546	8			

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	G	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	H	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	I	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	J	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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		
3	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	J	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	135	Total	O	0	0
			135	135		
4	B	123	Total	O	0	0
			123	123		

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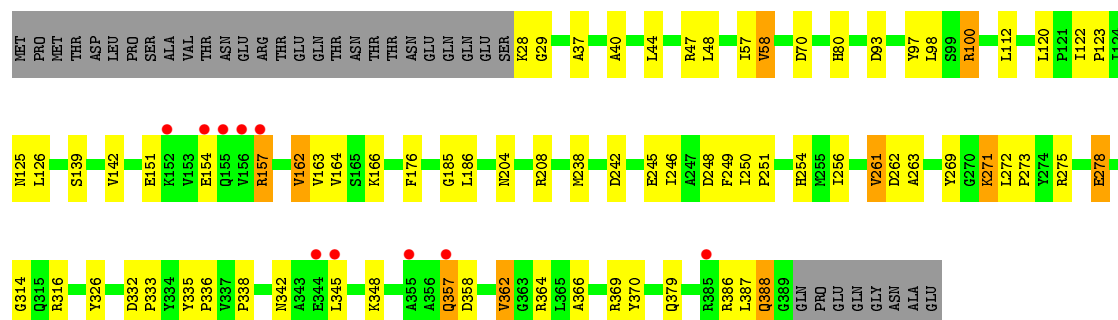
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	94	Total 94	O 94	0	0
4	D	95	Total 95	O 95	0	0
4	E	79	Total 79	O 79	0	0
4	F	107	Total 107	O 107	0	0
4	G	104	Total 104	O 104	0	0
4	H	133	Total 133	O 133	0	0
4	I	110	Total 110	O 110	0	0
4	J	112	Total 112	O 112	0	0

- Molecule 1: UDP-galactopyranose mutase

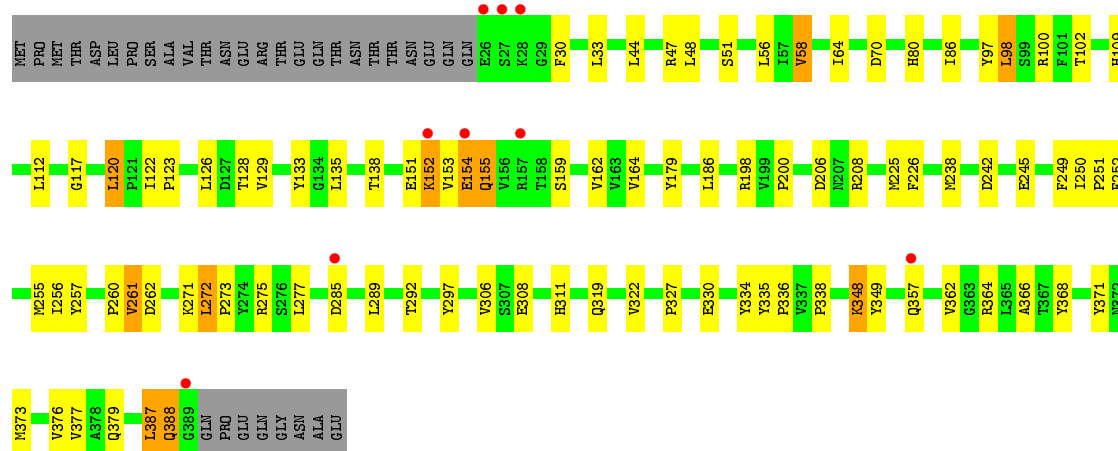




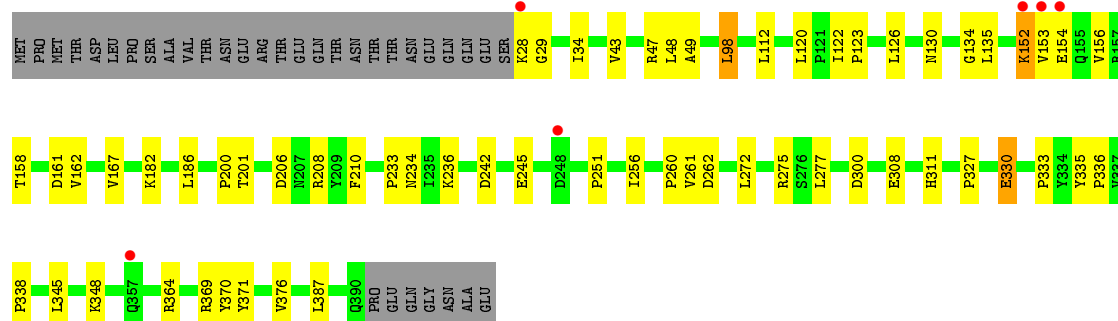
• Molecule 1: UDP-galactopyranose mutase



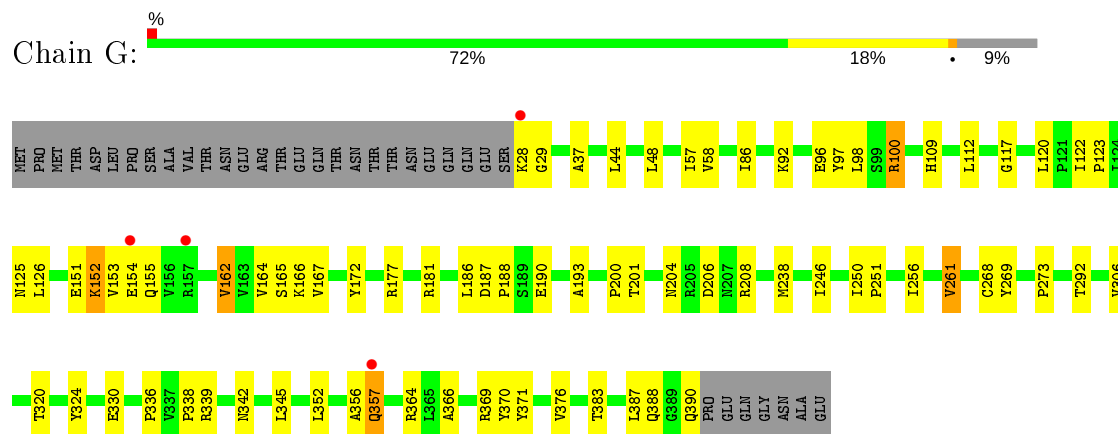
• Molecule 1: UDP-galactopyranose mutase



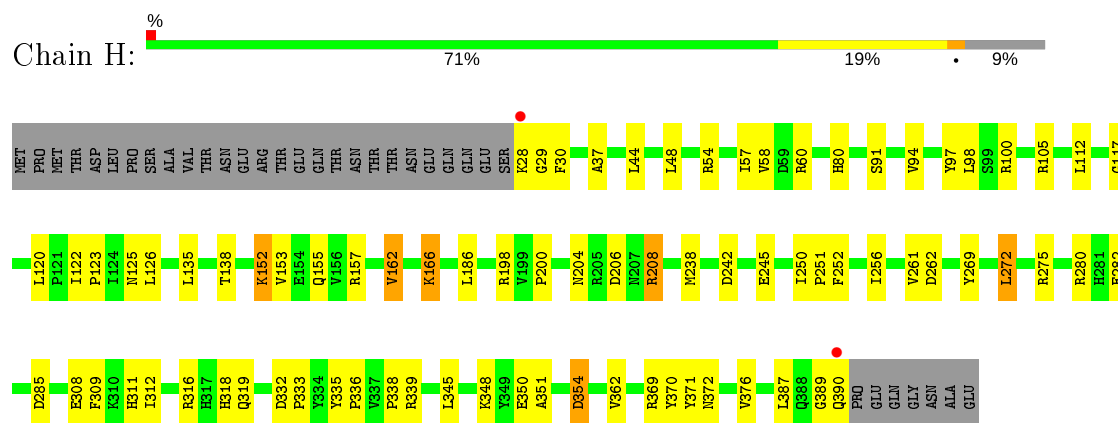
• Molecule 1: UDP-galactopyranose mutase



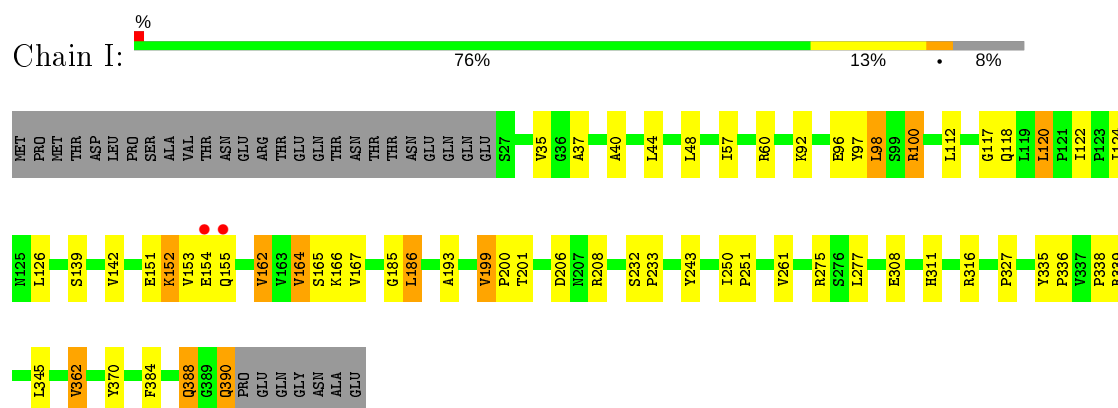
- Molecule 1: UDP-galactopyranose mutase



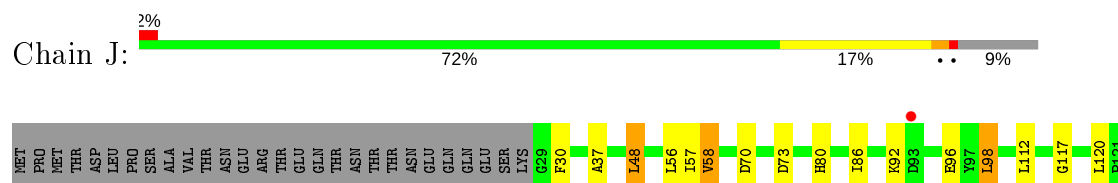
- Molecule 1: UDP-galactopyranose mutase

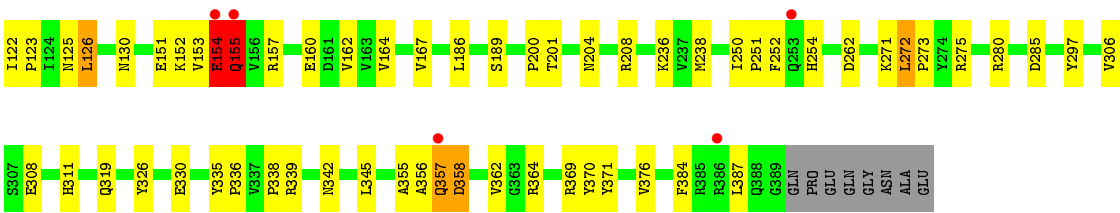


- Molecule 1: UDP-galactopyranose mutase



- Molecule 1: UDP-galactopyranose mutase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.05Å 176.87Å 222.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.88 – 2.40 39.88 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.88-2.40) 98.8 (39.88-2.40)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.208 , 0.254 0.202 , 0.245	Depositor DCC
R_{free} test set	10272 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31550	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, 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	0.32	0/3077	0.45	0/4183
1	B	0.26	0/3055	0.44	0/4155
1	C	0.27	0/3034	0.44	0/4127
1	D	0.25	0/3044	0.44	0/4139
1	E	0.33	0/3059	0.45	0/4159
1	F	0.28	0/3053	0.46	0/4151
1	G	0.28	0/3049	0.44	0/4146
1	H	0.31	0/3053	0.45	0/4151
1	I	0.29	0/3059	0.45	0/4159
1	J	0.39	0/3035	0.56	3/4128 (0.1%)
All	All	0.30	0/30518	0.46	3/41498 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	154	GLU	OE1-CD-OE2	-9.80	111.54	123.30
1	J	154	GLU	CA-CB-CG	-8.93	93.76	113.40
1	J	155	GLN	N-CA-CB	8.32	125.58	110.60

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	2993	0	2862	41	0
1	B	2971	0	2837	37	0
1	C	2950	0	2812	47	0
1	D	2960	0	2835	52	0
1	E	2975	0	2846	63	0
1	F	2969	0	2843	34	0
1	G	2965	0	2837	48	0
1	H	2969	0	2843	51	0
1	I	2975	0	2848	41	0
1	J	2951	0	2822	44	0
2	A	25	0	11	2	0
2	B	25	0	11	0	0
2	C	25	0	11	0	0
2	D	25	0	11	0	0
2	E	25	0	11	1	0
2	F	25	0	11	0	0
2	G	25	0	11	0	0
2	H	25	0	11	0	0
2	I	25	0	11	0	0
2	J	25	0	11	0	0
3	A	53	0	31	1	0
3	B	53	0	31	2	0
3	C	53	0	31	1	0
3	D	53	0	31	0	0
3	E	53	0	31	1	0
3	F	53	0	31	1	0
3	G	53	0	31	1	0
3	H	53	0	31	1	0
3	I	53	0	31	0	0
3	J	53	0	31	1	0
4	A	135	0	0	1	0
4	B	123	0	0	1	0
4	C	94	0	0	2	0
4	D	95	0	0	2	0
4	E	79	0	0	1	0
4	F	107	0	0	0	0
4	G	104	0	0	1	0
4	H	133	0	0	1	0
4	I	110	0	0	1	0
4	J	112	0	0	2	0
All	All	31550	0	28805	433	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 7.

The worst 5 of 433 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:154:GLU:CD	1:I:154:GLU:H	1.51	1.04
1:J:155:GLN:HG2	1:J:157:ARG:CZ	1.99	0.93
1:G:58:VAL:HG23	1:G:238:MET:HB3	1.53	0.87
1:H:162:VAL:O	1:H:166:LYS:HD2	1.76	0.85
1:G:154:GLU:HG3	1:G:155:GLN:H	1.44	0.83

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	364/397 (92%)	352 (97%)	12 (3%)	0	100	100
1	B	362/397 (91%)	355 (98%)	7 (2%)	0	100	100
1	C	360/397 (91%)	351 (98%)	8 (2%)	1 (0%)	41	55
1	D	360/397 (91%)	349 (97%)	10 (3%)	1 (0%)	41	55
1	E	362/397 (91%)	351 (97%)	10 (3%)	1 (0%)	41	55
1	F	361/397 (91%)	349 (97%)	12 (3%)	0	100	100
1	G	361/397 (91%)	349 (97%)	12 (3%)	0	100	100
1	H	361/397 (91%)	353 (98%)	8 (2%)	0	100	100
1	I	362/397 (91%)	347 (96%)	15 (4%)	0	100	100
1	J	359/397 (90%)	345 (96%)	13 (4%)	1 (0%)	41	55
All	All	3612/3970 (91%)	3501 (97%)	107 (3%)	4 (0%)	51	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	154	GLU
1	J	154	GLU
1	D	357	GLN
1	C	154	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/346 (92%)	295 (93%)	23 (7%)	14	23
1	B	315/346 (91%)	299 (95%)	16 (5%)	24	39
1	C	311/346 (90%)	296 (95%)	15 (5%)	25	41
1	D	314/346 (91%)	294 (94%)	20 (6%)	17	28
1	E	316/346 (91%)	296 (94%)	20 (6%)	18	28
1	F	315/346 (91%)	301 (96%)	14 (4%)	28	45
1	G	314/346 (91%)	295 (94%)	19 (6%)	18	30
1	H	315/346 (91%)	296 (94%)	19 (6%)	19	31
1	I	316/346 (91%)	294 (93%)	22 (7%)	15	24
1	J	313/346 (90%)	292 (93%)	21 (7%)	16	26
All	All	3147/3460 (91%)	2958 (94%)	189 (6%)	19	31

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	186	LEU
1	F	348	LYS
1	J	152	LYS
1	E	292	THR
1	F	98	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	108	GLN
1	F	311	HIS
1	I	357	GLN
1	D	311	HIS
1	E	311	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	E	450	-	51,58,58	1.31	5 (9%)	60,89,89	1.51	7 (11%)
3	FAD	C	450	-	51,58,58	1.31	5 (9%)	60,89,89	1.49	7 (11%)
3	FAD	A	450	-	51,58,58	1.33	6 (11%)	60,89,89	1.57	8 (13%)
2	UDP	G	400	-	20,26,26	1.10	1 (5%)	25,40,40	0.95	3 (12%)
2	UDP	D	400	-	20,26,26	1.13	1 (5%)	25,40,40	0.88	1 (4%)
2	UDP	F	400	-	20,26,26	1.12	1 (5%)	25,40,40	0.99	1 (4%)
2	UDP	C	400	-	20,26,26	1.16	1 (5%)	25,40,40	0.94	1 (4%)
2	UDP	E	400	-	20,26,26	1.15	1 (5%)	25,40,40	0.93	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	I	450	-	51,58,58	1.34	6 (11%)	60,89,89	1.50	7 (11%)
3	FAD	D	450	-	51,58,58	1.31	6 (11%)	60,89,89	1.53	7 (11%)
2	UDP	B	400	-	20,26,26	1.17	1 (5%)	25,40,40	0.89	1 (4%)
3	FAD	B	450	-	51,58,58	1.32	5 (9%)	60,89,89	1.51	8 (13%)
3	FAD	J	450	-	51,58,58	1.37	6 (11%)	60,89,89	1.56	9 (15%)
2	UDP	H	400	-	20,26,26	1.14	1 (5%)	25,40,40	0.93	1 (4%)
2	UDP	A	400	-	20,26,26	1.17	1 (5%)	25,40,40	1.02	1 (4%)
2	UDP	J	400	-	20,26,26	1.18	1 (5%)	25,40,40	0.98	1 (4%)
2	UDP	I	400	-	20,26,26	1.14	1 (5%)	25,40,40	0.88	1 (4%)
3	FAD	H	450	-	51,58,58	1.33	6 (11%)	60,89,89	1.49	7 (11%)
3	FAD	F	450	-	51,58,58	1.33	5 (9%)	60,89,89	1.58	9 (15%)
3	FAD	G	450	-	51,58,58	1.34	6 (11%)	60,89,89	1.48	7 (11%)

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	FAD	E	450	-	-	3/30/50/50	0/6/6/6
3	FAD	C	450	-	-	5/30/50/50	0/6/6/6
3	FAD	A	450	-	-	5/30/50/50	0/6/6/6
2	UDP	G	400	-	-	2/14/32/32	0/2/2/2
2	UDP	D	400	-	-	2/14/32/32	0/2/2/2
2	UDP	F	400	-	-	1/14/32/32	0/2/2/2
2	UDP	C	400	-	-	1/14/32/32	0/2/2/2
2	UDP	E	400	-	-	2/14/32/32	0/2/2/2
3	FAD	I	450	-	-	7/30/50/50	0/6/6/6
3	FAD	D	450	-	-	4/30/50/50	0/6/6/6
2	UDP	B	400	-	-	3/14/32/32	0/2/2/2
3	FAD	B	450	-	-	2/30/50/50	0/6/6/6
3	FAD	J	450	-	-	3/30/50/50	0/6/6/6
2	UDP	H	400	-	-	2/14/32/32	0/2/2/2
2	UDP	A	400	-	-	3/14/32/32	0/2/2/2
2	UDP	J	400	-	-	2/14/32/32	0/2/2/2
2	UDP	I	400	-	-	0/14/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	H	450	-	-	3/30/50/50	0/6/6/6
3	FAD	F	450	-	-	1/30/50/50	0/6/6/6
3	FAD	G	450	-	-	7/30/50/50	0/6/6/6

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	450	FAD	C10-N1	4.22	1.38	1.33
3	J	450	FAD	C2A-N3A	4.18	1.38	1.32
3	A	450	FAD	C2A-N3A	4.11	1.38	1.32
3	G	450	FAD	C10-N1	4.09	1.38	1.33
3	H	450	FAD	C2A-N3A	4.07	1.38	1.32

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	450	FAD	C4-N3-C2	6.41	120.55	115.14
3	E	450	FAD	C4-N3-C2	6.24	120.41	115.14
3	D	450	FAD	C4-N3-C2	6.18	120.36	115.14
3	A	450	FAD	C4-N3-C2	6.11	120.31	115.14
3	H	450	FAD	C4-N3-C2	5.99	120.20	115.14

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	450	FAD	O4'-C4'-C5'-O5'
2	G	400	UDP	PA-O3A-PB-O3B
2	A	400	UDP	PA-O3A-PB-O3B
2	H	400	UDP	PA-O3A-PB-O2B
2	H	400	UDP	PA-O3A-PB-O3B

There are no ring outliers.

10 monomers are involved in 12 short contacts:

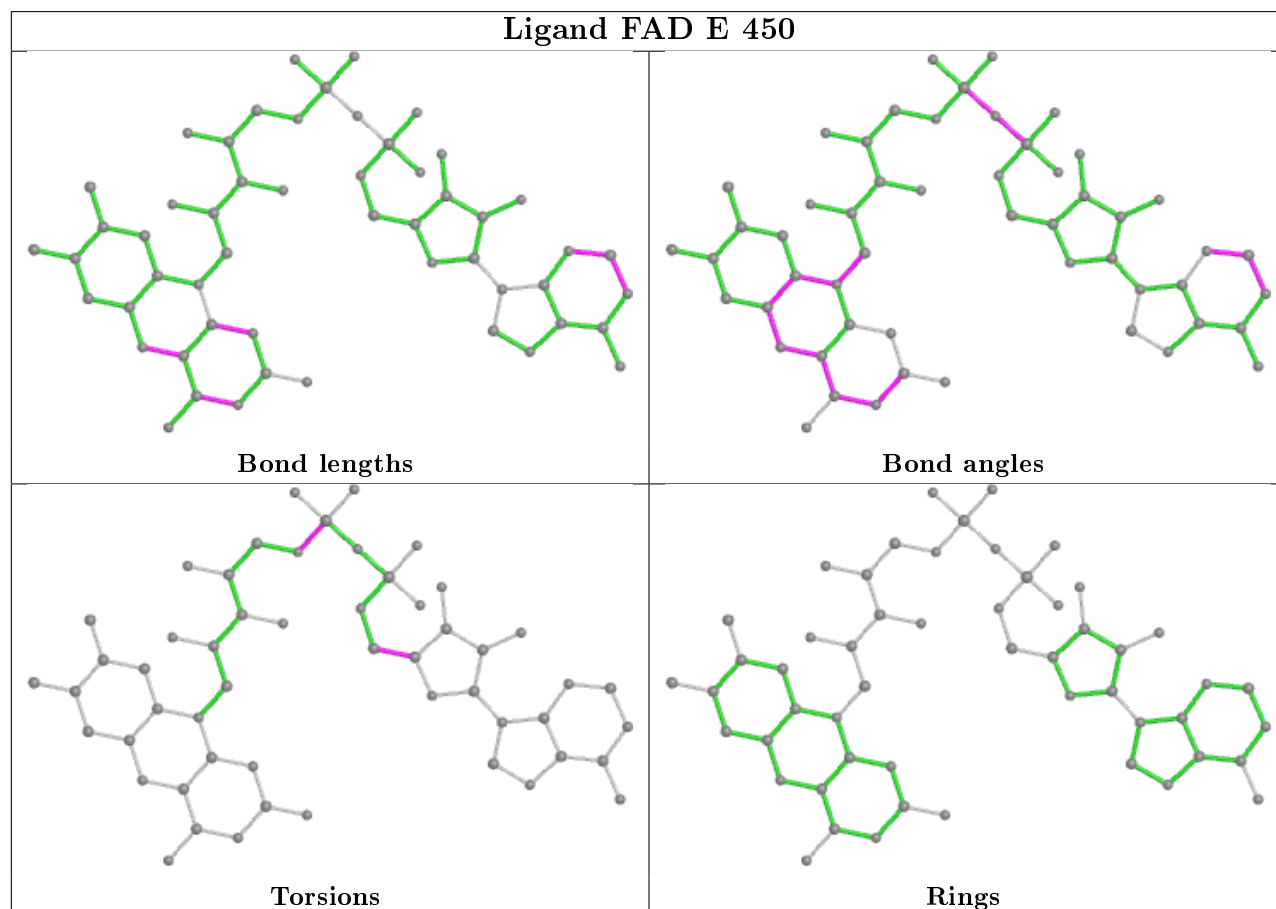
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	450	FAD	1	0
3	C	450	FAD	1	0
3	A	450	FAD	1	0
2	E	400	UDP	1	0

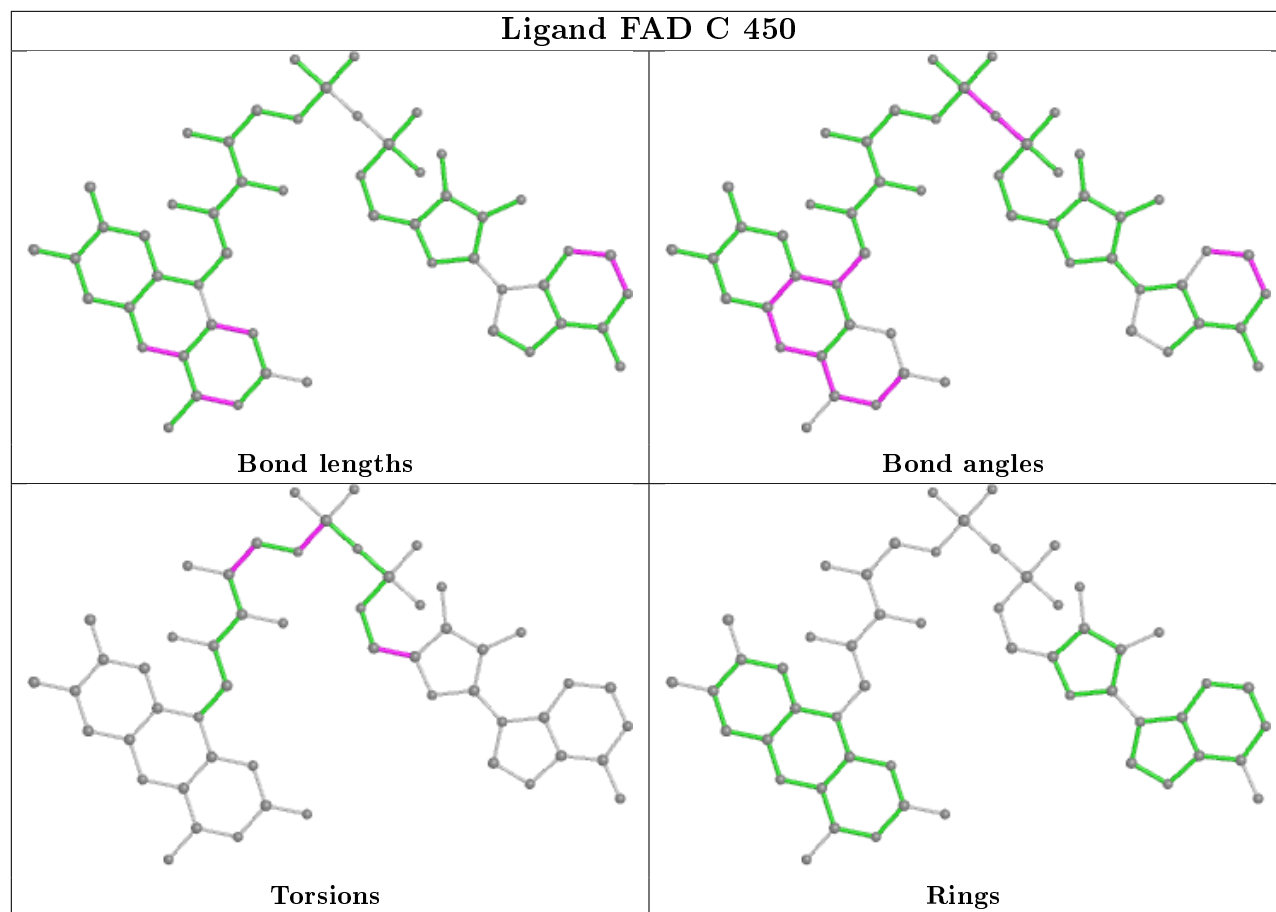
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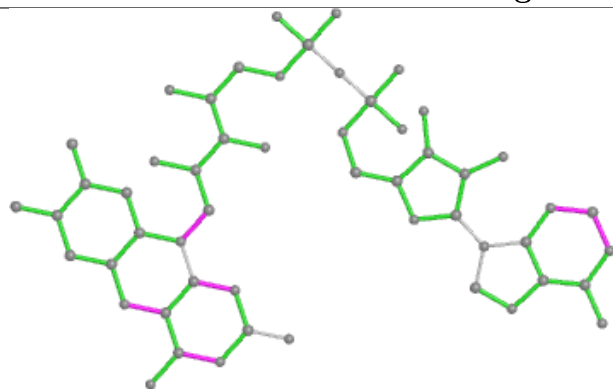
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	450	FAD	2	0
3	J	450	FAD	1	0
2	A	400	UDP	2	0
3	H	450	FAD	1	0
3	F	450	FAD	1	0
3	G	450	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

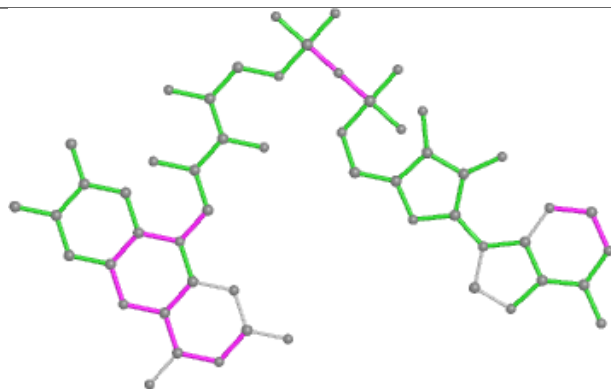




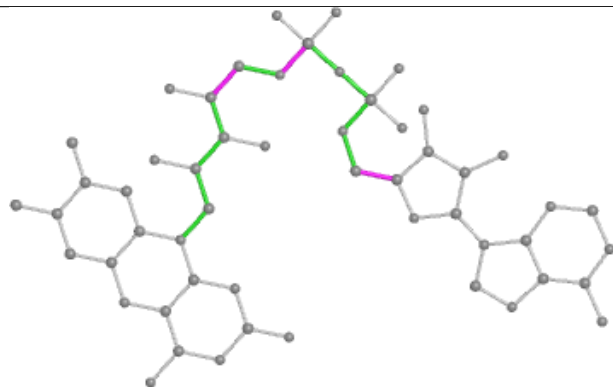
Ligand FAD A 450



Bond lengths



Bond angles

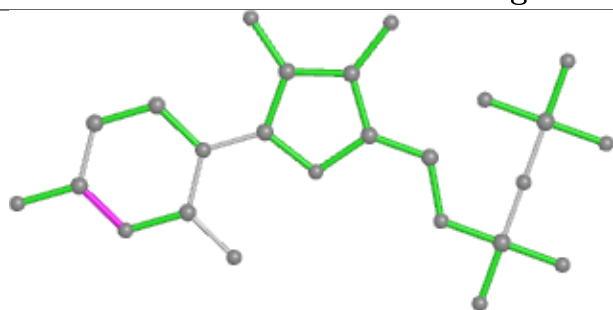


Torsions

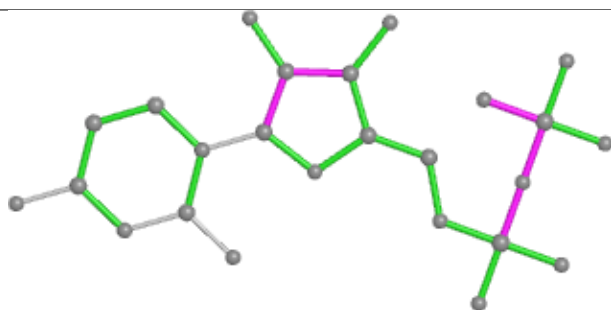


Rings

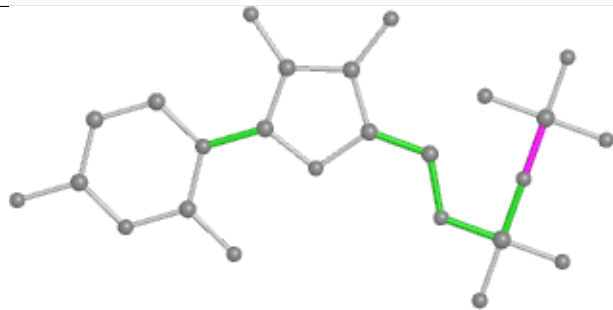
Ligand UDP G 400



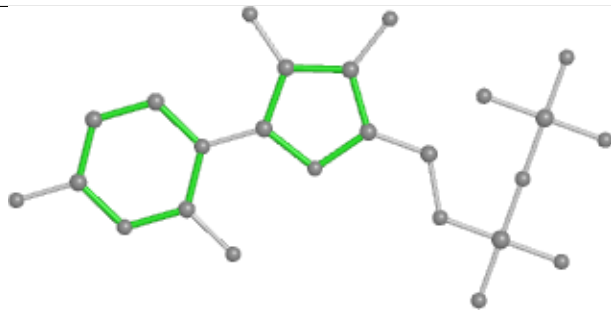
Bond lengths



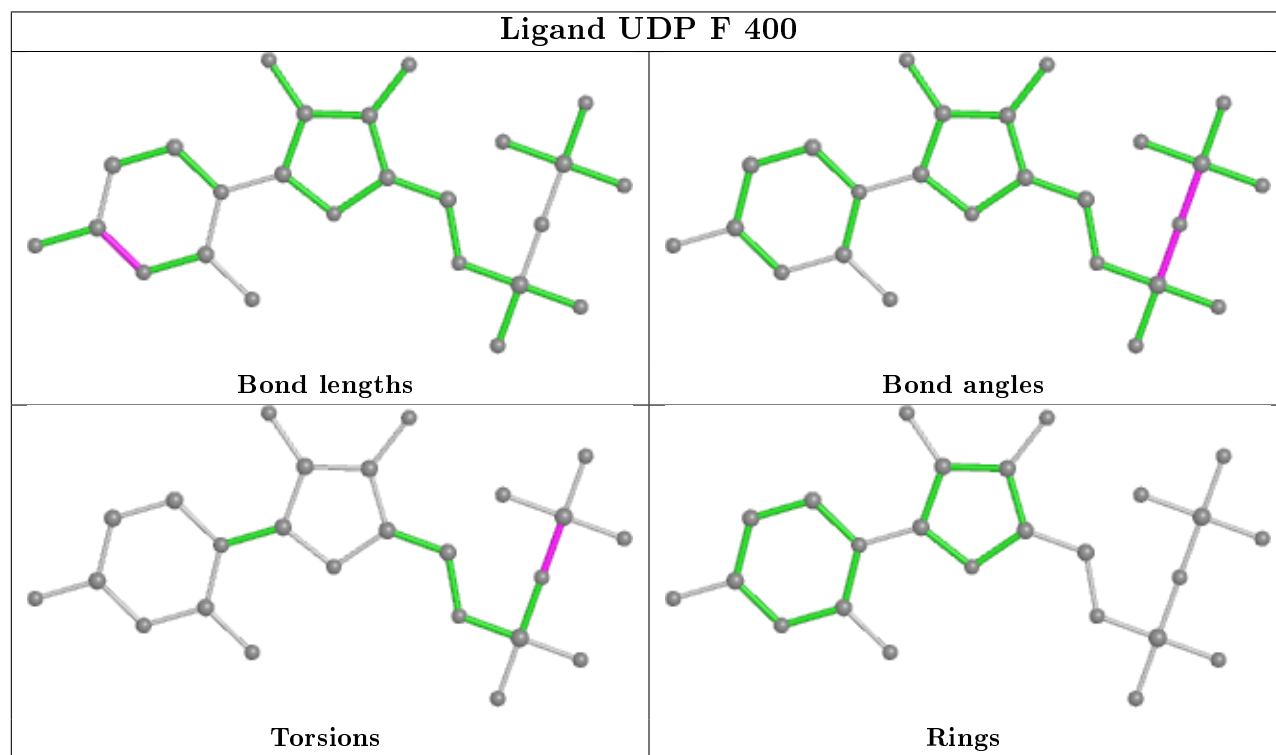
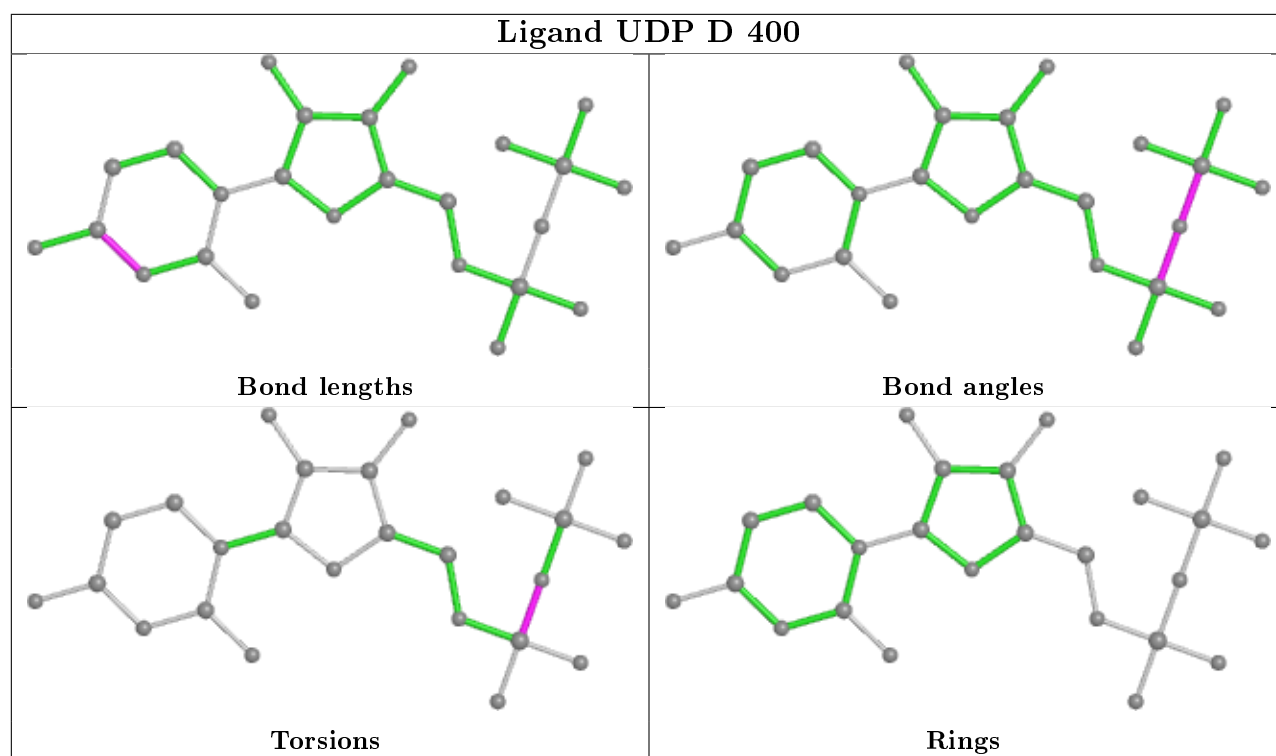
Bond angles

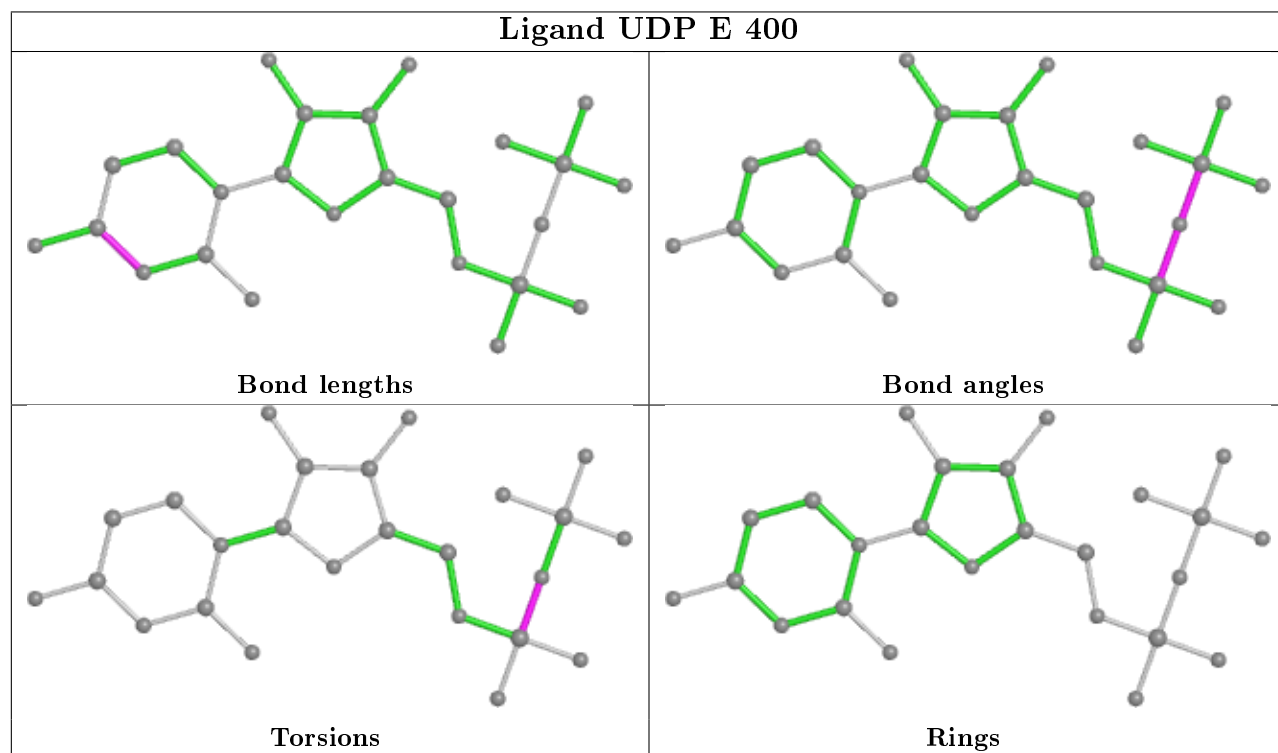
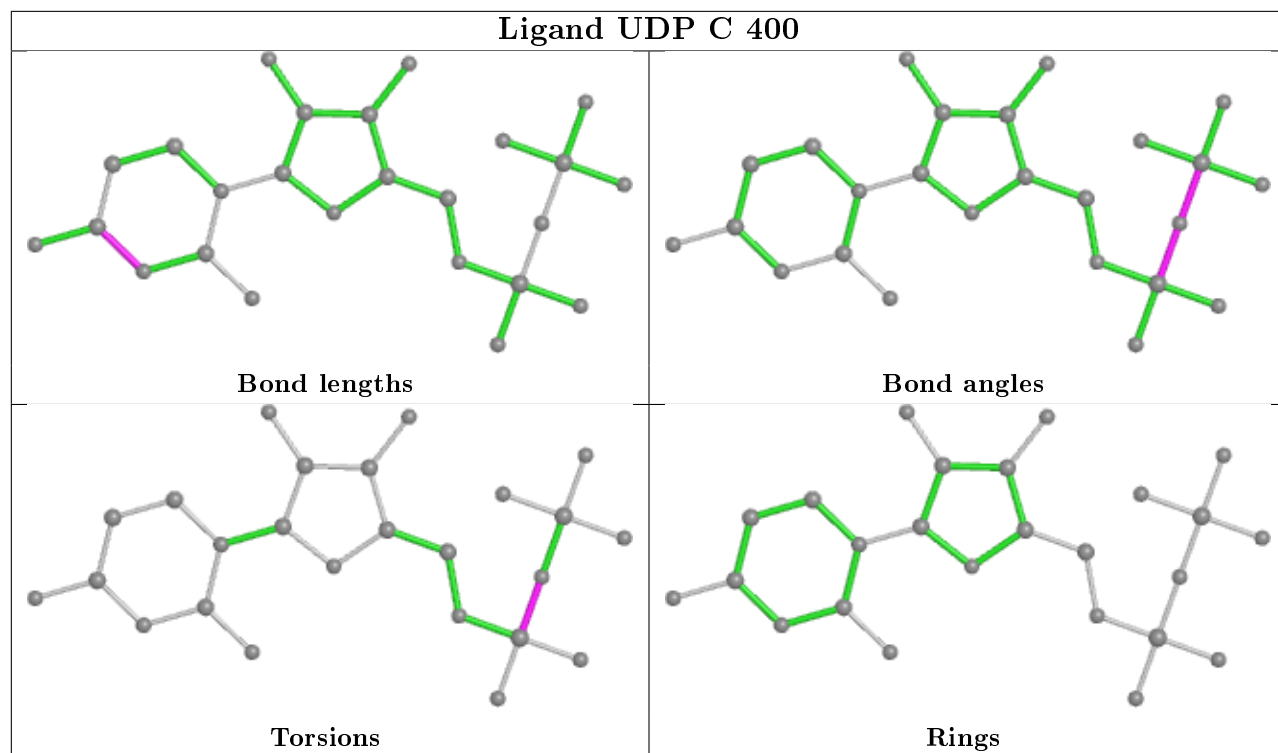


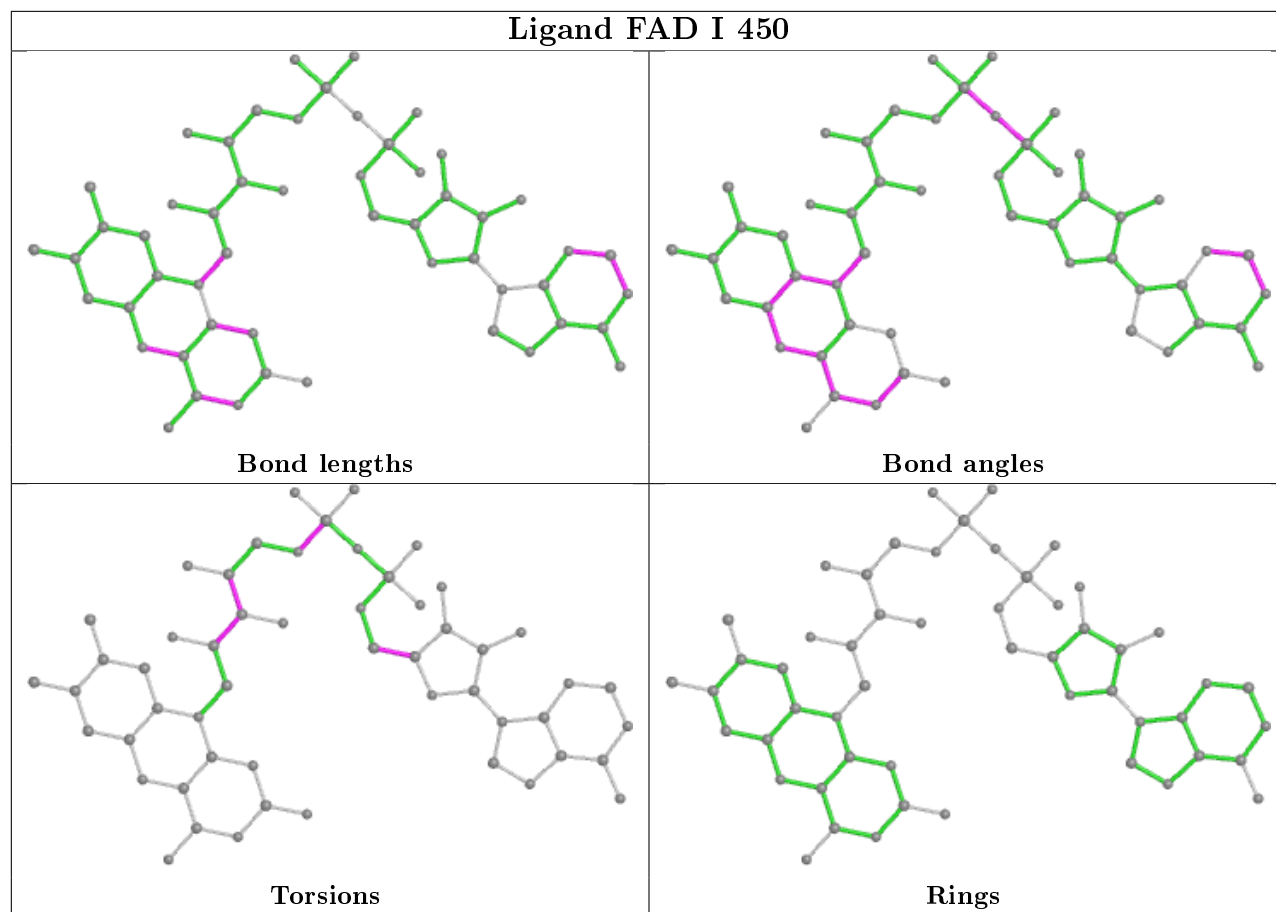
Torsions



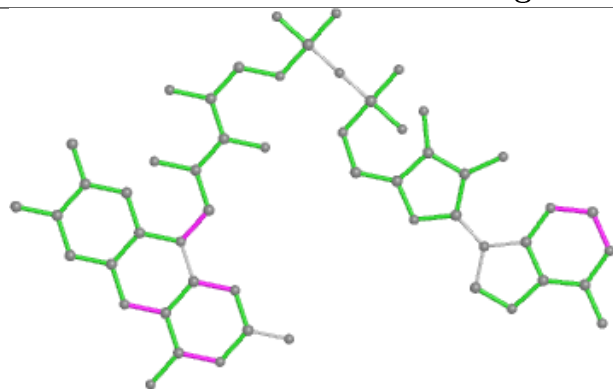
Rings



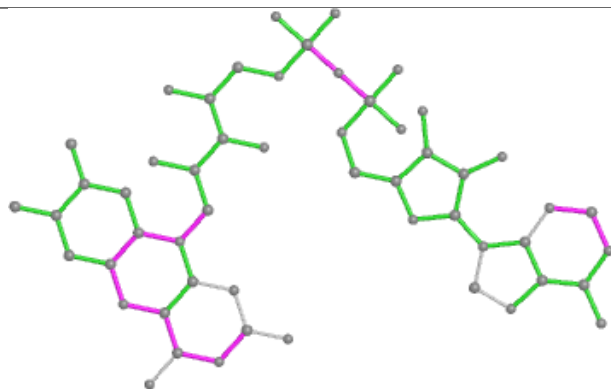




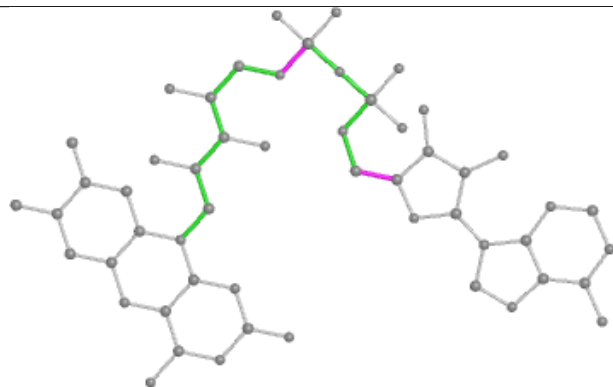
Ligand FAD D 450



Bond lengths



Bond angles

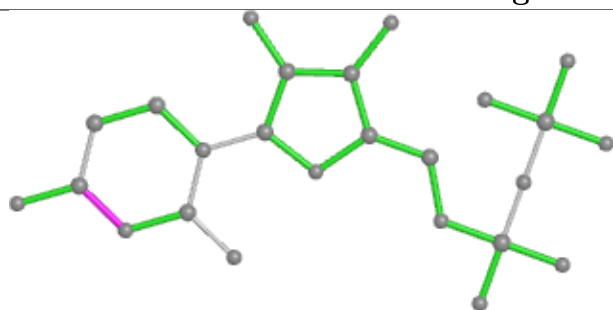


Torsions

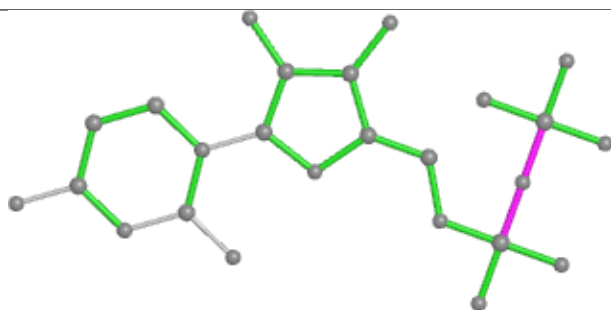


Rings

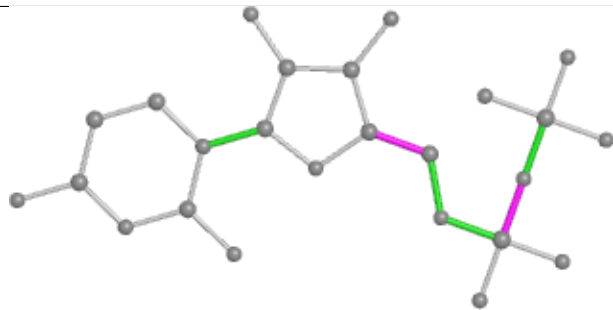
Ligand UDP B 400



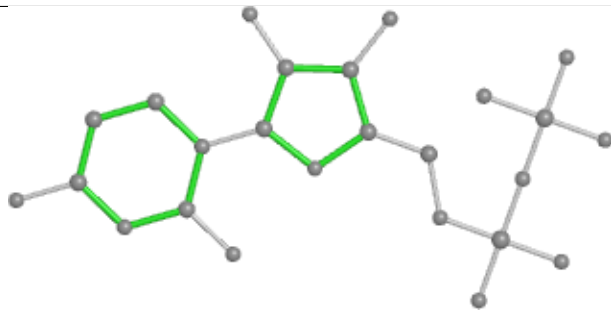
Bond lengths



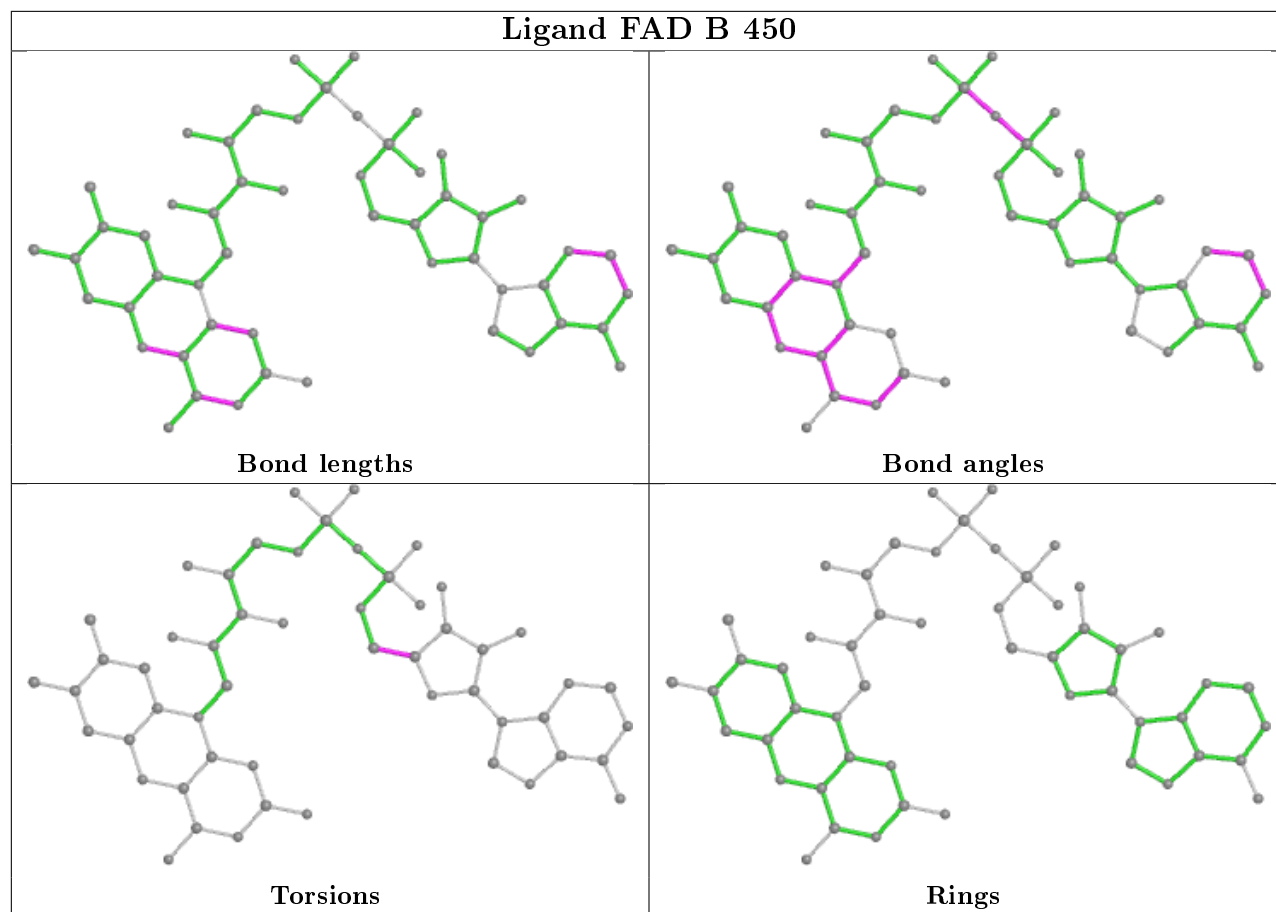
Bond angles



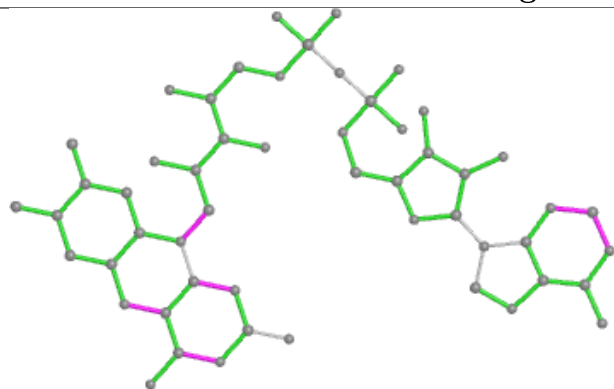
Torsions



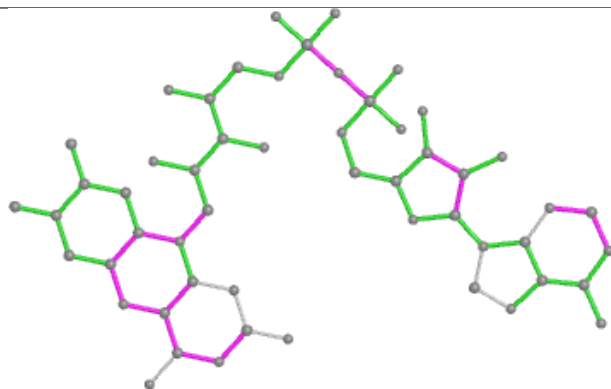
Rings



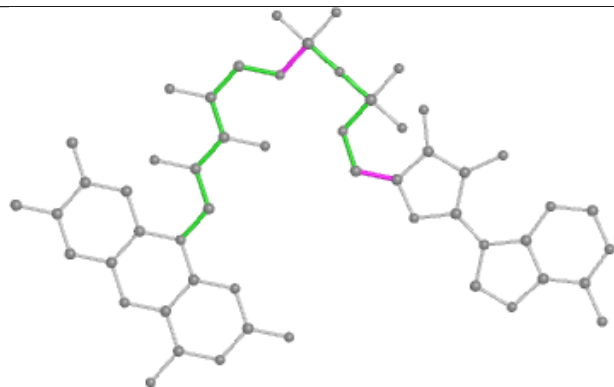
Ligand FAD J 450



Bond lengths



Bond angles

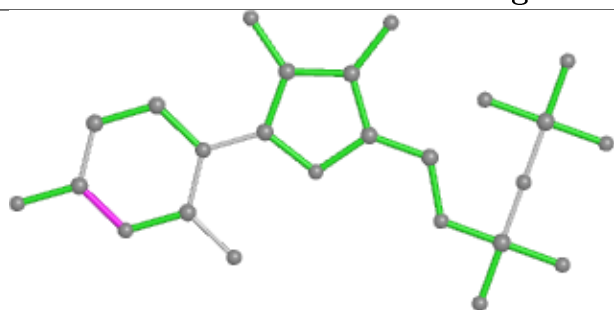


Torsions

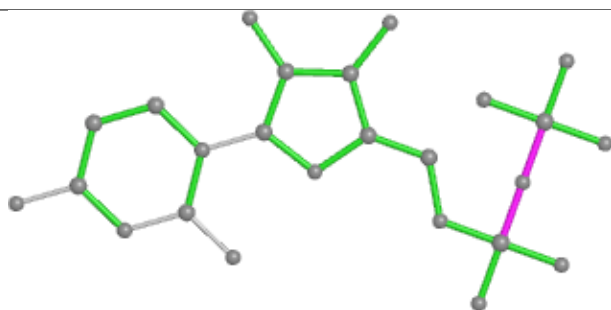


Rings

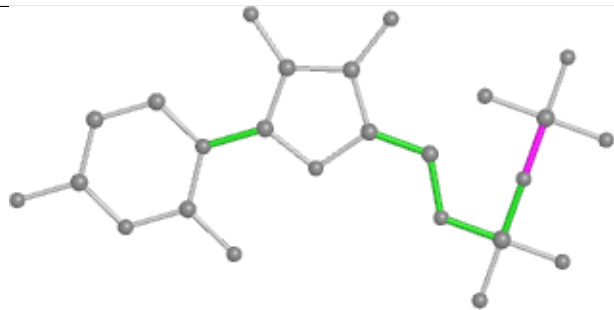
Ligand UDP H 400



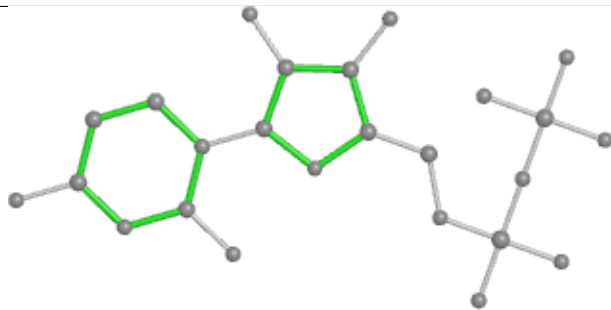
Bond lengths



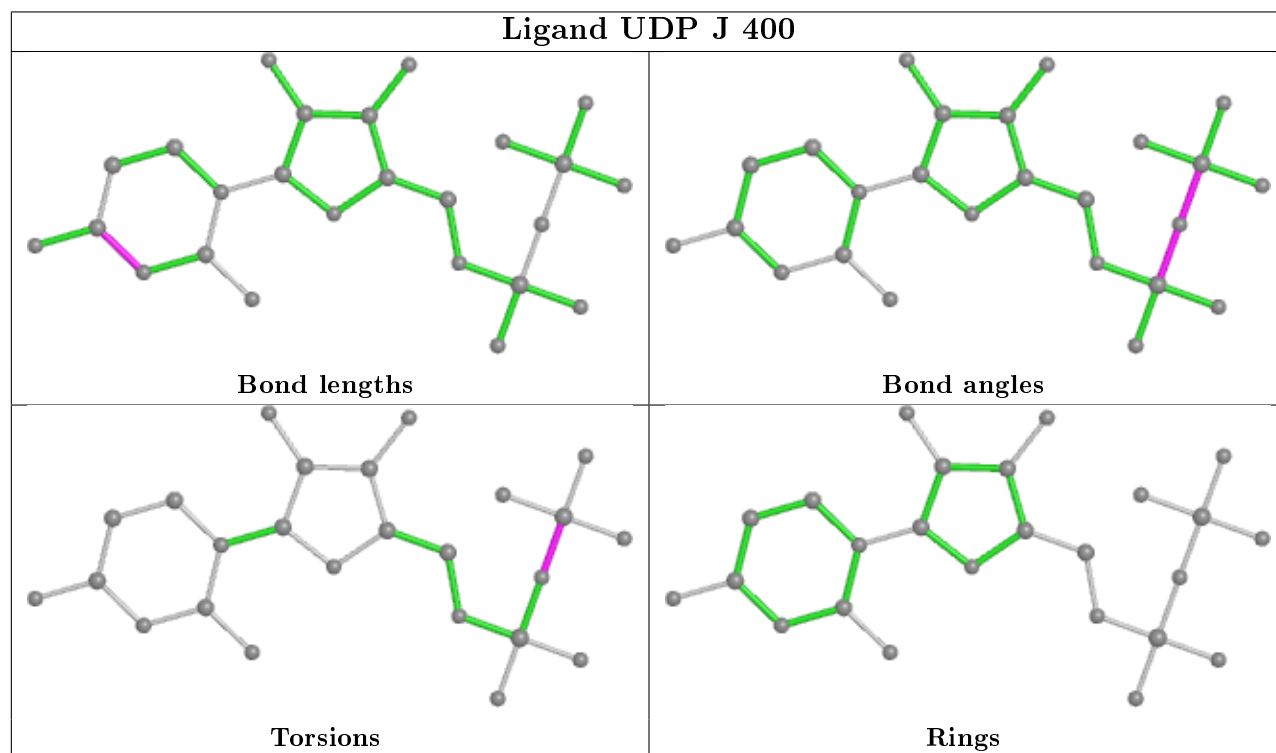
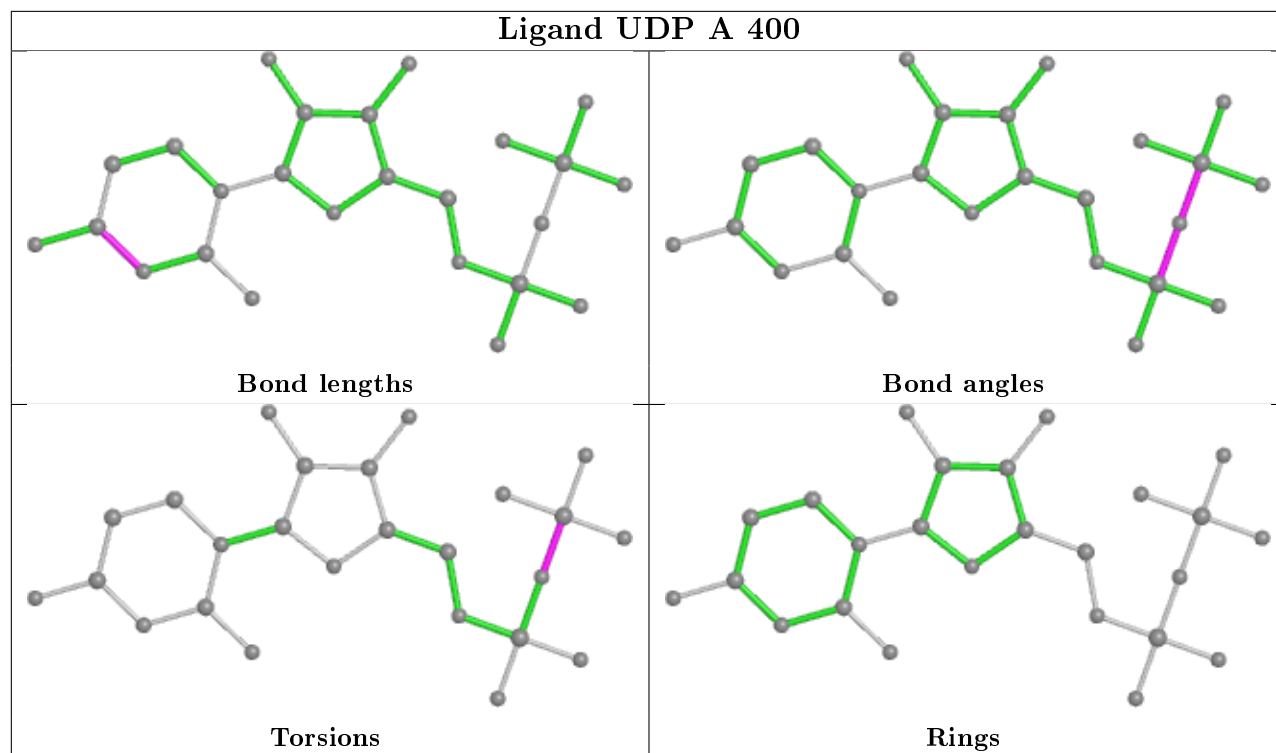
Bond angles

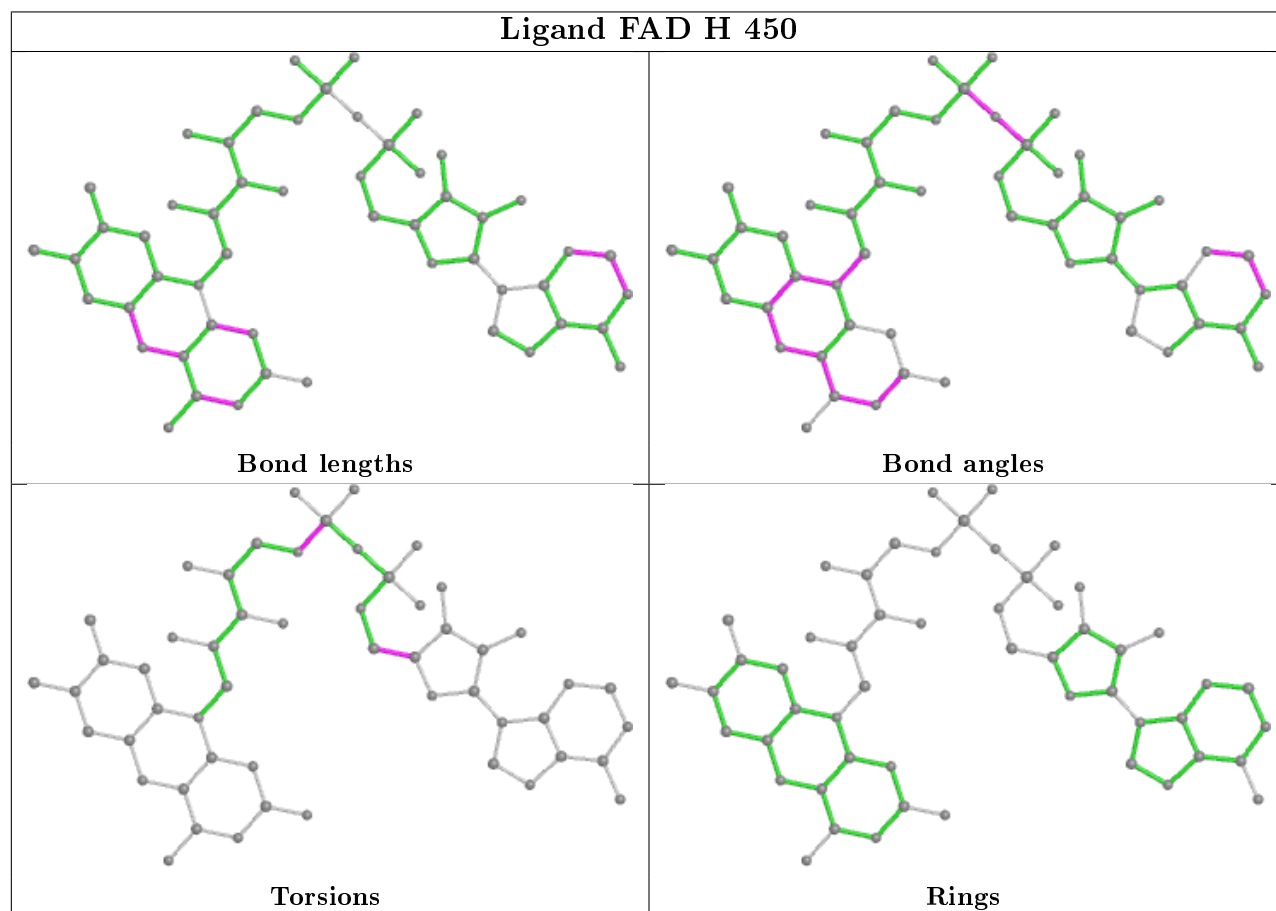
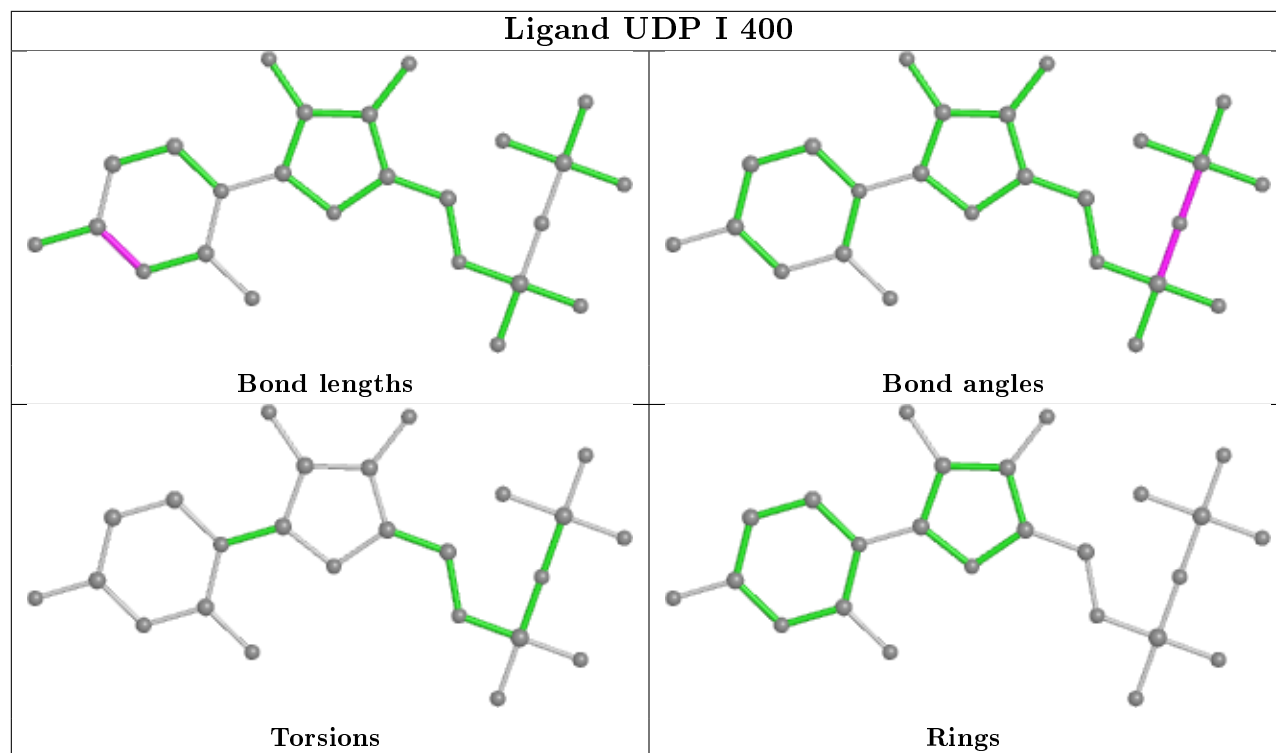


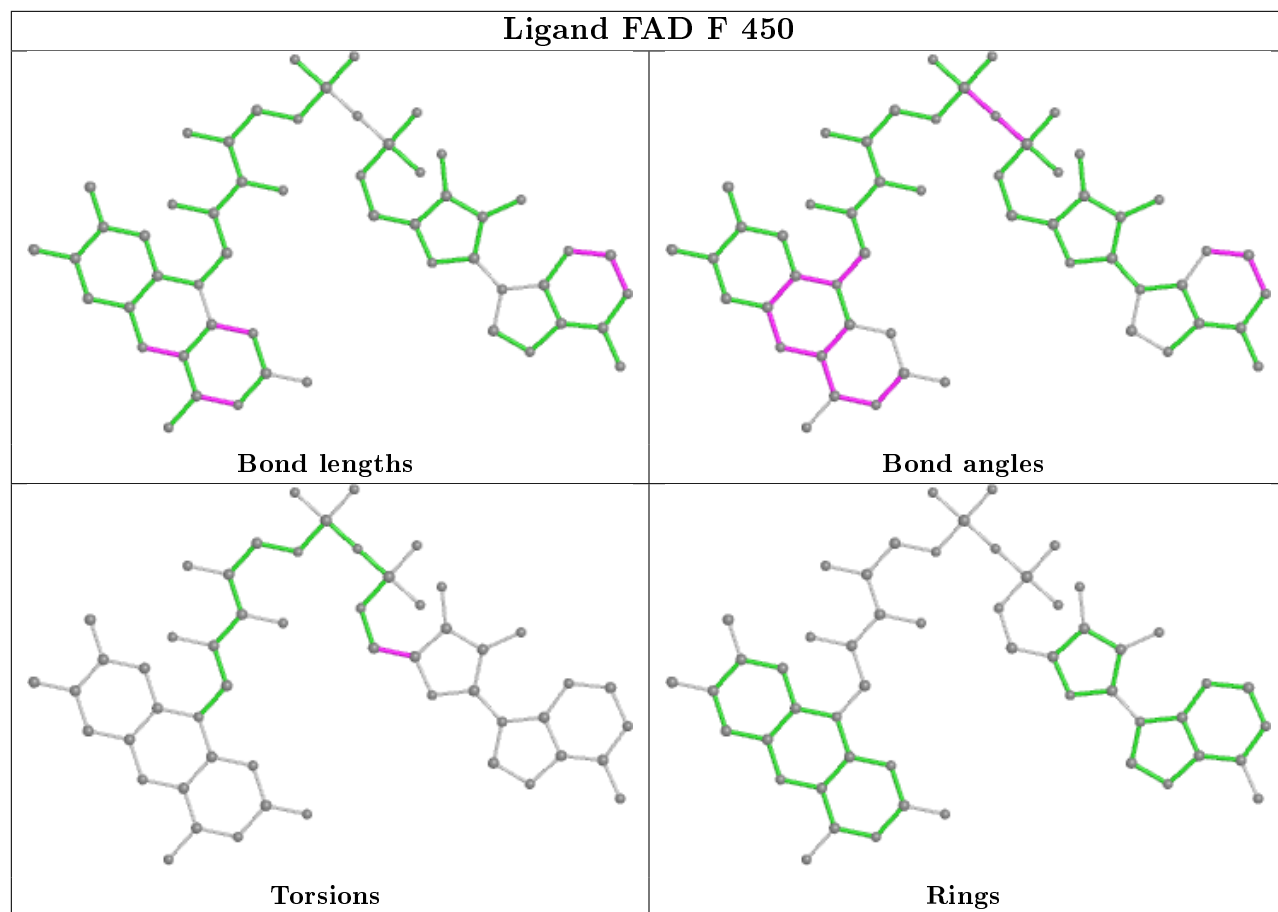
Torsions

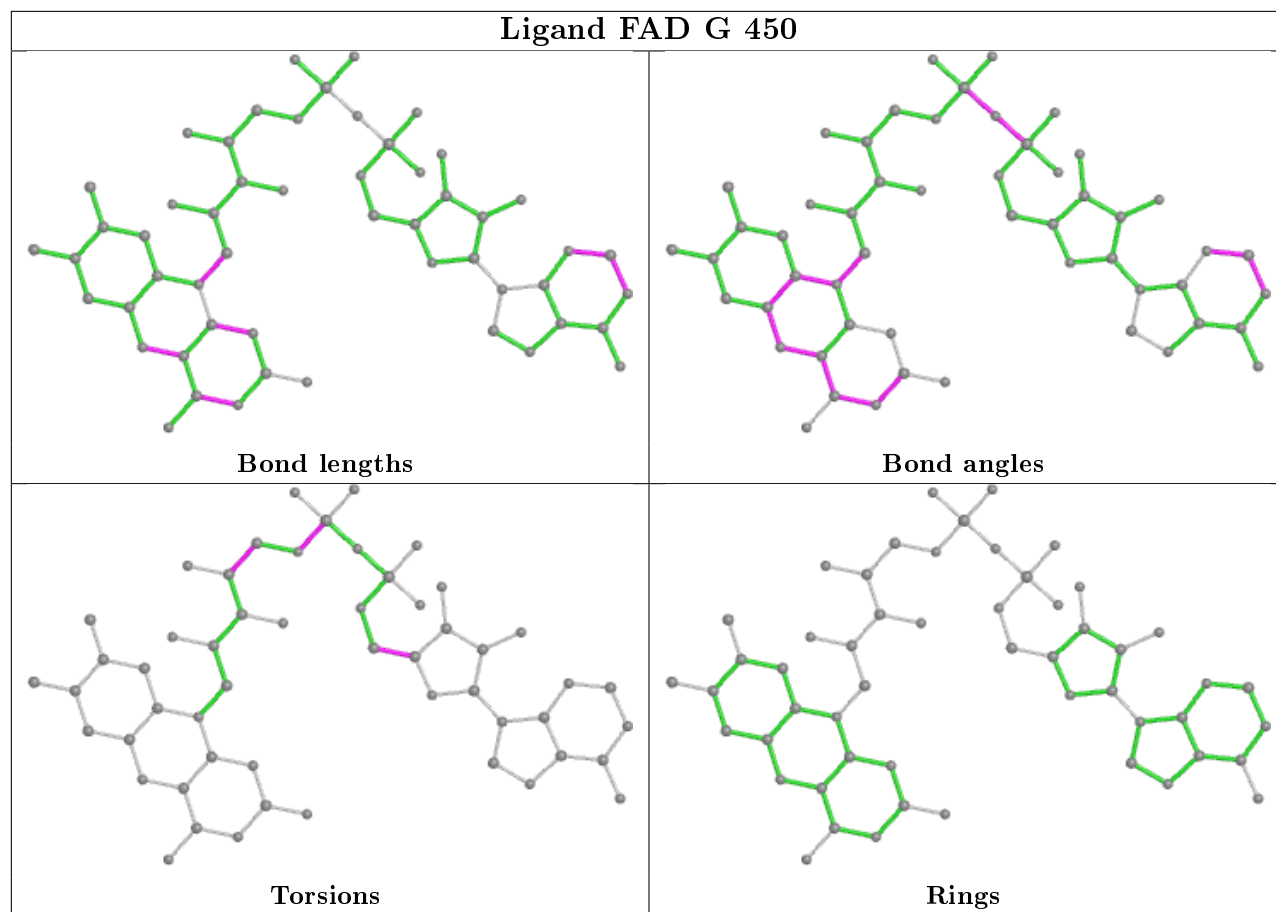


Rings









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, 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	366/397 (92%)	-0.44	5 (1%) 75 73	29, 38, 55, 90	1 (0%)
1	B	364/397 (91%)	-0.34	8 (2%) 62 60	30, 39, 59, 102	1 (0%)
1	C	362/397 (91%)	-0.34	3 (0%) 86 84	31, 44, 63, 78	1 (0%)
1	D	362/397 (91%)	-0.11	10 (2%) 53 51	33, 49, 72, 94	1 (0%)
1	E	364/397 (91%)	-0.22	9 (2%) 57 55	20, 49, 70, 107	0
1	F	363/397 (91%)	-0.40	6 (1%) 70 68	31, 41, 57, 82	1 (0%)
1	G	363/397 (91%)	-0.37	4 (1%) 80 79	32, 46, 67, 93	0
1	H	363/397 (91%)	-0.40	2 (0%) 89 88	20, 41, 61, 91	0
1	I	364/397 (91%)	-0.46	2 (0%) 91 89	30, 41, 60, 75	1 (0%)
1	J	361/397 (90%)	-0.29	6 (1%) 70 68	30, 43, 64, 80	1 (0%)
All	All	3632/3970 (91%)	-0.34	55 (1%) 73 72	20, 42, 66, 107	7 (0%)

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	154	GLU	5.2
1	B	357	GLN	4.2
1	E	154	GLU	4.1
1	F	154	GLU	4.1
1	B	155	GLN	4.1

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

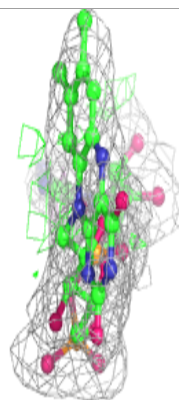
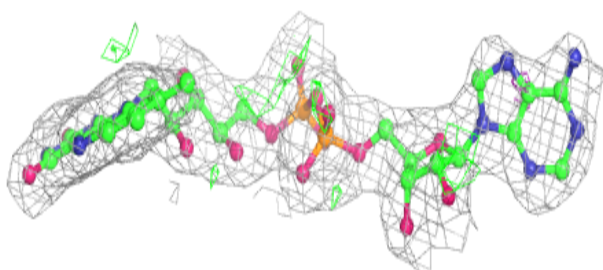
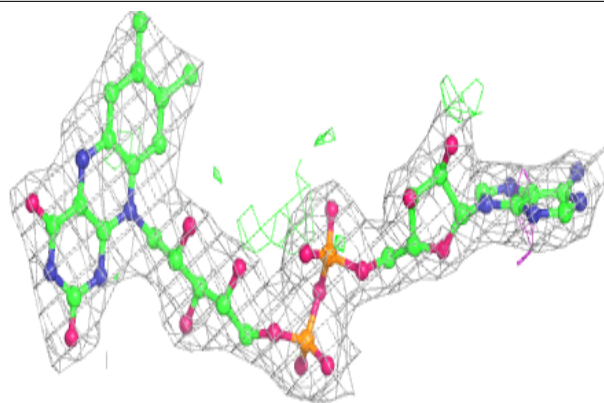
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FAD	G	450	53/53	0.96	0.13	38,50,57,61	0
3	FAD	C	450	53/53	0.97	0.16	36,46,57,61	0
3	FAD	A	450	53/53	0.97	0.15	31,37,42,45	0
2	UDP	F	400	25/25	0.97	0.11	38,41,46,50	0
2	UDP	E	400	25/25	0.97	0.16	37,44,53,61	0
3	FAD	D	450	53/53	0.97	0.17	38,49,62,66	0
3	FAD	E	450	53/53	0.97	0.15	41,51,59,65	0
3	FAD	J	450	53/53	0.97	0.14	37,43,54,58	0
3	FAD	I	450	53/53	0.97	0.12	34,42,47,52	0
2	UDP	B	400	25/25	0.98	0.12	33,39,49,51	0
2	UDP	D	400	25/25	0.98	0.15	41,46,55,57	0
3	FAD	B	450	53/53	0.98	0.14	32,39,44,52	0
2	UDP	A	400	25/25	0.98	0.15	34,38,46,52	0
2	UDP	C	400	25/25	0.98	0.12	35,41,51,59	0
2	UDP	H	400	25/25	0.98	0.12	35,42,50,55	0
2	UDP	J	400	25/25	0.98	0.15	32,38,48,52	0
2	UDP	I	400	25/25	0.98	0.13	35,40,51,55	0
3	FAD	H	450	53/53	0.98	0.14	33,39,45,49	0
3	FAD	F	450	53/53	0.98	0.14	31,40,46,47	0
2	UDP	G	400	25/25	0.98	0.12	38,40,53,59	0

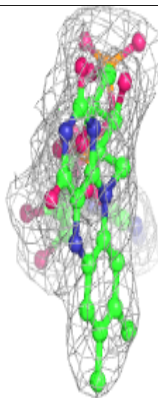
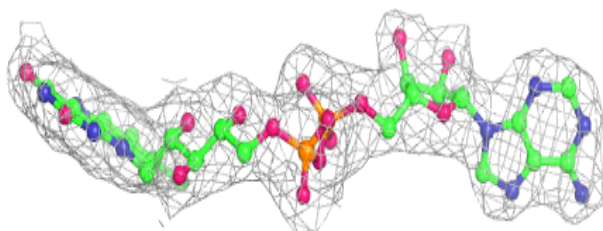
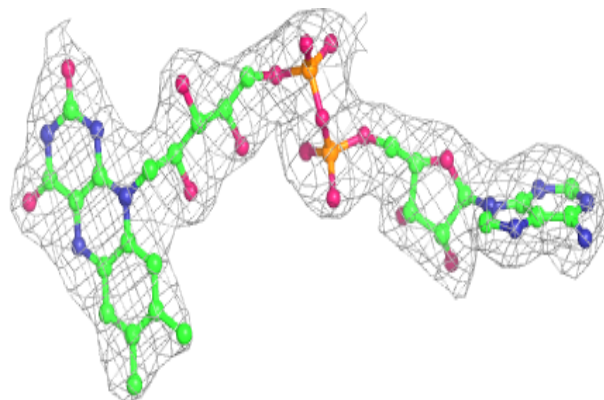
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD G 450:

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

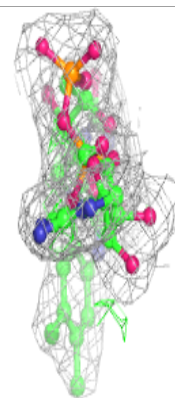
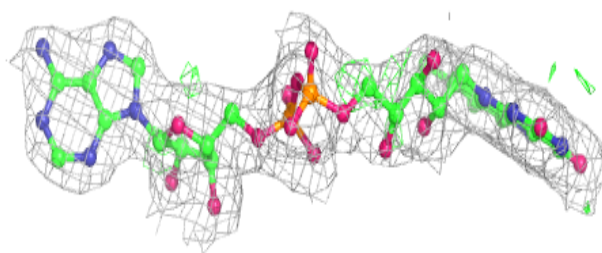
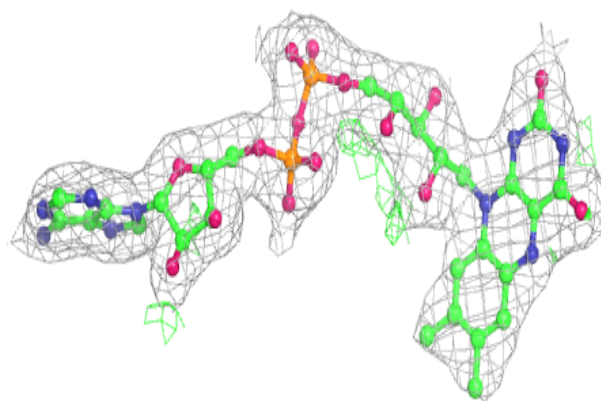
**Electron density around FAD C 450:**

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and green (positive)

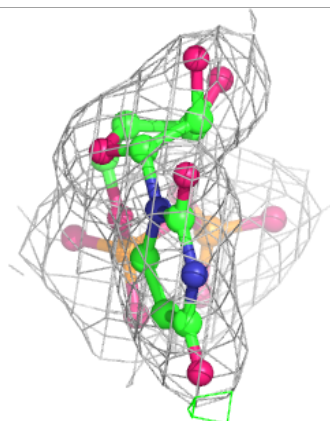
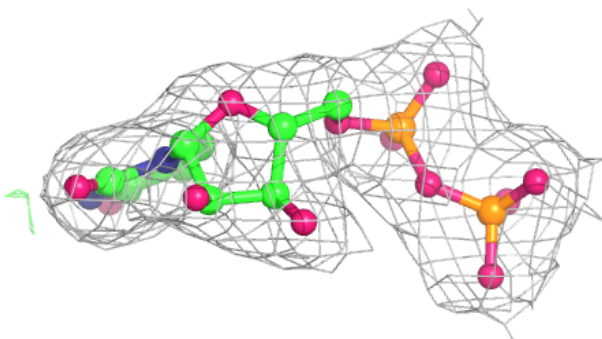
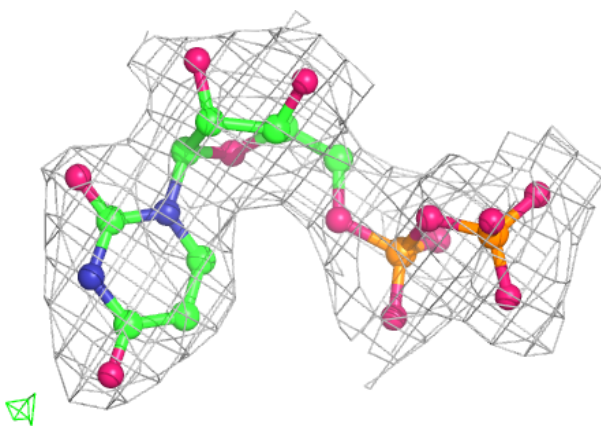


Electron density around FAD A 450:

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and green (positive)

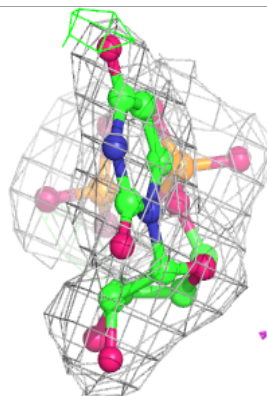
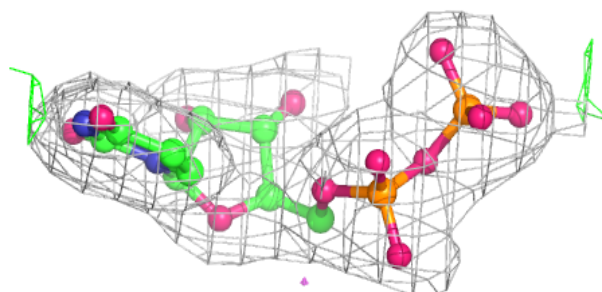
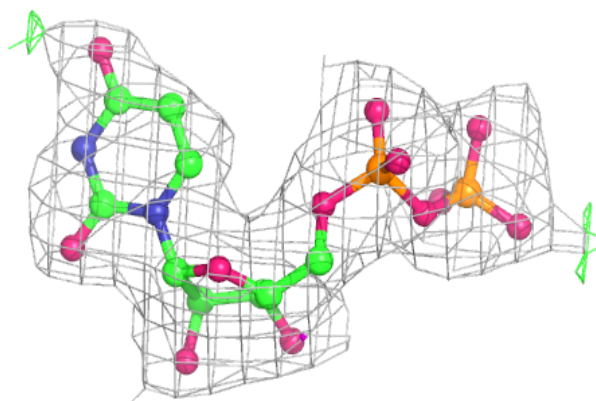
**Electron density around UDP F 400:**

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

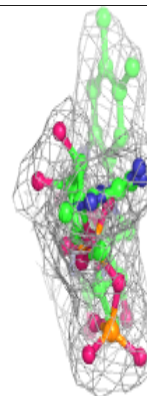
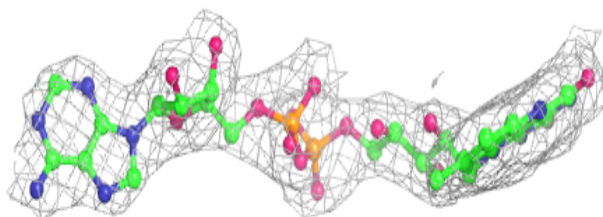
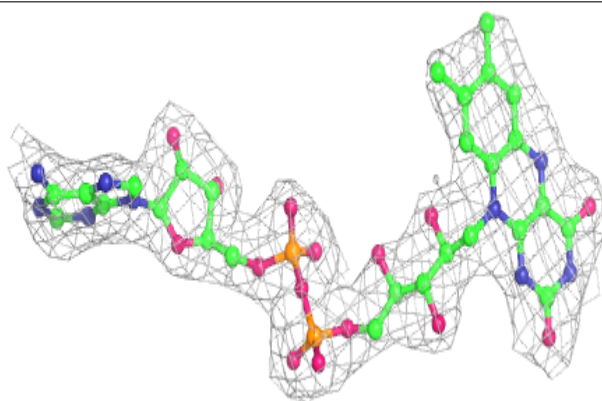


Electron density around UDP E 400:

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

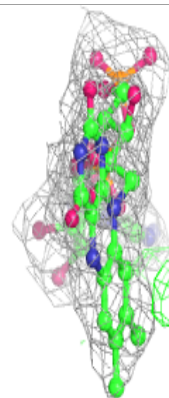
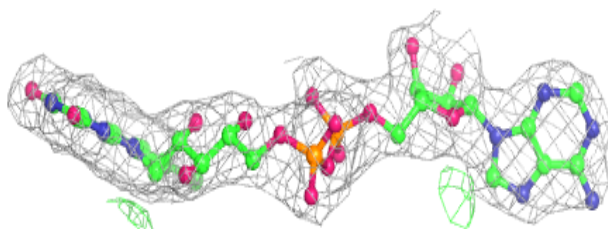
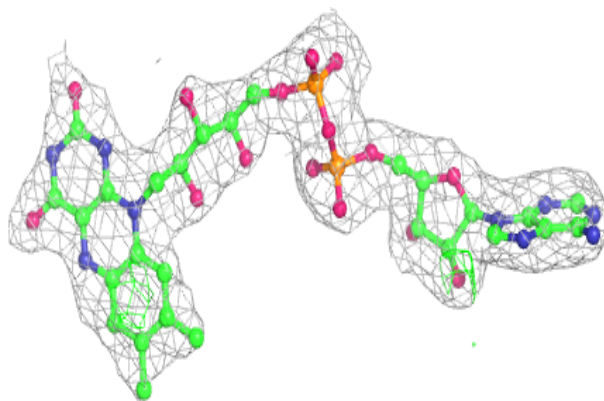
**Electron density around FAD D 450:**

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

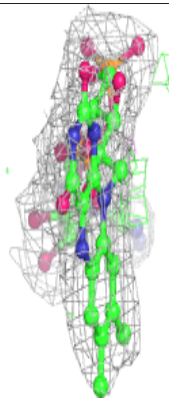
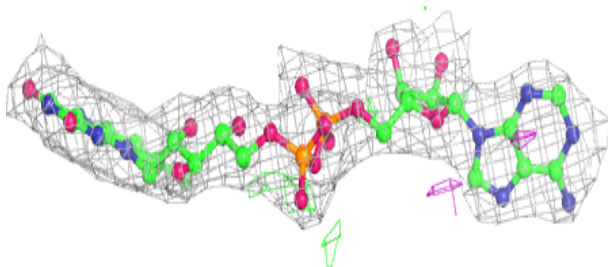
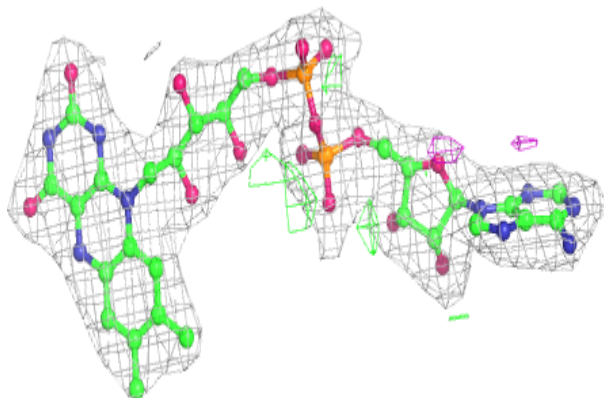


Electron density around FAD E 450:

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

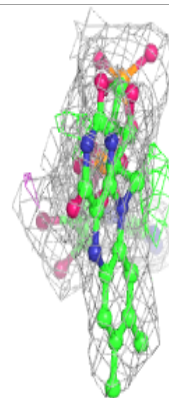
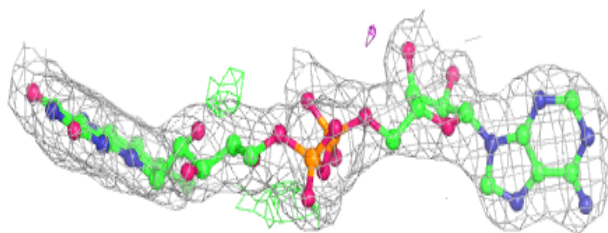
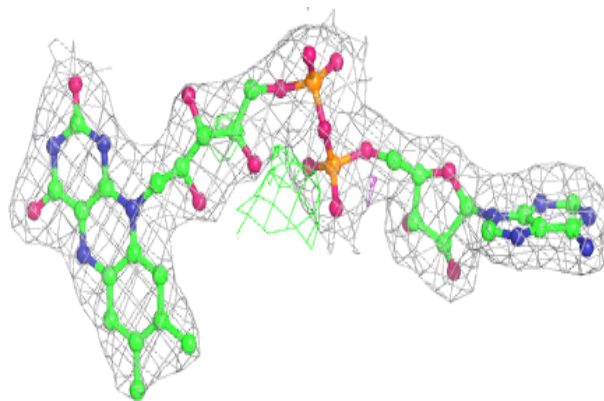
**Electron density around FAD J 450:**

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

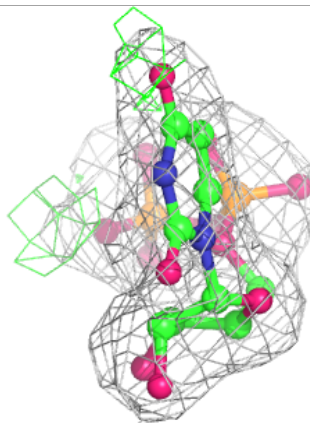
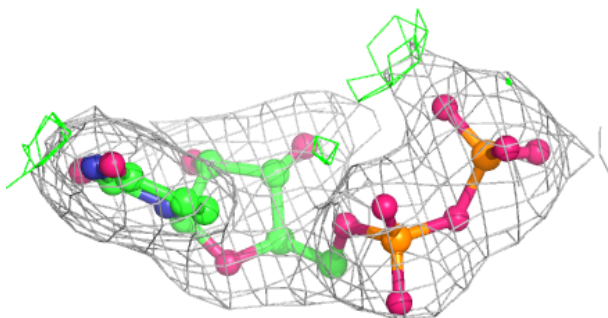
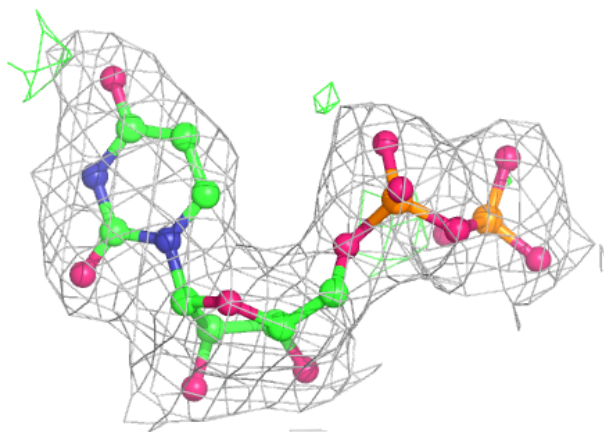


Electron density around FAD I 450:

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

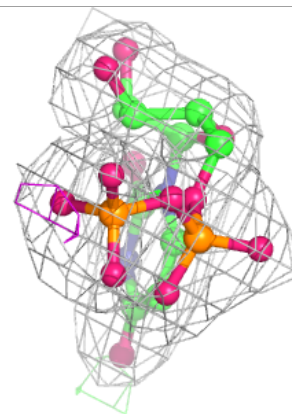
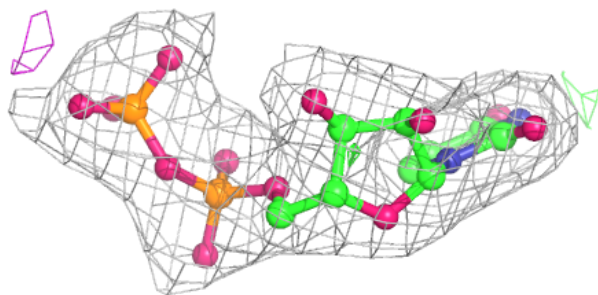
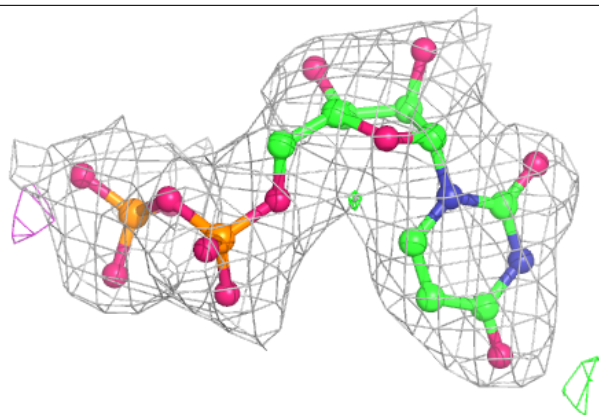
**Electron density around UDP B 400:**

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

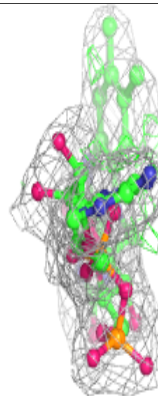
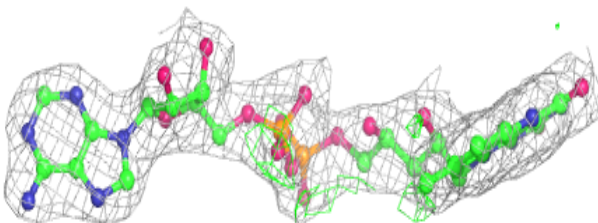
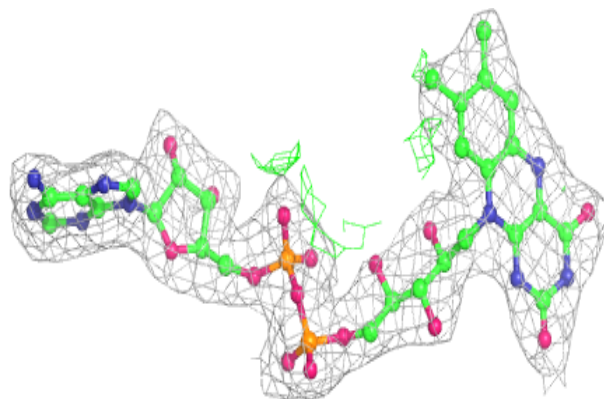


Electron density around UDP D 400:

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

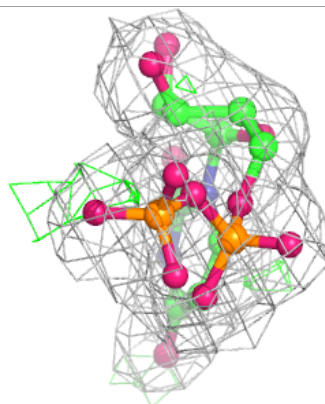
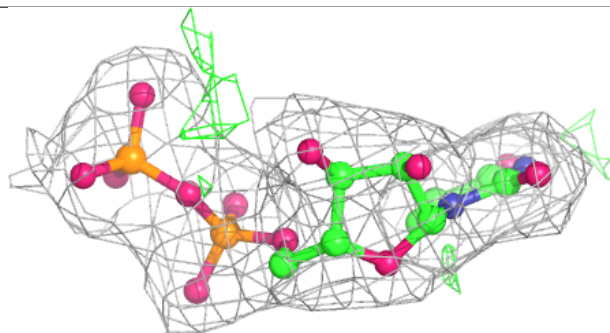
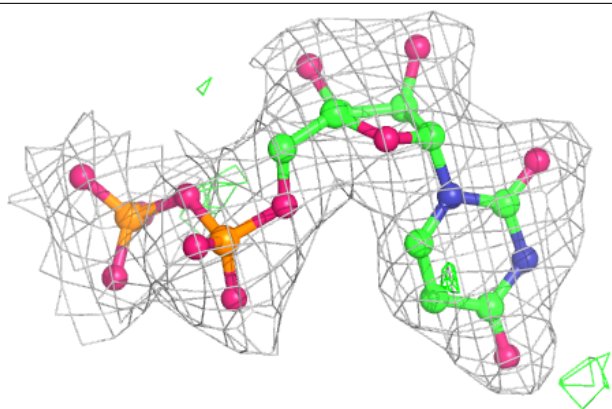
**Electron density around FAD B 450:**

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

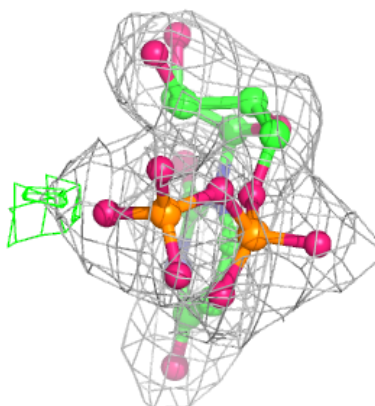
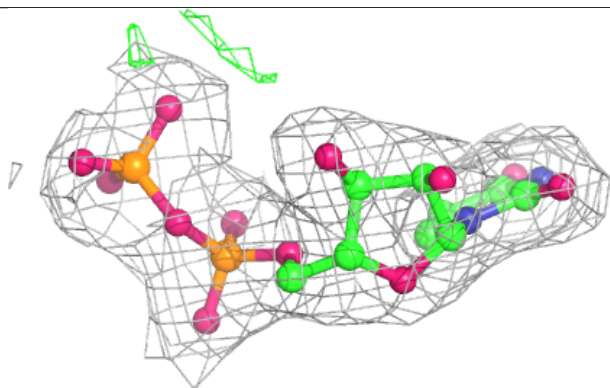
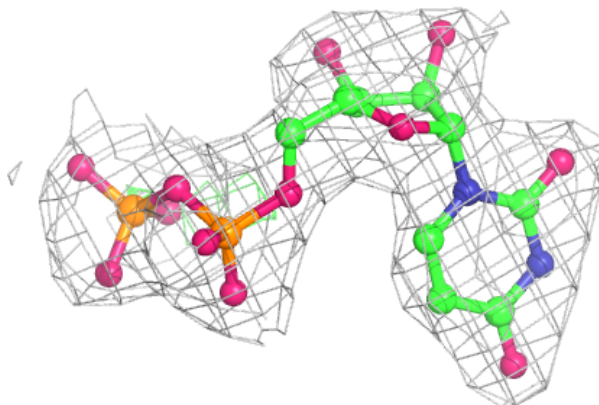


Electron density around UDP A 400:

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

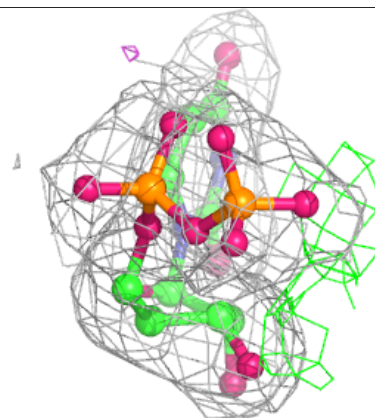
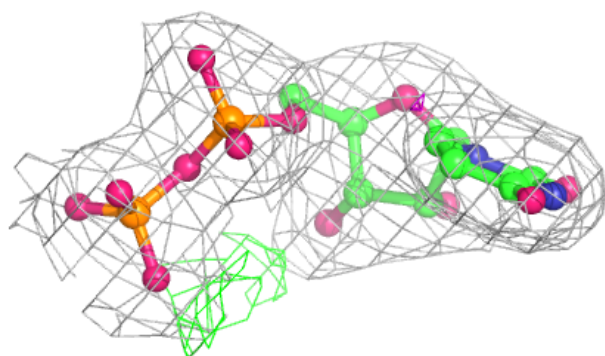
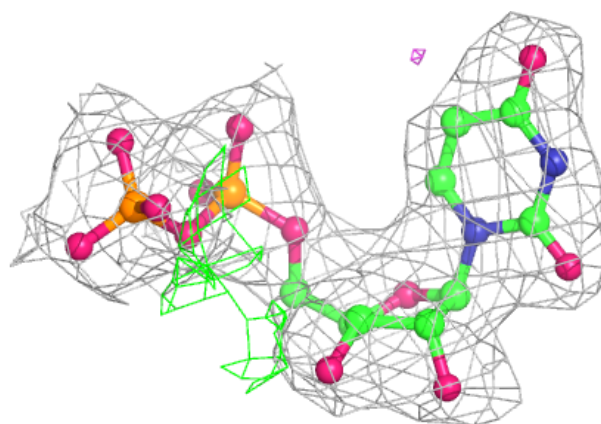
**Electron density around UDP C 400:**

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

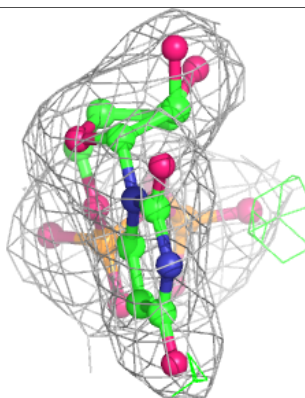
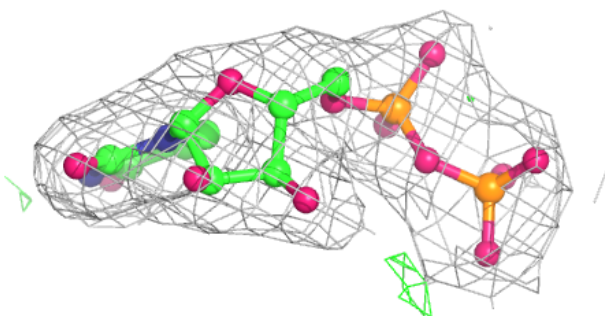
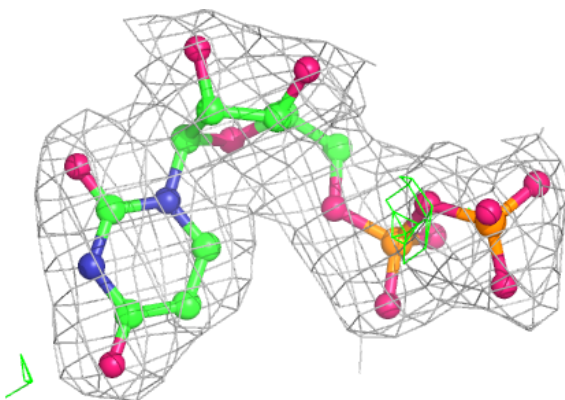


Electron density around UDP H 400:

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

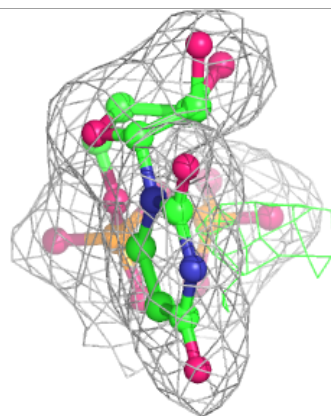
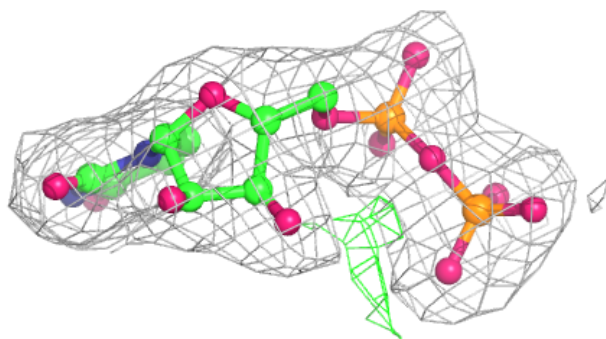
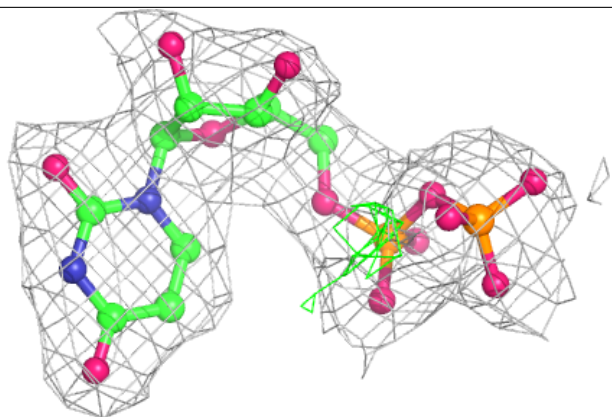
**Electron density around UDP J 400:**

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

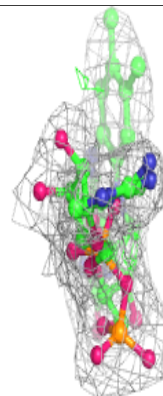
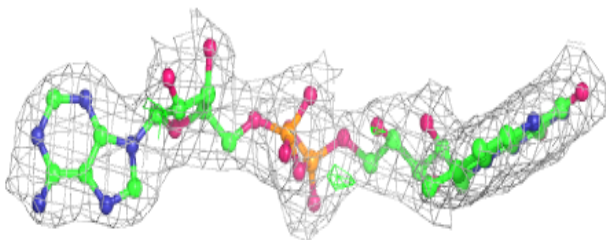
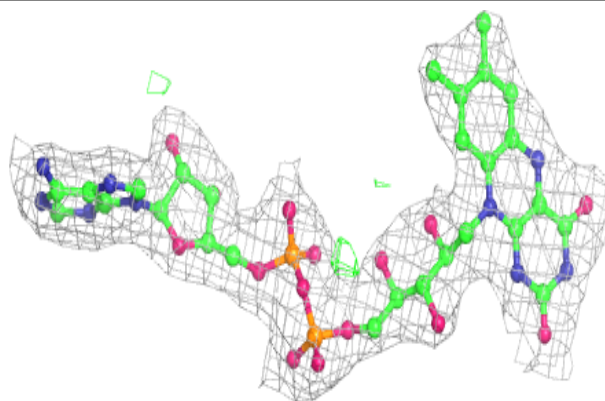


Electron density around UDP I 400:

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

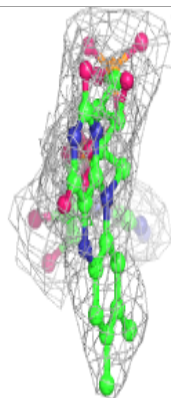
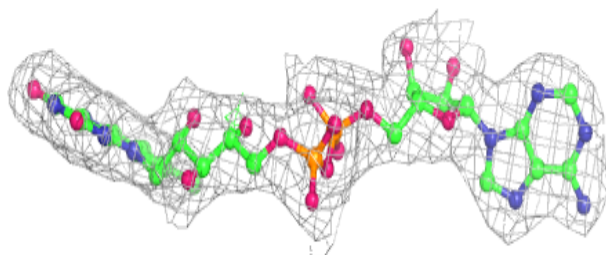
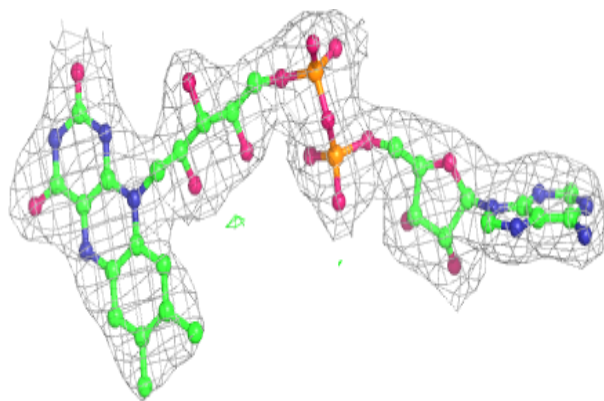
**Electron density around FAD H 450:**

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

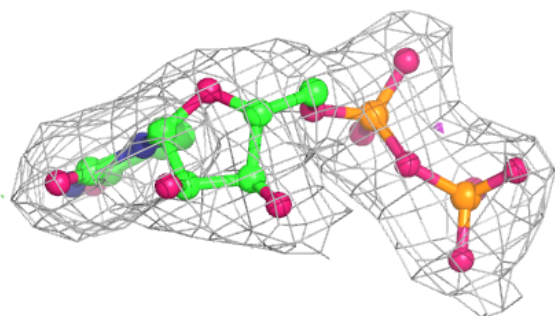
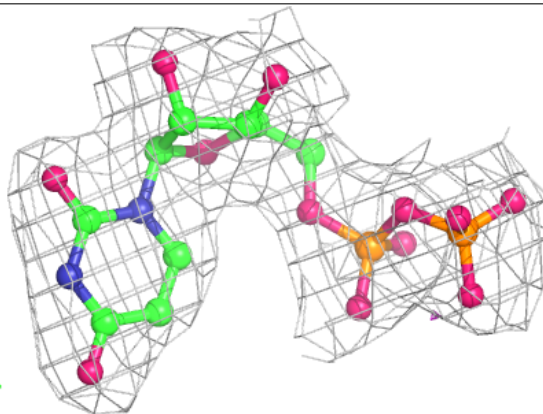


Electron density around FAD F 450:

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

**Electron density around UDP G 400:**

$2mF_o-DF_c$ (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.