



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2021 – 06:15 AM EDT

PDB ID : 3EYA  
Title : Structural basis for membrane binding and catalytic activation of the peripheral membrane enzyme pyruvate oxidase from Escherichia coli  
Authors : Neumann, P.; Weidner, A.; Pech, A.; Stubbs, M.T.; Tittmann, K.  
Deposited on : 2008-10-20  
Resolution : 2.50 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 : 2.23.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.1

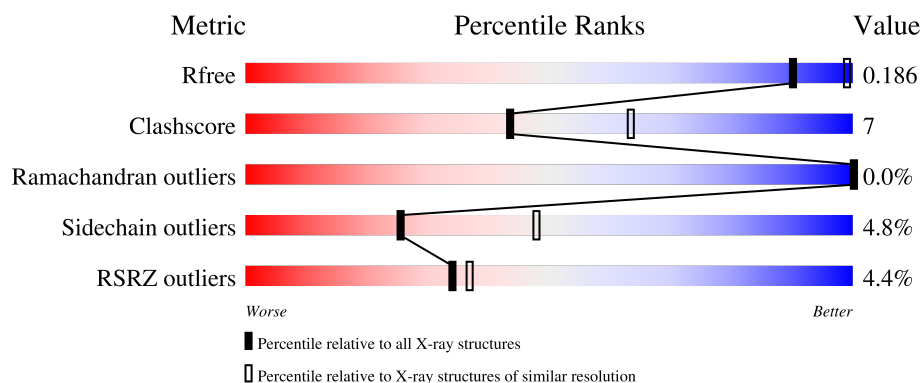
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	549	<div> <div>3%</div> <div>81% 12% . .</div> </div>
1	B	549	<div> <div>4%</div> <div>82% 11% . 5%</div> </div>
1	C	549	<div> <div>4%</div> <div>82% 11% . 5%</div> </div>
1	D	549	<div> <div>3%</div> <div>81% 12% . 5%</div> </div>
1	E	549	<div> <div>5%</div> <div>82% 10% . 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	549	
1	G	549	
1	H	549	
1	I	549	
1	J	549	
1	K	549	
1	L	549	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	616	-	-	X	-
5	PO4	A	618	-	-	X	-
5	PO4	A	619	-	-	X	-
5	PO4	D	616	-	-	-	X

## 2 Entry composition

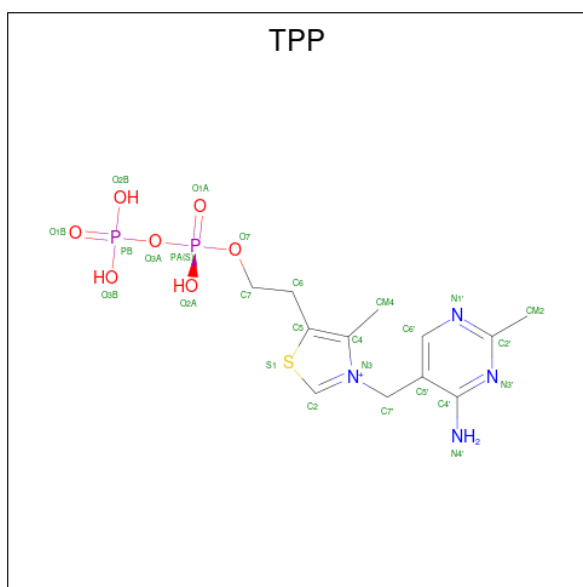
There are 6 unique types of molecules in this entry. The entry contains 50360 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyruvate dehydrogenase [cytochrome].

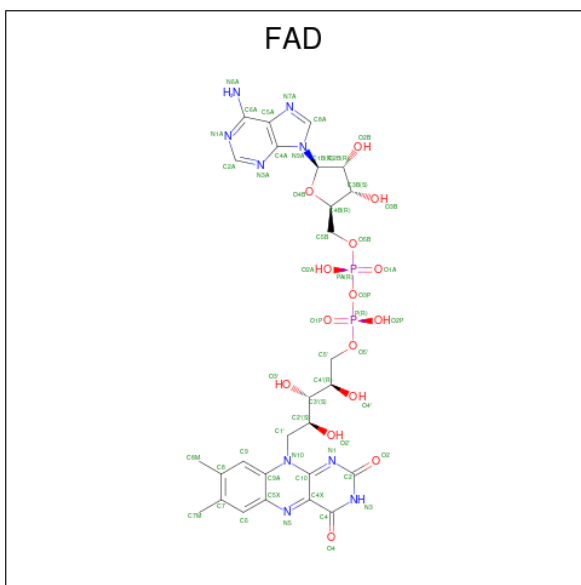
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	12	0
			4066	2579	708	752	27			
1	B	524	Total	C	N	O	S	0	5	0
			3999	2529	694	749	27			
1	C	522	Total	C	N	O	S	0	6	0
			4001	2530	697	748	26			
1	D	520	Total	C	N	O	S	0	6	0
			3977	2516	693	741	27			
1	E	522	Total	C	N	O	S	0	3	0
			3975	2513	693	743	26			
1	F	521	Total	C	N	O	S	0	3	0
			3969	2510	693	739	27			
1	G	519	Total	C	N	O	S	0	2	0
			3939	2490	684	738	27			
1	H	522	Total	C	N	O	S	0	4	0
			3973	2515	688	743	27			
1	I	523	Total	C	N	O	S	0	2	0
			3978	2516	694	741	27			
1	J	522	Total	C	N	O	S	0	6	0
			3993	2527	696	743	27			
1	K	523	Total	C	N	O	S	0	5	0
			4005	2533	702	743	27			
1	L	523	Total	C	N	O	S	0	8	0
			4016	2541	704	744	27			

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	E	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	F	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	G	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	H	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	I	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	J	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	K	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	L	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

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

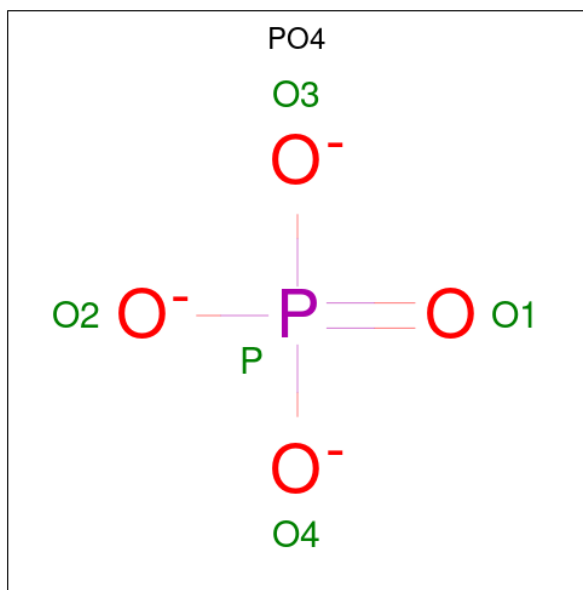


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	D	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	E	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	F	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	G	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	H	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	I	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	J	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	K	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	L	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	I	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0
4	K	1	Total Mg 1 1	0	0
4	L	1	Total Mg 1 1	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	I	1	Total	O	P	0	0
			5	4	1		
5	I	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		
5	K	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	280	Total	O	0	0
			280	280		
6	B	60	Total	O	0	0
			60	60		
6	C	73	Total	O	0	0
			73	73		
6	D	88	Total	O	0	0
			88	88		
6	E	43	Total	O	0	0
			43	43		

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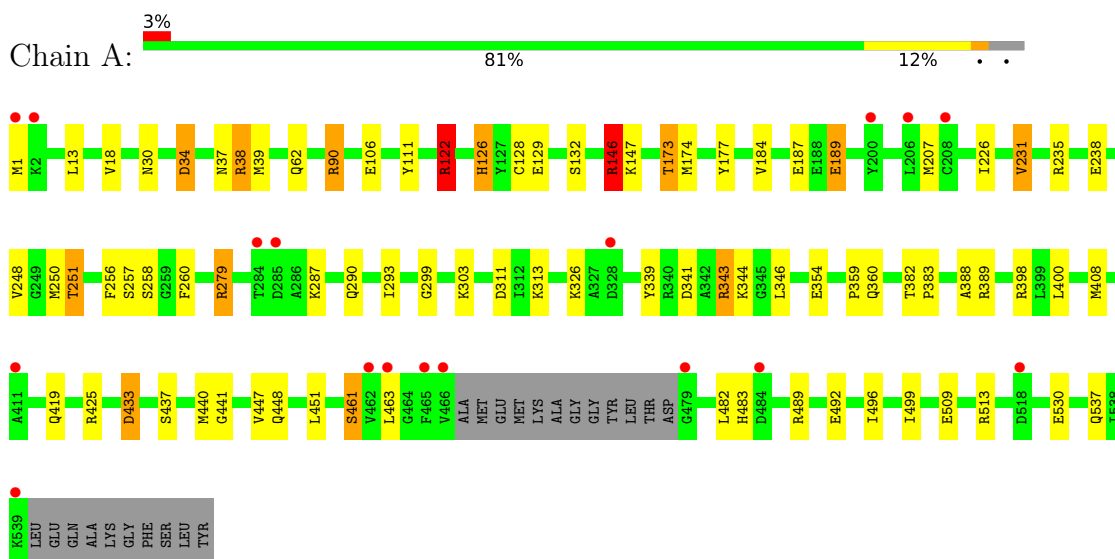
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	41	Total 41	O 41	0	0
6	G	40	Total 40	O 40	0	0
6	H	64	Total 64	O 64	0	0
6	I	62	Total 62	O 62	0	0
6	J	50	Total 50	O 50	0	0
6	K	77	Total 77	O 77	0	0
6	L	451	Total 451	O 451	0	0

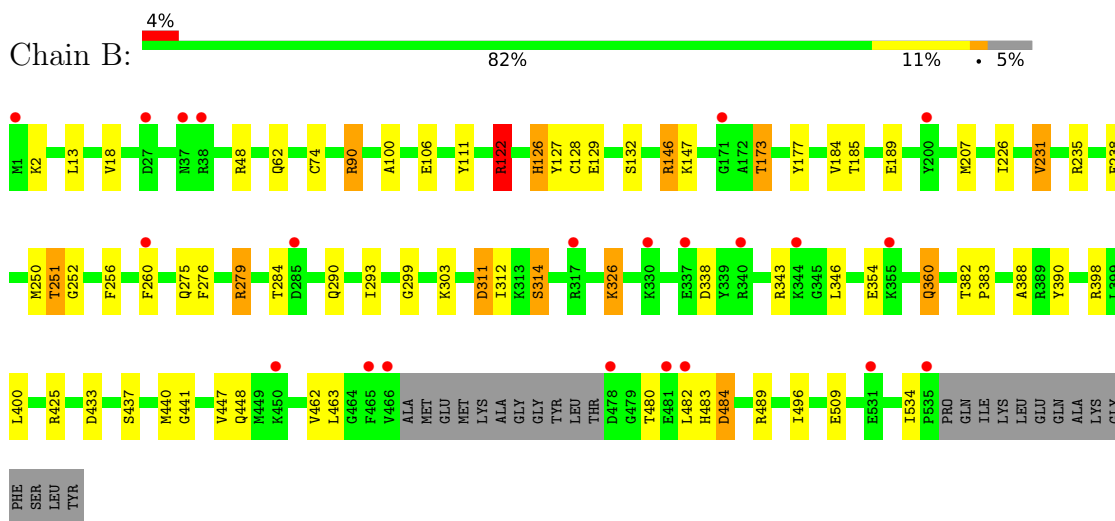
### 3 Residue-property plots [i](#)

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.

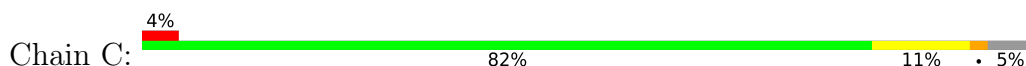
- Molecule 1: Pyruvate dehydrogenase [cytochrome]

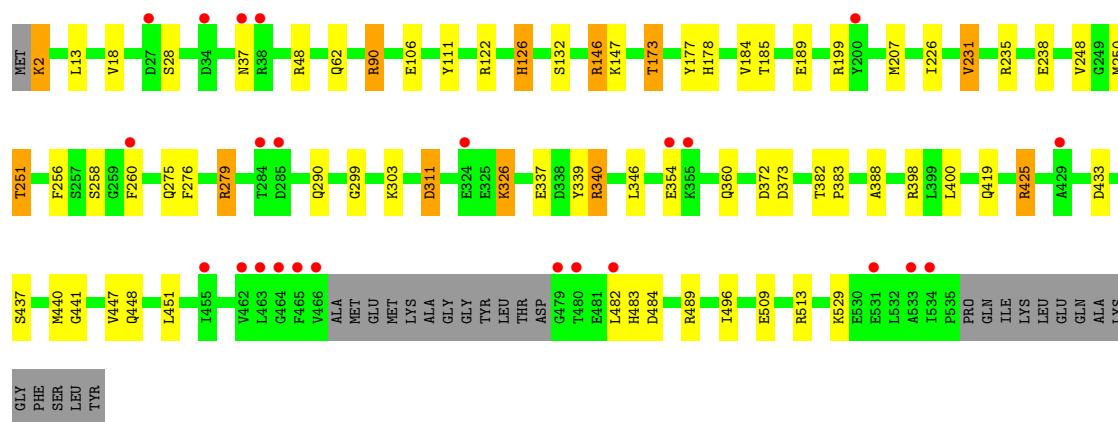


- Molecule 1: Pyruvate dehydrogenase [cytochrome]

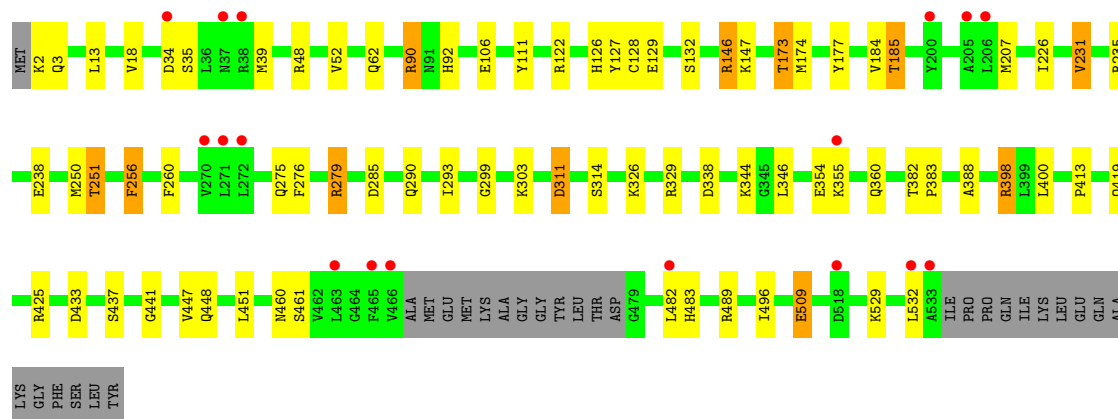
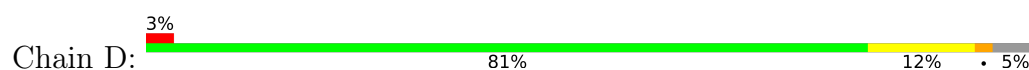


- Molecule 1: Pyruvate dehydrogenase [cytochrome]

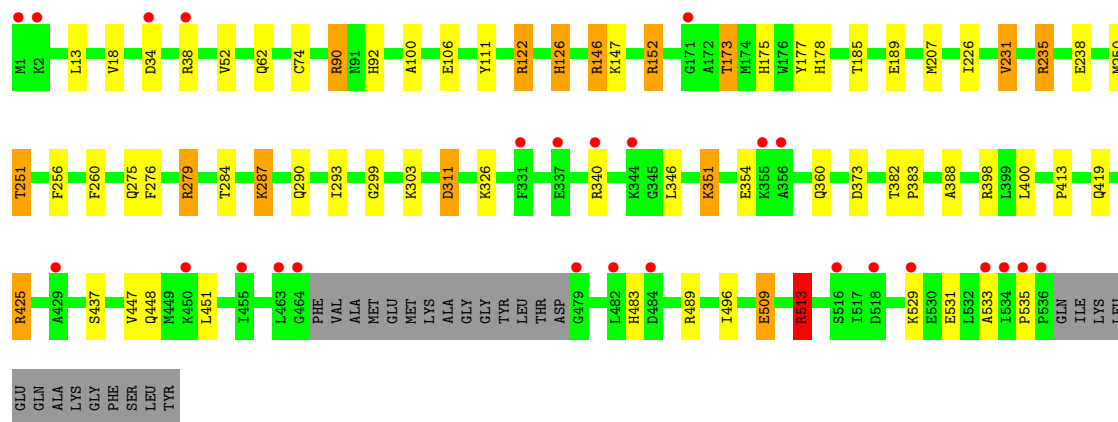
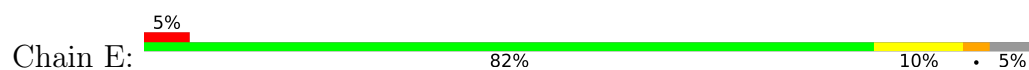




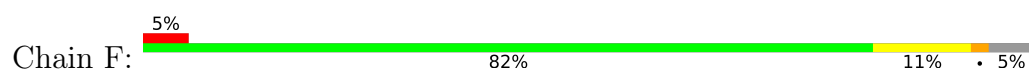
• Molecule 1: Pyruvate dehydrogenase [cytochrome]

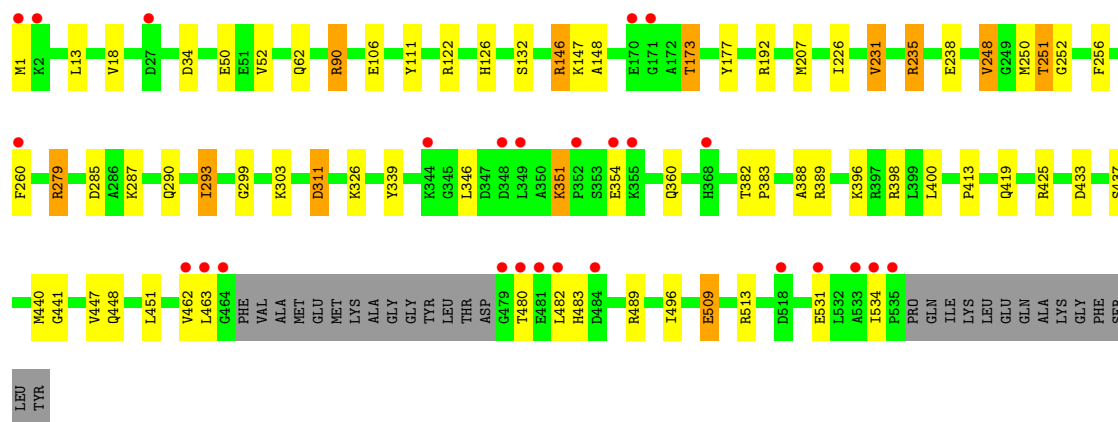


• Molecule 1: Pyruvate dehydrogenase [cytochrome]

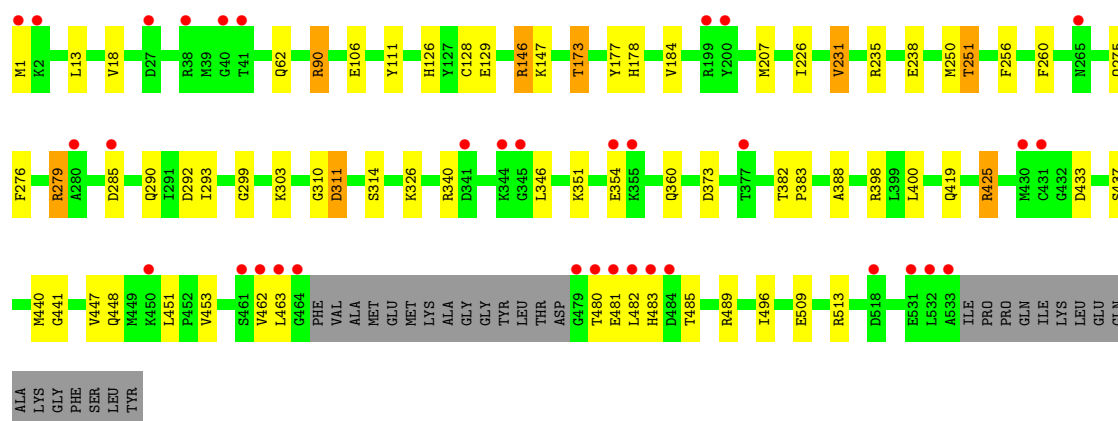
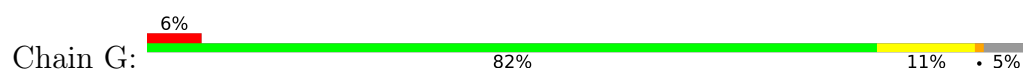


• Molecule 1: Pyruvate dehydrogenase [cytochrome]

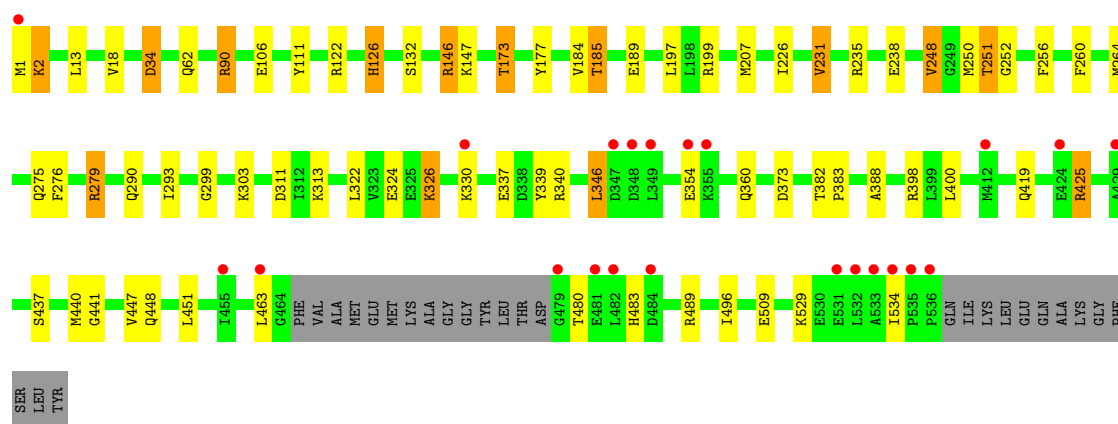
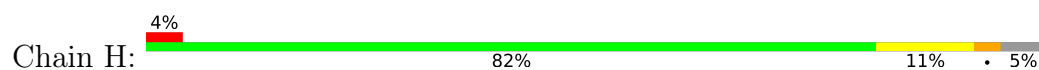




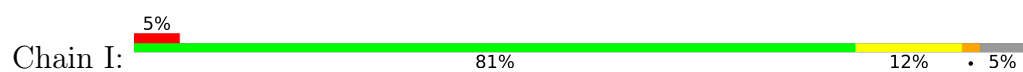
• Molecule 1: Pyruvate dehydrogenase [cytochrome]

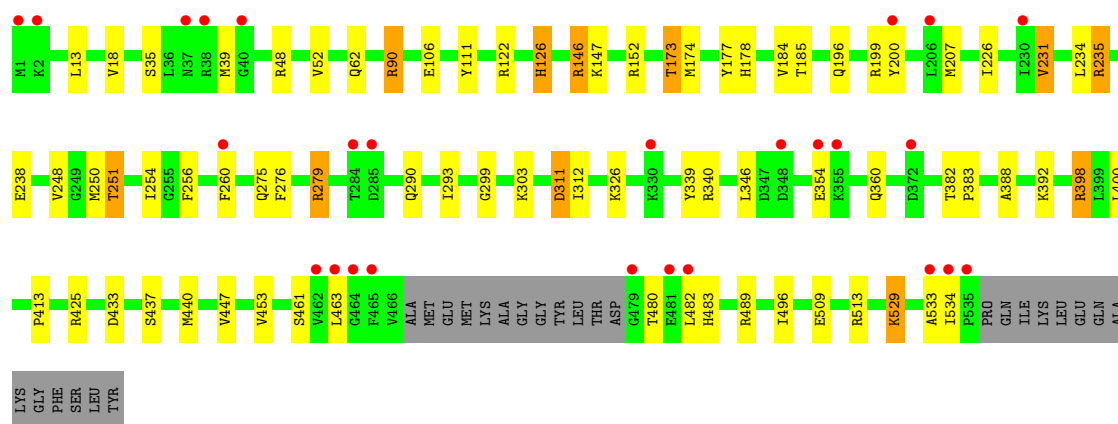


• Molecule 1: Pyruvate dehydrogenase [cytochrome]

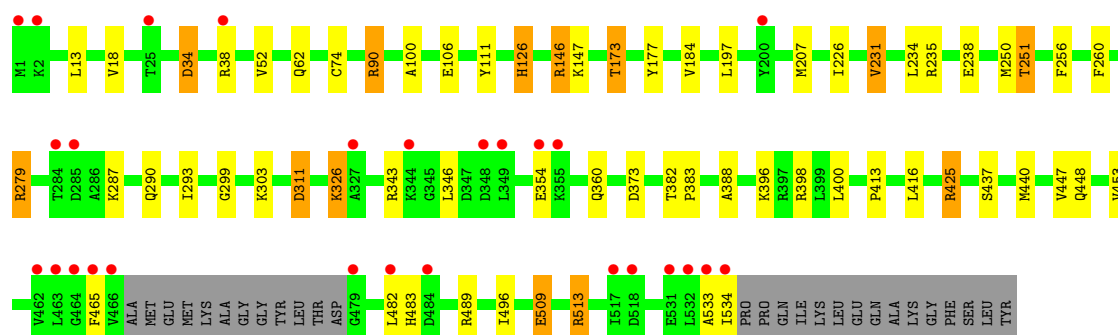
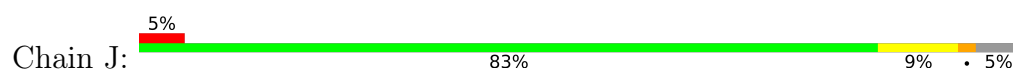


• Molecule 1: Pyruvate dehydrogenase [cytochrome]

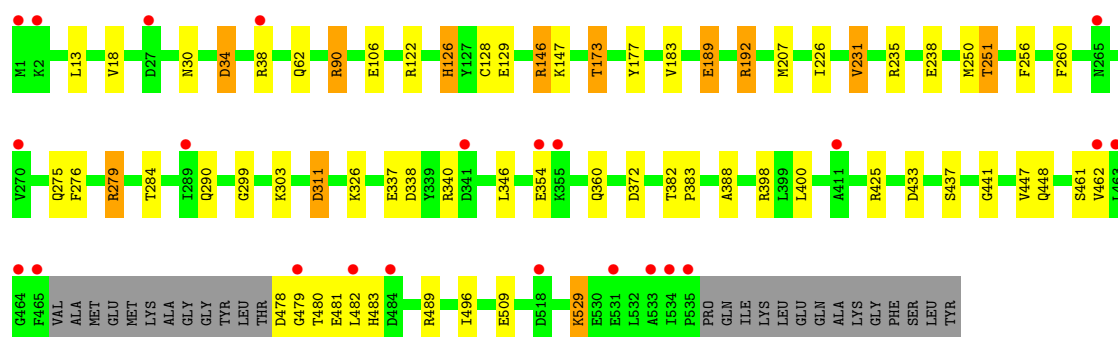
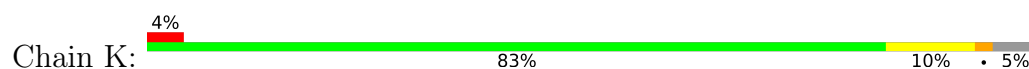




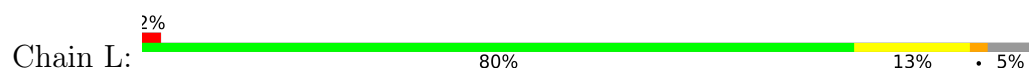
• Molecule 1: Pyruvate dehydrogenase [cytochrome]

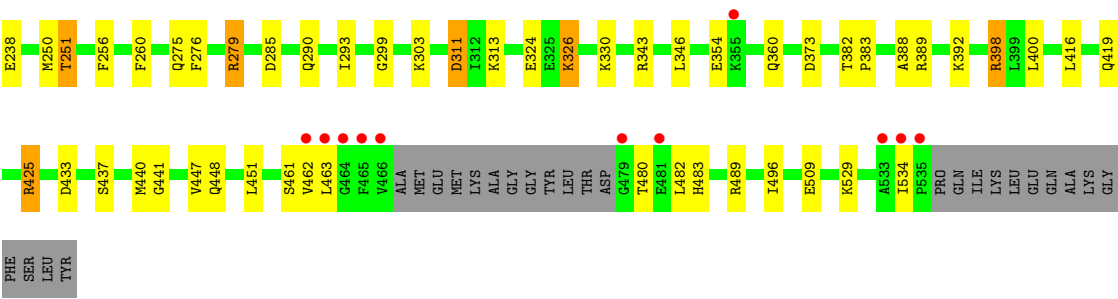


• Molecule 1: Pyruvate dehydrogenase [cytochrome]



• Molecule 1: Pyruvate dehydrogenase [cytochrome]





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.24Å 207.05Å 214.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.50) 99.6 (29.99-2.50)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.183 , 0.198 0.186 , 0.186	Depositor DCC
$R_{free}$ test set	15607 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	50360	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, MG, PO4, TPP

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	0.68	1/4186 (0.0%)	0.76	12/5670 (0.2%)
1	B	0.61	0/4096	0.73	10/5550 (0.2%)
1	C	0.66	3/4088 (0.1%)	0.77	12/5540 (0.2%)
1	D	0.65	0/4076	0.74	8/5522 (0.1%)
1	E	0.63	4/4063 (0.1%)	0.70	8/5508 (0.1%)
1	F	0.57	1/4060 (0.0%)	0.69	9/5502 (0.2%)
1	G	0.55	1/4024 (0.0%)	0.67	6/5453 (0.1%)
1	H	0.62	1/4066 (0.0%)	0.72	9/5513 (0.2%)
1	I	0.66	8/4065 (0.2%)	0.81	16/5507 (0.3%)
1	J	0.64	6/4092 (0.1%)	0.82	11/5543 (0.2%)
1	K	0.64	0/4102	0.75	9/5556 (0.2%)
1	L	0.68	2/4123 (0.0%)	0.75	10/5584 (0.2%)
All	All	0.63	27/49041 (0.1%)	0.74	120/66448 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	351	LYS	CG-CD	12.22	1.94	1.52
1	E	351	LYS	CE-NZ	12.20	1.79	1.49
1	E	513[A]	ARG	CD-NE	11.85	1.66	1.46
1	E	513[B]	ARG	CD-NE	11.85	1.66	1.46
1	I	513[A]	ARG	NE-CZ	9.84	1.45	1.33
1	I	513[B]	ARG	NE-CZ	9.84	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	340	ARG	CZ-NH1	8.49	1.44	1.33
1	J	513[A]	ARG	CZ-NH1	8.40	1.44	1.33
1	J	513[B]	ARG	CZ-NH1	8.40	1.44	1.33
1	I	513[A]	ARG	CG-CD	-6.77	1.35	1.51
1	I	513[B]	ARG	CG-CD	-6.77	1.35	1.51
1	J	513[A]	ARG	CG-CD	6.28	1.67	1.51
1	J	513[B]	ARG	CG-CD	6.28	1.67	1.51
1	C	340	ARG	CD-NE	6.06	1.56	1.46
1	C	340	ARG	CZ-NH2	6.00	1.40	1.33
1	J	513[A]	ARG	CD-NE	-5.93	1.36	1.46
1	J	513[B]	ARG	CD-NE	-5.93	1.36	1.46
1	I	513[A]	ARG	CZ-NH1	-5.91	1.25	1.33
1	I	513[B]	ARG	CZ-NH1	-5.91	1.25	1.33
1	E	351	LYS	CG-CD	5.73	1.72	1.52
1	L	189	GLU	CG-CD	5.72	1.60	1.51
1	H	122	ARG	CG-CD	5.45	1.65	1.51
1	I	513[A]	ARG	CB-CG	-5.40	1.38	1.52
1	I	513[B]	ARG	CB-CG	-5.40	1.38	1.52
1	L	129	GLU	CD-OE1	5.15	1.31	1.25
1	G	351	LYS	CE-NZ	5.08	1.61	1.49
1	A	187	GLU	CD-OE2	5.03	1.31	1.25

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	513[A]	ARG	NE-CZ-NH1	18.57	129.59	120.30
1	J	513[B]	ARG	NE-CZ-NH1	18.57	129.59	120.30
1	C	340	ARG	NE-CZ-NH1	-14.26	113.17	120.30
1	I	513[A]	ARG	NE-CZ-NH1	14.22	127.41	120.30
1	I	513[B]	ARG	NE-CZ-NH1	14.22	127.41	120.30
1	J	513[A]	ARG	NE-CZ-NH2	-12.43	114.08	120.30
1	J	513[B]	ARG	NE-CZ-NH2	-12.43	114.08	120.30
1	L	90	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	B	90	ARG	NE-CZ-NH2	-11.35	114.63	120.30
1	K	90	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	A	90	ARG	NE-CZ-NH2	-10.91	114.85	120.30
1	D	90	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	I	90	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	J	90	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	H	90	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	I	513[A]	ARG	NH1-CZ-NH2	-10.49	107.86	119.40
1	I	513[B]	ARG	NH1-CZ-NH2	-10.49	107.86	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	G	90	ARG	NE-CZ-NH2	-10.05	115.27	120.30
1	E	90	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	F	90	ARG	NE-CZ-NH2	-9.67	115.47	120.30
1	A	235	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	I	513[A]	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	I	513[B]	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	I	279	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	C	279	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	D	279	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	L	279	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	K	279	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	K	192[A]	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	K	192[B]	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	L	235	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	H	279	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	A	279	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	B	279	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	B	235	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	D	235	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	E	122	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	H	235	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	G	279	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	C	90	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	E	279	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	E	235	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	J	279	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	D	235	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	D	90	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	G	235	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	C	235	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	C	279	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	I	235	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	F	279	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	K	235	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	F	235	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	B	235	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	C	122	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	J	90	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	L	279	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	B	90	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	K	90	ARG	NE-CZ-NH1	6.66	123.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	351	LYS	CB-CG-CD	-6.65	94.31	111.60
1	A	235	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	L	235	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	K	279	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	I	90	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	122	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	B	122	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	F	235	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	B	484	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	L	90	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	C	513[A]	ARG	NE-CZ-NH1	-6.09	117.26	120.30
1	C	513[B]	ARG	NE-CZ-NH1	-6.09	117.26	120.30
1	C	513[A]	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	C	513[B]	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	B	279	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	I	279	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	E	90	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	H	90	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	90	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	90	ARG	CG-CD-NE	-5.95	99.31	111.80
1	F	90	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	K	235	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	D	90	ARG	CG-CD-NE	-5.85	99.51	111.80
1	L	398	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	I	90	ARG	CG-CD-NE	-5.80	99.61	111.80
1	L	122	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	279	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	90	ARG	CG-CD-NE	-5.74	99.74	111.80
1	J	235	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	E	90	ARG	CG-CD-NE	-5.67	99.90	111.80
1	I	122[A]	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	I	122[B]	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	H	279	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	279	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	H	122	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	K	90	ARG	CG-CD-NE	-5.58	100.08	111.80
1	L	90	ARG	CG-CD-NE	-5.57	100.10	111.80
1	F	279	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	G	90	ARG	CG-CD-NE	-5.55	100.14	111.80
1	J	235	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	H	90	ARG	CG-CD-NE	-5.49	100.27	111.80
1	G	279	ARG	NE-CZ-NH1	5.48	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	E	152	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	G	90	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	L	38	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	H	235	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	I	235	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	I	398	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	90	ARG	CG-CD-NE	-5.34	100.59	111.80
1	D	398	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	146	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	J	90	ARG	CG-CD-NE	-5.29	100.70	111.80
1	F	90	ARG	CG-CD-NE	-5.23	100.83	111.80
1	J	279	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	433	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	38	ARG	CB-CA-C	5.10	120.61	110.40
1	F	293	ILE	CB-CA-C	-5.07	101.46	111.60
1	A	122	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	H	34	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	E	351	LYS	CD-CE-NZ	-5.01	100.19	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	513[A]	ARG	Sidechain
1	E	513[B]	ARG	Sidechain

## 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	4066	0	4095	79	2
1	B	3999	0	3991	51	0
1	C	4001	0	3990	63	0
1	D	3977	0	3975	71	0
1	E	3975	0	3967	57	0
1	F	3969	0	3969	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3939	0	3938	56	0
1	H	3973	0	3982	65	0
1	I	3978	0	3978	47	0
1	J	3993	0	3999	43	0
1	K	4005	0	4014	69	0
1	L	4016	0	4027	61	2
2	A	26	0	16	3	0
2	B	26	0	16	1	0
2	C	26	0	16	2	0
2	D	26	0	16	1	0
2	E	26	0	16	2	0
2	F	26	0	16	2	0
2	G	26	0	16	2	0
2	H	26	0	16	2	0
2	I	26	0	16	3	0
2	J	26	0	16	2	0
2	K	26	0	16	6	0
2	L	26	0	16	4	0
3	A	53	0	31	1	0
3	B	53	0	31	3	0
3	C	53	0	31	1	0
3	D	53	0	31	3	0
3	E	53	0	31	5	0
3	F	53	0	31	4	0
3	G	53	0	31	4	0
3	H	53	0	31	2	0
3	I	53	0	31	6	0
3	J	53	0	31	4	0
3	K	53	0	31	2	0
3	L	53	0	31	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	30	0	0	8	0
5	B	15	0	0	1	0
5	C	10	0	0	0	0
5	D	35	0	0	3	0
5	E	10	0	0	1	0
5	F	10	0	0	1	0
5	G	15	0	0	0	0
5	H	10	0	0	1	0
5	I	10	0	0	1	0
5	J	5	0	0	0	0
5	K	5	0	0	1	0
5	L	25	0	0	2	0
6	A	280	0	0	15	0
6	B	60	0	0	0	0
6	C	73	0	0	4	0
6	D	88	0	0	6	0
6	E	43	0	0	8	0
6	F	41	0	0	2	0
6	G	40	0	0	1	0
6	H	64	0	0	4	0
6	I	62	0	0	1	0
6	J	50	0	0	3	0
6	K	77	0	0	4	0
6	L	451	0	0	28	0
All	All	50360	0	48489	649	2

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.

All (649) 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:K:337:GLU:CG	1:K:340:ARG:HH22	1.26	1.49
1:C:337:GLU:CG	1:C:340:ARG:HH21	1.25	1.46
1:F:351:LYS:CD	1:F:351:LYS:CG	1.94	1.42
1:E:351:LYS:NZ	1:E:351:LYS:CE	1.79	1.41
1:C:337:GLU:CG	1:C:340:ARG:NH2	1.80	1.40
1:K:337:GLU:CG	1:K:340:ARG:NH2	1.97	1.27
1:D:355:LYS:CE	1:H:322:LEU:HA	1.64	1.25
1:C:337:GLU:HG3	1:C:340:ARG:NH2	0.93	1.24
1:K:337:GLU:HG3	1:K:340:ARG:NH2	1.52	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:509:GLU:OE2	1:J:513[A]:ARG:NH1	1.78	1.16
1:F:396:LYS:NZ	6:F:625:HOH:O	1.80	1.14
6:A:682:HOH:O	1:J:251:THR:HG21	1.48	1.12
1:K:337:GLU:HG3	1:K:340:ARG:HH22	0.98	1.11
6:A:699:HOH:O	1:L:251:THR:HG21	1.50	1.10
1:D:355:LYS:HE2	1:H:322:LEU:HA	1.27	1.09
1:D:355:LYS:HE3	1:H:322:LEU:HD23	1.34	1.09
1:C:251:THR:HG21	6:L:721:HOH:O	1.50	1.09
6:D:672:HOH:O	1:H:330:LYS:HE2	1.49	1.08
1:C:248:VAL:HG23	1:C:339:TYR:HB2	1.32	1.07
6:A:684:HOH:O	1:G:251:THR:HG21	1.53	1.07
6:A:760:HOH:O	1:D:251:THR:HG21	1.54	1.06
1:K:478:ASP:OD2	1:K:480:THR:HB	1.57	1.05
1:A:251:THR:HG21	6:A:696:HOH:O	1.56	1.04
1:E:178[B]:HIS:HD2	6:E:770:HOH:O	1.39	1.03
1:H:2:LYS:N	1:H:2:LYS:HE2	1.79	0.98
1:K:337:GLU:HG3	1:K:340:ARG:CZ	1.92	0.97
1:A:39:MET:O	1:L:11:LYS:HE3	1.63	0.97
1:A:122:ARG:HG3	1:A:122:ARG:HH11	1.27	0.96
1:H:2:LYS:HE2	1:H:2:LYS:H	1.29	0.95
1:K:251:THR:HG21	6:L:634:HOH:O	1.64	0.95
1:I:251:THR:HG23	1:I:260:PHE:HA	1.49	0.95
1:K:337:GLU:HG2	1:K:340:ARG:NH2	1.82	0.94
1:H:251:THR:HG21	6:L:949:HOH:O	1.65	0.94
1:C:248:VAL:CG2	1:C:339:TYR:HB2	2.00	0.91
1:D:251:THR:HG23	1:D:260:PHE:HA	1.52	0.91
1:I:251:THR:CG2	1:I:260:PHE:HA	2.00	0.90
1:H:251:THR:HG23	1:H:260:PHE:HA	1.52	0.90
1:L:324:GLU:HG2	5:L:617:PO4:O4	1.72	0.89
1:K:337:GLU:HG3	1:K:340:ARG:NH1	1.86	0.89
1:A:39:MET:O	1:L:11:LYS:CE	2.21	0.88
1:C:448:GLN:HE21	1:D:483:HIS:H	1.20	0.88
1:L:250:MET:HE2	6:L:1043:HOH:O	1.74	0.88
1:A:251:THR:HG23	1:A:260[A]:PHE:HA	1.56	0.88
2:G:611:TPP:H7'2	5:H:615:PO4:O3	1.74	0.88
1:J:251:THR:HG23	1:J:260:PHE:HA	1.57	0.87
1:J:251:THR:CG2	1:J:260:PHE:HA	2.04	0.87
1:K:251:THR:HG23	1:K:260:PHE:HA	1.57	0.86
1:C:251:THR:HG23	1:C:260:PHE:HA	1.58	0.86
1:K:251:THR:CG2	1:K:260:PHE:HA	2.05	0.86
1:H:251:THR:CG2	1:H:260:PHE:HA	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:THR:CG2	1:E:260:PHE:HA	2.06	0.86
1:A:248[B]:VAL:HG13	1:A:339:TYR:HB2	1.56	0.86
1:C:251:THR:CG2	1:C:260:PHE:HA	2.07	0.85
1:E:251:THR:HG23	1:E:260:PHE:HA	1.58	0.85
1:G:251:THR:HG23	1:G:260:PHE:HA	1.59	0.84
1:H:324:GLU:OE2	6:H:663:HOH:O	1.94	0.84
1:E:311:ASP:HB3	6:E:1065:HOH:O	1.77	0.84
1:D:251:THR:CG2	1:D:260:PHE:HA	2.07	0.84
1:A:313:LYS:NZ	5:A:619:PO4:O2	2.09	0.84
1:K:337:GLU:CD	1:K:340:ARG:HH22	1.81	0.84
1:L:251:THR:CG2	1:L:260:PHE:HA	2.08	0.84
1:G:251:THR:CG2	1:G:260:PHE:HA	2.07	0.83
1:C:337:GLU:HG3	1:C:340:ARG:HH22	1.40	0.83
1:L:251:THR:HG23	1:L:260:PHE:HA	1.59	0.83
1:K:483:HIS:H	1:L:448:GLN:HE21	1.24	0.83
1:B:251:THR:HG23	1:B:260:PHE:HA	1.61	0.83
1:C:337:GLU:HA	1:C:340:ARG:HE	1.43	0.82
1:A:251:THR:CG2	1:A:260[A]:PHE:HA	2.08	0.82
1:B:251:THR:CG2	1:B:260:PHE:HA	2.09	0.81
1:C:433:ASP:OD2	1:C:482:LEU:HD12	1.78	0.81
1:K:462:VAL:CG2	1:K:480:THR:HG22	2.11	0.81
1:G:483:HIS:H	1:H:448:GLN:HE21	1.29	0.81
1:K:478:ASP:OD2	1:K:480:THR:CB	2.28	0.81
1:E:311:ASP:OD2	6:E:1065:HOH:O	2.00	0.80
1:F:251:THR:HG23	1:F:260:PHE:HA	1.62	0.80
1:F:251:THR:CG2	1:F:260:PHE:HA	2.11	0.80
1:G:433:ASP:OD2	1:G:482:LEU:HD12	1.81	0.80
1:E:483:HIS:H	1:F:448:GLN:HE21	1.29	0.80
1:I:174:MET:N	5:I:614:PO4:O2	2.11	0.79
1:D:250:MET:HE2	6:L:629:HOH:O	1.83	0.79
1:A:174:MET:N	5:A:618:PO4:O2	2.13	0.79
1:A:344:LYS:HD3	1:A:537:GLN:NE2	1.98	0.78
1:I:483:HIS:H	1:J:448:GLN:HE21	1.31	0.78
1:K:337:GLU:HG3	1:K:340:ARG:HH12	1.45	0.78
1:C:184[A]:VAL:HG23	1:C:311:ASP:HB3	1.65	0.77
2:K:611:TPP:H2	2:K:611:TPP:HN42	1.49	0.77
1:A:448:GLN:HE21	1:B:483:HIS:H	1.32	0.77
1:D:355:LYS:HE3	1:H:322:LEU:HA	1.64	0.77
1:F:462:VAL:HG23	1:F:480:THR:O	1.84	0.76
1:H:2:LYS:H	1:H:2:LYS:CE	1.98	0.76
1:F:351:LYS:CD	1:F:351:LYS:CB	2.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:465:PHE:O	1:J:465:PHE:CD2	2.38	0.76
1:G:448:GLN:HE21	1:H:483:HIS:H	1.34	0.76
1:K:448:GLN:HE21	1:L:483:HIS:H	1.34	0.75
6:A:685:HOH:O	1:C:250:MET:HE2	1.87	0.74
1:C:448:GLN:NE2	1:D:483:HIS:H	1.84	0.74
1:K:337:GLU:HA	1:K:340:ARG:NH1	2.02	0.74
1:B:433:ASP:OD2	1:B:482:LEU:HD12	1.88	0.74
5:E:614:PO4:O2	2:F:611:TPP:H7'2	1.88	0.74
1:G:279:ARG:HD3	1:H:106:GLU:OE1	1.88	0.74
6:A:825:HOH:O	1:D:146:ARG:HD2	1.88	0.73
1:K:279:ARG:HD3	1:L:106:GLU:OE1	1.88	0.73
1:H:185:THR:HG21	6:H:670:HOH:O	1.89	0.73
6:E:1066:HOH:O	1:H:146:ARG:HD2	1.89	0.73
1:L:433:ASP:OD2	1:L:482:LEU:HD12	1.89	0.73
1:A:448:GLN:NE2	1:B:483:HIS:H	1.86	0.73
1:A:106:GLU:OE1	1:B:279:ARG:HD3	1.89	0.72
1:A:251:THR:CG2	1:A:260[B]:PHE:HA	2.20	0.72
1:K:483:HIS:H	1:L:448:GLN:NE2	1.87	0.72
1:E:483:HIS:H	1:F:448:GLN:NE2	1.87	0.71
1:C:173:THR:CG2	6:C:619:HOH:O	2.39	0.71
1:D:355:LYS:HE3	1:H:322:LEU:CD2	2.16	0.71
1:C:279:ARG:HD3	1:D:106:GLU:OE1	1.92	0.70
1:E:279:ARG:HD3	1:F:106:GLU:OE1	1.90	0.70
1:G:178:HIS:HB3	6:G:630:HOH:O	1.91	0.70
1:I:199:ARG:HD3	1:I:200:TYR:CE2	2.26	0.70
1:I:483:HIS:H	1:J:448:GLN:NE2	1.89	0.70
1:D:355:LYS:HE2	1:H:322:LEU:CA	2.15	0.70
1:I:392:LYS:HE3	6:L:931:HOH:O	1.91	0.70
1:D:355:LYS:CE	1:H:322:LEU:HD23	2.18	0.69
1:L:28[B]:SER:HG	1:L:74:CYS:HG	1.37	0.69
1:E:351:LYS:NZ	1:E:351:LYS:CG	2.56	0.69
6:A:756:HOH:O	1:K:250:MET:HE2	1.91	0.69
1:A:447:VAL:HG23	1:A:496:ILE:HD11	1.75	0.69
1:G:447:VAL:HG23	1:G:496:ILE:HD11	1.75	0.69
1:C:447:VAL:HG23	1:C:496:ILE:HD11	1.75	0.68
1:A:339:TYR:OH	1:A:343[B]:ARG:HD3	1.93	0.68
1:B:311:ASP:OD2	1:B:314:SER:HB3	1.92	0.68
1:E:351:LYS:NZ	1:E:351:LYS:CD	2.57	0.68
1:I:447:VAL:HG23	1:I:496:ILE:HD11	1.76	0.68
1:J:447:VAL:HG23	1:J:496:ILE:HD11	1.75	0.68
1:F:248:VAL:HG22	1:F:339:TYR:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:313:LYS:NZ	6:H:650:HOH:O	2.27	0.68
1:I:279:ARG:HD3	1:J:106:GLU:OE1	1.93	0.68
1:L:447:VAL:HG23	1:L:496:ILE:HD11	1.74	0.68
1:D:344:LYS:HD3	6:D:672:HOH:O	1.94	0.67
1:H:447:VAL:HG23	1:H:496:ILE:HD11	1.76	0.67
1:C:337:GLU:HA	1:C:340:ARG:NE	2.09	0.67
1:A:250:MET:HE2	6:A:632:HOH:O	1.94	0.67
1:B:447:VAL:HG23	1:B:496:ILE:HD11	1.76	0.67
1:A:146:ARG:HD2	6:A:625:HOH:O	1.95	0.67
1:A:251:THR:HG23	1:A:260[B]:PHE:HA	1.76	0.67
1:A:343[A]:ARG:NH1	1:A:389:ARG:O	2.25	0.67
1:D:509:GLU:HG2	6:D:637:HOH:O	1.94	0.67
1:K:448:GLN:NE2	1:L:483:HIS:H	1.93	0.67
1:D:173:THR:HG23	6:D:641:HOH:O	1.95	0.67
1:D:447:VAL:HG23	1:D:496:ILE:HD11	1.77	0.66
1:C:337:GLU:HG2	1:C:340:ARG:NH2	2.04	0.66
1:E:311:ASP:CB	6:E:1065:HOH:O	2.38	0.66
1:E:447:VAL:HG23	1:E:496:ILE:HD11	1.76	0.66
1:F:447:VAL:HG23	1:F:496:ILE:HD11	1.77	0.66
1:H:337:GLU:HG3	1:H:340:ARG:HH22	1.61	0.66
1:D:173:THR:CG2	6:D:641:HOH:O	2.44	0.65
1:K:447:VAL:HG23	1:K:496:ILE:HD11	1.76	0.65
1:E:146:ARG:HD2	6:L:877:HOH:O	1.97	0.65
1:H:146:ARG:NH2	1:H:177:TYR:O	2.28	0.65
1:E:351:LYS:NZ	1:E:351:LYS:HG2	2.12	0.64
1:L:313:LYS:NZ	6:L:1062:HOH:O	2.30	0.64
1:F:462:VAL:CG2	1:F:480:THR:O	2.44	0.64
1:G:448:GLN:NE2	1:H:483:HIS:H	1.94	0.64
2:C:611:TPP:H7'2	5:D:615:PO4:O2	1.97	0.64
1:H:463:LEU:HB3	2:H:611:TPP:H61	1.80	0.64
2:J:611:TPP:H2	2:J:611:TPP:HN42	1.63	0.63
6:A:751:HOH:O	1:B:146:ARG:HD2	1.98	0.63
1:A:483:HIS:H	1:B:448:GLN:HE21	1.46	0.63
1:A:251:THR:HG22	1:A:260[B]:PHE:HD1	1.64	0.62
1:I:303:LYS:HD3	1:L:173:THR:HG21	1.81	0.62
1:C:106:GLU:OE1	1:D:279:ARG:HD3	1.98	0.62
1:H:248:VAL:HG22	1:H:339:TYR:HB2	1.80	0.62
1:B:462:VAL:HG23	1:B:480:THR:O	1.99	0.62
1:D:355:LYS:CE	1:H:322:LEU:CA	2.60	0.62
1:J:303:LYS:HD3	1:K:173:THR:HG21	1.80	0.62
1:A:38:ARG:HB2	1:L:38:ARG:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:HB2	6:L:800:HOH:O	1.99	0.61
1:A:38:ARG:HA	1:L:38:ARG:O	2.01	0.61
1:C:337:GLU:CG	1:C:340:ARG:HH22	2.02	0.61
1:A:257:SER:HA	1:A:260[B]:PHE:CD2	2.36	0.61
1:F:146:ARG:NH2	1:F:177:TYR:O	2.31	0.61
1:F:303:LYS:HD3	1:G:173:THR:HG21	1.81	0.61
1:E:173:THR:HG21	1:H:303:LYS:HD3	1.83	0.61
1:J:173:THR:HG21	1:K:303:LYS:HD3	1.82	0.61
1:H:337:GLU:HG3	1:H:340:ARG:NH2	2.16	0.60
1:E:250:MET:HE2	6:L:688:HOH:O	2.01	0.60
1:F:433:ASP:OD2	1:F:482:LEU:HD12	1.99	0.60
1:J:396:LYS:NZ	6:J:1235:HOH:O	2.35	0.60
1:A:122:ARG:HG3	1:A:122:ARG:NH1	2.05	0.60
1:G:482:LEU:O	1:G:483:HIS:C	2.39	0.60
2:K:611:TPP:HN42	2:K:611:TPP:C2	2.15	0.60
1:A:492:GLU:OE2	5:A:617:PO4:O4	2.19	0.60
1:B:173:THR:HG21	1:C:303:LYS:HD3	1.84	0.59
1:B:303:LYS:HD3	1:C:173:THR:HG21	1.83	0.59
1:K:122[B]:ARG:CG	1:K:122[B]:ARG:HH11	2.15	0.59
1:K:189:GLU:HA	1:K:192[B]:ARG:NH1	2.17	0.59
1:D:146:ARG:NH2	1:D:177:TYR:O	2.33	0.59
1:I:173:THR:HG21	1:L:303:LYS:HD3	1.83	0.59
1:L:250:MET:CE	6:L:1043:HOH:O	2.43	0.59
1:L:392:LYS:HE3	6:L:713:HOH:O	2.02	0.59
1:E:106:GLU:OE1	1:F:279:ARG:HD3	2.02	0.59
1:A:483:HIS:H	1:B:448:GLN:NE2	2.01	0.59
1:C:173:THR:HG23	6:C:619:HOH:O	1.99	0.59
1:D:355:LYS:NZ	1:H:322:LEU:HA	2.16	0.59
1:G:483:HIS:O	1:G:485:THR:OG1	2.21	0.58
1:K:433:ASP:OD2	1:K:482:LEU:HD12	2.03	0.58
1:K:461:SER:HB2	6:K:622:HOH:O	2.02	0.58
1:G:483:HIS:H	1:H:448:GLN:NE2	2.01	0.58
1:A:339:TYR:CZ	1:A:343[B]:ARG:HD3	2.38	0.58
1:J:146:ARG:NH2	1:J:177:TYR:O	2.31	0.58
1:C:248:VAL:HG23	1:C:339:TYR:CB	2.19	0.57
1:D:532:LEU:CG	1:D:532:LEU:O	2.50	0.57
1:I:248:VAL:HG22	1:I:339:TYR:HB2	1.86	0.57
2:I:611:TPP:HN42	2:I:611:TPP:H2	1.69	0.57
1:L:152[A]:ARG:HD2	6:L:1046:HOH:O	2.04	0.57
1:L:146:ARG:NH2	1:L:177:TYR:O	2.31	0.57
1:K:337:GLU:HA	1:K:340:ARG:HH12	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:106:GLU:OE1	1:J:279:ARG:HD3	2.05	0.57
1:K:462:VAL:HG22	1:K:480:THR:HG22	1.85	0.57
1:C:178:HIS:HB3	6:C:646:HOH:O	2.05	0.56
1:H:251:THR:HG23	1:H:260:PHE:CA	2.32	0.56
1:B:462:VAL:CG2	1:B:480:THR:O	2.52	0.56
1:E:303:LYS:HD3	1:H:173:THR:HG21	1.86	0.56
1:F:351:LYS:CG	1:F:351:LYS:CE	2.81	0.56
1:F:463:LEU:HB3	2:F:611:TPP:H61	1.86	0.56
1:K:106:GLU:OE1	1:L:279:ARG:HD3	2.05	0.56
2:K:611:TPP:H7'2	5:L:616:PO4:O4	2.05	0.56
1:L:285:ASP:OD1	1:L:285:ASP:N	2.37	0.56
1:I:90:ARG:NH2	1:J:111:TYR:O	2.38	0.56
1:G:106:GLU:OE1	1:H:279:ARG:HD3	2.06	0.56
1:H:199:ARG:NH1	1:H:324:GLU:OE1	2.38	0.56
1:B:146:ARG:NH2	1:B:177:TYR:O	2.34	0.56
1:E:92:HIS:HE1	3:E:612:FAD:O2A	1.89	0.56
1:J:173:THR:CG2	6:J:1258:HOH:O	2.53	0.56
1:A:146:ARG:NH2	1:A:177:TYR:O	2.35	0.55
1:G:90:ARG:NH2	1:H:111:TYR:O	2.39	0.55
1:I:146:ARG:NH2	1:I:177:TYR:O	2.32	0.55
1:K:529:LYS:HD3	1:K:529:LYS:N	2.21	0.55
1:A:238:GLU:OE1	1:A:398:ARG:HD2	2.06	0.55
1:D:185[B]:THR:OG1	1:D:314:SER:OG	2.24	0.55
1:D:532:LEU:O	1:D:532:LEU:HD12	2.07	0.55
1:D:532:LEU:O	1:D:532:LEU:HG	2.05	0.55
1:E:311:ASP:CG	6:E:1065:HOH:O	2.41	0.55
1:A:30:ASN:O	1:A:34:ASP:HB2	2.06	0.55
1:C:483:HIS:H	1:D:448:GLN:HE21	1.55	0.55
1:J:173:THR:HG23	6:J:1258:HOH:O	2.07	0.55
1:J:238:GLU:OE1	1:J:398:ARG:HD2	2.07	0.55
1:K:90:ARG:NH2	1:L:111:TYR:O	2.40	0.55
1:A:279:ARG:HD3	1:B:106:GLU:OE1	2.06	0.55
1:K:146:ARG:NH2	1:K:177:TYR:O	2.32	0.55
1:K:238:GLU:OE1	1:K:398:ARG:HD2	2.07	0.55
1:E:146:ARG:NH2	1:E:177:TYR:O	2.33	0.54
1:G:146:ARG:NH2	1:G:177:TYR:O	2.33	0.54
1:D:238:GLU:OE1	1:D:398:ARG:HD2	2.08	0.54
6:F:627:HOH:O	1:G:146:ARG:HD2	2.05	0.54
1:A:313:LYS:HZ1	5:A:619:PO4:P	2.25	0.54
1:C:146:ARG:NH2	1:C:177:TYR:O	2.32	0.54
1:G:437:SER:O	1:H:441:GLY:HA3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:462:VAL:CG2	1:G:480:THR:O	2.55	0.54
1:F:290:GLN:HE22	1:F:299:GLY:H	1.56	0.54
1:C:238:GLU:OE1	1:C:398:ARG:HD2	2.08	0.53
1:G:173:THR:CG2	6:L:806:HOH:O	2.55	0.53
1:K:462:VAL:HG22	1:K:480:THR:CG2	2.37	0.53
1:A:313:LYS:NZ	5:A:619:PO4:P	2.81	0.53
1:I:126:HIS:O	1:I:147:LYS:HE3	2.08	0.53
1:A:111:TYR:O	1:B:90:ARG:NH2	2.41	0.53
1:C:126:HIS:O	1:C:147:LYS:HE3	2.08	0.53
1:E:448:GLN:HE21	1:F:483:HIS:HB2	1.74	0.53
1:F:238:GLU:OE1	1:F:398:ARG:HD2	2.08	0.53
1:L:238:GLU:OE1	1:L:398:ARG:HD2	2.09	0.53
1:D:251:THR:HG23	1:D:260:PHE:CA	2.32	0.53
1:L:251:THR:HG23	1:L:260:PHE:CA	2.36	0.53
1:D:126:HIS:O	1:D:147:LYS:HE3	2.09	0.53
1:H:238:GLU:OE1	1:H:398:ARG:HD2	2.09	0.53
1:I:238:GLU:OE1	1:I:398:ARG:HD2	2.09	0.53
1:B:238:GLU:OE1	1:B:398:ARG:HD2	2.08	0.52
1:G:462:VAL:HG23	1:G:480:THR:O	2.09	0.52
1:L:207:MET:SD	1:L:231:VAL:HG22	2.50	0.52
1:E:126:HIS:O	1:E:147:LYS:HE3	2.09	0.52
1:L:461:SER:HB3	6:L:752:HOH:O	2.10	0.52
1:I:251:THR:HG23	1:I:260:PHE:CA	2.31	0.52
1:J:465:PHE:O	1:J:465:PHE:HD2	1.91	0.52
1:A:248[B]:VAL:CG1	1:A:258:SER:HB2	2.39	0.52
1:D:293:ILE:HG12	3:D:612:FAD:C4A	2.39	0.52
1:E:238:GLU:OE1	1:E:398:ARG:HD2	2.10	0.52
1:F:248:VAL:HG13	1:F:248:VAL:O	2.10	0.52
1:H:90:ARG:HD2	6:L:892:HOH:O	2.09	0.52
1:I:290:GLN:HE22	1:I:299:GLY:H	1.58	0.52
1:J:34:ASP:O	1:J:38[B]:ARG:HG3	2.10	0.52
1:K:437:SER:O	1:L:441:GLY:HA3	2.10	0.52
1:G:238:GLU:OE1	1:G:398:ARG:HD2	2.09	0.51
1:D:185[A]:THR:HG23	6:L:731:HOH:O	2.10	0.51
1:K:337:GLU:CG	1:K:340:ARG:CZ	2.66	0.51
1:E:251:THR:HG23	1:E:260:PHE:CA	2.37	0.51
1:E:90:ARG:NH2	1:F:111:TYR:O	2.43	0.51
1:A:303:LYS:HD3	1:D:173:THR:HG21	1.93	0.51
1:D:174:MET:N	5:D:614:PO4:O2	2.31	0.51
1:K:337:GLU:CG	1:K:340:ARG:HH12	2.21	0.51
1:K:478:ASP:C	1:K:480:THR:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ILE:HD11	1:A:513[B]:ARG:HD3	1.92	0.50
1:C:207:MET:SD	1:C:231:VAL:HG22	2.51	0.50
2:E:611:TPP:H7'2	5:F:614:PO4:O3	2.11	0.50
1:L:3:GLN:NE2	6:L:743:HOH:O	2.44	0.50
1:A:122:ARG:HH11	1:A:122:ARG:CG	2.11	0.50
1:C:337:GLU:CB	1:C:340:ARG:HH21	2.13	0.50
1:H:290:GLN:HE22	1:H:299:GLY:H	1.60	0.50
1:F:126[B]:HIS:CE1	1:F:148:ALA:HA	2.47	0.50
1:B:132:SER:HB3	1:D:132:SER:HB3	1.94	0.50
5:K:614:PO4:O1	2:L:611:TPP:H7'2	2.12	0.50
1:I:463:LEU:HB3	2:I:611:TPP:H61	1.94	0.50
1:L:392:LYS:CE	6:L:713:HOH:O	2.60	0.50
1:G:126:HIS:O	1:G:147:LYS:HE3	2.12	0.50
1:F:226:ILE:HA	1:F:326:LYS:HG3	1.94	0.50
1:J:146:ARG:HD2	6:K:624:HOH:O	2.10	0.49
1:K:441:GLY:HA3	1:L:437:SER:O	2.12	0.49
1:B:184:VAL:HG22	1:C:184[A]:VAL:HG12	1.94	0.49
1:C:290:GLN:HE22	1:C:299:GLY:H	1.60	0.49
1:J:251:THR:HG23	1:J:260:PHE:CA	2.36	0.49
2:J:611:TPP:HN42	2:J:611:TPP:C2	2.24	0.49
1:K:483:HIS:HD2	6:K:687:HOH:O	1.94	0.49
1:D:460:ASN:O	1:D:461:SER:HB3	2.11	0.49
1:L:290:GLN:HE22	1:L:299:GLY:H	1.60	0.49
1:E:178[B]:HIS:CD2	6:E:770:HOH:O	2.28	0.49
1:G:226:ILE:HA	1:G:326:LYS:HG3	1.95	0.49
2:H:611:TPP:HN42	2:H:611:TPP:H2	1.77	0.49
1:J:290:GLN:HE22	1:J:299:GLY:H	1.60	0.49
1:K:126:HIS:O	1:K:147:LYS:HE3	2.11	0.49
1:D:290:GLN:HE22	1:D:299:GLY:H	1.61	0.49
1:E:351:LYS:CG	1:E:351:LYS:HZ3	2.26	0.49
1:K:290:GLN:HE22	1:K:299:GLY:H	1.58	0.49
1:G:207:MET:SD	1:G:231:VAL:HG22	2.53	0.49
1:J:126:HIS:O	1:J:147:LYS:HE3	2.11	0.49
1:G:441:GLY:HA3	1:H:437:SER:O	2.12	0.49
1:C:90:ARG:NH2	1:D:111:TYR:O	2.45	0.49
1:D:461:SER:HB2	6:L:679:HOH:O	2.13	0.49
1:G:481:GLU:O	1:G:482:LEU:HD23	2.12	0.49
1:E:290:GLN:HE22	1:E:299:GLY:H	1.60	0.49
1:F:173:THR:HG21	1:G:303:LYS:HD3	1.93	0.49
1:F:207:MET:SD	1:F:231:VAL:HG22	2.53	0.49
1:A:461[A]:SER:HB3	6:L:785:HOH:O	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:178:HIS:HB3	6:I:636:HOH:O	2.13	0.48
1:K:462:VAL:CG2	1:K:480:THR:CG2	2.87	0.48
1:A:37:ASN:O	1:L:38:ARG:HD2	2.13	0.48
1:H:226:ILE:HA	1:H:326:LYS:HG3	1.95	0.48
1:A:290:GLN:HE22	1:A:299:GLY:H	1.61	0.48
1:B:290:GLN:HE22	1:B:299:GLY:H	1.59	0.48
1:C:251:THR:HG23	1:C:260:PHE:CA	2.37	0.48
1:A:207:MET:SD	1:A:231:VAL:HG22	2.53	0.48
6:A:756:HOH:O	1:K:250:MET:CE	2.56	0.48
1:D:250:MET:CE	6:L:629:HOH:O	2.52	0.48
1:F:290:GLN:NE2	1:F:299:GLY:H	2.11	0.48
3:E:612:FAD:N1	3:E:612:FAD:H2'	2.29	0.48
1:A:126:HIS:O	1:A:147:LYS:HE3	2.12	0.48
1:G:251:THR:HG23	1:G:260:PHE:CA	2.37	0.48
1:I:290:GLN:NE2	1:I:299:GLY:H	2.12	0.48
1:K:34:ASP:O	1:K:38:ARG:HG2	2.14	0.48
1:E:290:GLN:NE2	1:E:299:GLY:H	2.12	0.48
1:B:127:TYR:CZ	1:B:129[A]:GLU:HG3	2.49	0.48
1:B:207:MET:SD	1:B:231:VAL:HG22	2.54	0.48
1:D:344:LYS:CD	6:D:672:HOH:O	2.59	0.48
1:G:290:GLN:HE22	1:G:299:GLY:H	1.60	0.48
1:I:207:MET:SD	1:I:231:VAL:HG22	2.54	0.48
1:K:311:ASP:HA	3:K:612:FAD:N1A	2.29	0.48
1:K:337:GLU:CG	1:K:340:ARG:NH1	2.68	0.48
1:L:199:ARG:HG2	1:L:200:TYR:CD2	2.49	0.48
1:B:311:ASP:HA	3:B:612:FAD:N1A	2.28	0.47
1:K:290:GLN:NE2	1:K:299:GLY:H	2.11	0.47
1:L:126:HIS:O	1:L:147:LYS:HE3	2.13	0.47
1:A:132:SER:HB3	1:C:132:SER:HB3	1.97	0.47
1:B:126:HIS:O	1:B:147:LYS:HE3	2.13	0.47
1:B:290:GLN:NE2	1:B:299:GLY:H	2.12	0.47
1:C:248:VAL:HG22	1:C:258:SER:HB2	1.96	0.47
1:C:290:GLN:NE2	1:C:299:GLY:H	2.12	0.47
1:H:126:HIS:O	1:H:147:LYS:HE3	2.13	0.47
2:K:611:TPP:C2	2:K:611:TPP:N4'	2.77	0.47
1:A:226:ILE:HA	1:A:326:LYS:HG3	1.96	0.47
1:B:251:THR:HG23	1:B:260:PHE:CA	2.38	0.47
1:G:290:GLN:NE2	1:G:299:GLY:H	2.13	0.47
1:A:250:MET:CE	1:A:388:ALA:HB1	2.45	0.47
1:B:312:ILE:HG12	3:B:612:FAD:C2A	2.45	0.47
1:K:251:THR:HG23	1:K:260:PHE:CA	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189[B]:GLU:H	1:C:189[B]:GLU:CD	2.17	0.47
1:G:250:MET:CE	1:G:388:ALA:HB1	2.45	0.47
1:G:463:LEU:HB3	2:G:611:TPP:H61	1.96	0.47
1:I:226:ILE:HA	1:I:326:LYS:HG3	1.97	0.47
1:J:290:GLN:NE2	1:J:299:GLY:H	2.12	0.47
1:L:226:ILE:HA	1:L:326:LYS:HG3	1.97	0.47
1:A:359:PRO:HD2	1:A:530:GLU:OE2	2.15	0.47
1:E:207:MET:SD	1:E:231:VAL:HG22	2.55	0.47
1:K:226:ILE:HA	1:K:326:LYS:HG3	1.96	0.47
1:L:250:MET:CE	1:L:388:ALA:HB1	2.45	0.47
1:A:447:VAL:CG2	1:A:496:ILE:HD11	2.45	0.47
1:D:226:ILE:HA	1:D:326:LYS:HG3	1.96	0.47
1:H:290:GLN:NE2	1:H:299:GLY:H	2.13	0.47
1:B:226:ILE:HA	1:B:326:LYS:HG3	1.96	0.47
1:I:146:ARG:HD2	6:L:741:HOH:O	2.15	0.47
1:D:92:HIS:HE1	3:D:612:FAD:O2A	1.98	0.46
1:J:226:ILE:HA	1:J:326:LYS:HG3	1.96	0.46
6:A:739:HOH:O	1:C:90:ARG:HD2	2.15	0.46
1:F:389:ARG:NH1	1:F:534:ILE:HD11	2.30	0.46
1:K:207:MET:SD	1:K:231:VAL:HG22	2.55	0.46
1:D:128:CYS:C	1:D:129:GLU:HG2	2.35	0.46
1:K:250:MET:CE	1:K:388:ALA:HB1	2.45	0.46
1:H:207:MET:SD	1:H:231:VAL:HG22	2.55	0.46
1:I:311:ASP:HA	3:I:612:FAD:N1A	2.30	0.46
2:L:611:TPP:H2	2:L:611:TPP:HN42	1.81	0.46
1:C:111:TYR:O	1:D:90:ARG:NH2	2.48	0.46
1:G:482:LEU:HA	1:H:448:GLN:NE2	2.31	0.46
1:L:463:LEU:HB3	2:L:611:TPP:H61	1.98	0.46
1:D:285:ASP:OD1	1:D:285:ASP:N	2.47	0.46
1:D:433:ASP:OD2	1:D:482:LEU:HD12	2.16	0.46
1:E:351:LYS:HG2	1:E:351:LYS:HZ2	1.81	0.46
1:F:132:SER:HB3	1:H:132:SER:HB3	1.98	0.46
1:D:311:ASP:HA	3:D:612:FAD:N1A	2.31	0.46
1:A:290:GLN:NE2	1:A:299:GLY:H	2.14	0.46
1:I:62:GLN:HG2	1:I:400:LEU:HD22	1.98	0.46
1:A:173:THR:HB	5:A:618:PO4:O1	2.16	0.46
1:A:257:SER:HA	1:A:260[B]:PHE:HD2	1.78	0.46
1:E:250:MET:CE	1:E:388:ALA:HB1	2.46	0.46
1:G:482:LEU:HA	1:H:448:GLN:HE22	1.81	0.46
1:C:437:SER:O	1:D:441:GLY:HA3	2.17	0.45
1:D:207:MET:SD	1:D:231:VAL:HG22	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:207:MET:SD	1:J:231:VAL:HG22	2.56	0.45
1:C:184[A]:VAL:HG23	1:C:311:ASP:CB	2.41	0.45
1:I:250:MET:CE	1:I:388:ALA:HB1	2.46	0.45
1:A:90:ARG:NH2	1:B:111:TYR:O	2.50	0.45
1:C:226:ILE:HA	1:C:326:LYS:HG3	1.97	0.45
1:D:256:PHE:HA	5:D:618:PO4:O1	2.16	0.45
1:E:226:ILE:HA	1:E:326:LYS:HG3	1.97	0.45
1:F:146:ARG:HD2	6:L:923:HOH:O	2.15	0.45
1:J:482:LEU:O	1:J:483:HIS:C	2.53	0.45
1:B:463:LEU:HB3	2:B:611:TPP:H61	1.98	0.45
1:C:2:LYS:O	1:C:2:LYS:HG3	2.16	0.45
1:L:383:PRO:HD3	2:L:611:TPP:O1B	2.17	0.45
1:A:441:GLY:HA3	1:B:437:SER:O	2.16	0.45
1:I:111:TYR:O	1:J:90:ARG:NH2	2.49	0.45
1:J:62:GLN:HG2	1:J:400:LEU:HD22	1.99	0.45
1:C:483:HIS:H	1:D:448:GLN:NE2	2.13	0.45
1:D:382:THR:N	1:D:383:PRO:CD	2.79	0.45
1:F:62:GLN:HG2	1:F:400:LEU:HD22	1.99	0.45
1:F:351:LYS:CD	1:F:351:LYS:HB2	2.45	0.45
1:K:447:VAL:CG2	1:K:496:ILE:HD11	2.46	0.45
1:D:62:GLN:HG2	1:D:400:LEU:HD22	1.99	0.45
1:D:250:MET:CE	1:D:388:ALA:HB1	2.47	0.45
1:A:408:MET:SD	2:A:611:TPP:HM42	2.57	0.45
1:A:448:GLN:HE21	1:B:483:HIS:N	2.07	0.45
1:J:533:ALA:C	1:J:534:ILE:HG13	2.37	0.45
1:L:293:ILE:HG12	3:L:612:FAD:C4A	2.47	0.45
1:F:90:ARG:HD2	6:L:737:HOH:O	2.16	0.45
1:G:448:GLN:HE21	1:H:483:HIS:N	2.09	0.45
1:B:447:VAL:CG2	1:B:496:ILE:HD11	2.46	0.45
1:C:184[A]:VAL:CG2	1:C:311:ASP:HB3	2.42	0.45
1:G:293:ILE:HG12	3:G:612:FAD:C4A	2.47	0.45
1:L:290:GLN:NE2	1:L:299:GLY:H	2.14	0.45
1:B:250:MET:CE	1:B:388:ALA:HB1	2.47	0.44
1:E:92:HIS:CE1	3:E:612:FAD:O2A	2.68	0.44
3:H:612:FAD:H1'1	3:H:612:FAD:H9	1.84	0.44
1:I:13:LEU:O	1:I:18:VAL:HG13	2.17	0.44
3:I:612:FAD:H9	3:I:612:FAD:H1'1	1.79	0.44
1:J:250:MET:CE	1:J:388:ALA:HB1	2.47	0.44
1:K:13:LEU:O	1:K:18:VAL:HG13	2.17	0.44
1:K:462:VAL:HG23	1:K:480:THR:HG22	1.96	0.44
1:L:462:VAL:HG23	1:L:480:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ARG:HH12	1:D:122[A]:ARG:HH22	1.64	0.44
1:D:13:LEU:O	1:D:18:VAL:HG13	2.17	0.44
1:F:509:GLU:OE2	1:F:513:ARG:CD	2.65	0.44
1:H:293:ILE:HG12	3:H:612:FAD:C4A	2.47	0.44
1:L:389:ARG:NH1	1:L:534:ILE:HD11	2.33	0.44
1:L:447:VAL:CG2	1:L:496:ILE:HD11	2.45	0.44
1:D:290:GLN:NE2	1:D:299:GLY:H	2.15	0.44
1:E:447:VAL:CG2	1:E:496:ILE:HD11	2.46	0.44
2:K:611:TPP:H2	2:K:611:TPP:N4'	2.26	0.44
1:L:311:ASP:HA	3:L:612:FAD:N1A	2.32	0.44
1:B:251:THR:HB	1:B:252:GLY:H	1.56	0.44
1:C:37:ASN:HD22	1:C:37:ASN:HA	1.69	0.44
1:A:343[A]:ARG:NH2	5:A:616:PO4:P	2.91	0.44
1:C:447:VAL:CG2	1:C:496:ILE:HD11	2.46	0.44
1:E:62:GLN:HG2	1:E:400:LEU:HD22	1.98	0.44
1:F:13:LEU:O	1:F:18:VAL:HG13	2.18	0.44
1:F:251:THR:HB	1:F:252:GLY:H	1.54	0.44
1:F:293:ILE:HG12	3:F:612:FAD:C4A	2.48	0.44
1:K:30:ASN:O	1:K:34:ASP:HB2	2.17	0.44
1:K:483:HIS:CD2	6:K:687:HOH:O	2.69	0.44
1:C:250:MET:CE	1:C:388:ALA:HB1	2.48	0.44
1:F:447:VAL:CG2	1:F:496:ILE:HD11	2.47	0.44
1:G:62:GLN:HG2	1:G:400:LEU:HD22	1.99	0.44
1:G:382:THR:N	1:G:383:PRO:CD	2.81	0.44
1:H:447:VAL:CG2	1:H:496:ILE:HD11	2.46	0.44
1:K:382:THR:N	1:K:383:PRO:CD	2.81	0.44
1:A:341:ASP:HB3	1:A:537:GLN:HB2	1.99	0.44
1:A:433:ASP:OD2	1:A:482:LEU:HD12	2.17	0.44
2:A:611:TPP:H7'2	5:B:614:PO4:O4	2.18	0.44
1:C:311:ASP:HA	3:C:612:FAD:N1A	2.32	0.44
1:C:441:GLY:HA3	1:D:437:SER:O	2.18	0.44
1:E:437:SER:O	1:F:441:GLY:HA3	2.18	0.44
1:F:251:THR:HG23	1:F:260:PHE:CA	2.41	0.44
1:J:234:LEU:HB3	3:J:612:FAD:H1'2	2.00	0.44
1:C:62:GLN:HG2	1:C:400:LEU:HD22	2.00	0.44
1:E:509:GLU:OE2	1:E:513[A]:ARG:NE	2.49	0.44
2:E:611:TPP:N1'	1:F:50:GLU:OE2	2.51	0.44
1:G:311:ASP:OD2	1:G:314[A]:SER:HB3	2.17	0.44
1:H:250:MET:CE	1:H:388:ALA:HB1	2.48	0.44
1:E:152:ARG:HE	1:E:152:ARG:HB2	1.69	0.43
1:E:382:THR:N	1:E:383:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:612:FAD:H9	3:K:612:FAD:H1'1	1.77	0.43
1:F:248:VAL:O	1:F:248:VAL:CG1	2.66	0.43
1:J:373:ASP:O	1:J:425:ARG:NH1	2.45	0.43
1:J:382:THR:N	1:J:383:PRO:CD	2.80	0.43
1:J:437:SER:HA	1:J:440:MET:HB2	2.01	0.43
1:K:279:ARG:NH1	1:L:106:GLU:OE2	2.51	0.43
1:D:532:LEU:O	1:D:532:LEU:CD1	2.65	0.43
1:G:184[A]:VAL:HG23	1:G:310:GLY:HA2	2.00	0.43
1:I:196:GLN:O	1:I:199:ARG:HB3	2.18	0.43
1:G:279:ARG:NH1	1:H:106:GLU:OE2	2.51	0.43
1:L:382:THR:N	1:L:383:PRO:CD	2.82	0.43
1:G:437:SER:HA	1:G:440:MET:HB2	2.01	0.43
1:B:2:LYS:HE3	1:B:2:LYS:HB2	1.65	0.43
1:G:128:CYS:C	1:G:129:GLU:HG2	2.39	0.43
1:I:382:THR:N	1:I:383:PRO:CD	2.82	0.43
1:L:275:GLN:O	1:L:276:PHE:C	2.57	0.43
6:A:644:HOH:O	1:D:329:ARG:HA	2.18	0.43
1:B:62:GLN:HG2	1:B:400:LEU:HD22	1.99	0.43
1:H:62:GLN:HG2	1:H:400:LEU:HD22	2.00	0.43
1:A:128:CYS:C	1:A:129:GLU:HG2	2.39	0.43
1:E:34:ASP:O	1:E:38:ARG:HG3	2.19	0.43
1:F:250:MET:CE	1:F:388:ALA:HB1	2.49	0.43
1:G:447:VAL:CG2	1:G:496:ILE:HD11	2.45	0.43
1:I:437:SER:HA	1:I:440:MET:HB2	2.00	0.43
1:K:128:CYS:C	1:K:129:GLU:HG2	2.39	0.43
1:A:106:GLU:OE2	1:B:279:ARG:NH1	2.52	0.43
1:B:293:ILE:HG12	3:B:612:FAD:C4A	2.49	0.43
1:F:311:ASP:HA	3:F:612:FAD:N1A	2.34	0.43
1:H:251:THR:HB	1:H:252:GLY:H	1.55	0.43
1:J:13:LEU:O	1:J:18:VAL:HG13	2.19	0.43
1:K:62:GLN:HG2	1:K:400:LEU:HD22	1.99	0.43
1:A:62:GLN:HG2	1:A:400:LEU:HD22	2.01	0.42
1:A:173:THR:HG21	1:D:303:LYS:HD3	2.01	0.42
1:A:382:THR:N	1:A:383:PRO:CD	2.82	0.42
1:F:235:ARG:HB2	3:F:612:FAD:O1P	2.19	0.42
1:C:373:ASP:O	1:C:425:ARG:NH1	2.46	0.42
1:H:382:THR:N	1:H:383:PRO:CD	2.82	0.42
1:I:529:LYS:H	1:I:529:LYS:HG2	1.54	0.42
1:K:183:VAL:HA	6:L:856:HOH:O	2.19	0.42
1:B:382:THR:N	1:B:383:PRO:CD	2.82	0.42
2:D:611:TPP:H2	2:D:611:TPP:HN42	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:62:GLN:HG2	1:L:400:LEU:HD22	2.01	0.42
1:E:111:TYR:O	1:F:90:ARG:NH2	2.52	0.42
1:A:339:TYR:OH	1:A:343[B]:ARG:NH2	2.47	0.42
1:E:52:VAL:HG13	1:E:413:PRO:HB3	2.01	0.42
1:G:275:GLN:O	1:G:276:PHE:C	2.57	0.42
1:G:285:ASP:OD1	1:G:285:ASP:N	2.42	0.42
1:H:437:SER:HA	1:H:440:MET:HB2	2.00	0.42
1:B:275:GLN:O	1:B:276:PHE:C	2.58	0.42
1:E:311:ASP:HA	3:E:612:FAD:N1A	2.35	0.42
1:J:311:ASP:HA	3:J:612:FAD:N1A	2.34	0.42
1:A:437:SER:HA	1:A:440:MET:HB2	2.02	0.42
1:D:52:VAL:HG13	1:D:413:PRO:HB3	2.01	0.42
1:E:293:ILE:HG12	3:E:612:FAD:C4A	2.48	0.42
1:H:13:LEU:O	1:H:18:VAL:HG13	2.19	0.42
1:H:275:GLN:O	1:H:276:PHE:C	2.57	0.42
1:I:433:ASP:OD2	1:I:482:LEU:HD12	2.19	0.42
3:J:612:FAD:H1'1	3:J:612:FAD:H9	1.78	0.42
1:L:437:SER:HA	1:L:440:MET:HB2	2.02	0.42
6:A:735:HOH:O	1:I:235:ARG:HD2	2.20	0.42
1:B:13:LEU:O	1:B:18:VAL:HG13	2.19	0.42
1:E:419:GLN:HG2	1:E:451:LEU:HB3	2.02	0.42
1:K:189:GLU:HA	1:K:192[B]:ARG:CZ	2.49	0.42
3:F:612:FAD:H9	3:F:612:FAD:H1'1	1.63	0.42
1:G:111:TYR:O	1:H:90:ARG:NH2	2.53	0.42
1:I:48:ARG:HA	1:I:48:ARG:HD3	1.85	0.42
1:I:392:LYS:CE	6:L:931:HOH:O	2.59	0.42
1:A:419:GLN:HG2	1:A:451:LEU:HB3	2.02	0.42
1:A:499:ILE:CD1	1:A:513[B]:ARG:HD3	2.50	0.42
1:F:382:THR:N	1:F:383:PRO:CD	2.83	0.42
2:I:611:TPP:HN42	2:I:611:TPP:C2	2.31	0.42
1:J:52:VAL:HG13	1:J:413:PRO:HB3	2.01	0.42
1:J:416:LEU:HD12	1:J:416:LEU:HA	1.88	0.42
1:A:257:SER:O	1:A:260[B]:PHE:HB2	2.19	0.41
1:G:311:ASP:HA	3:G:612:FAD:N1A	2.35	0.41
1:J:293:ILE:HG12	3:J:612:FAD:C4A	2.50	0.41
1:E:373:ASP:O	1:E:425:ARG:NH1	2.47	0.41
1:G:373:ASP:O	1:G:425:ARG:NH1	2.48	0.41
1:A:463:LEU:HB3	2:A:611:TPP:H61	2.01	0.41
1:E:13:LEU:O	1:E:18:VAL:HG13	2.20	0.41
1:E:275:GLN:O	1:E:276:PHE:C	2.59	0.41
1:I:52:VAL:HG13	1:I:413:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:234:LEU:HB3	3:I:612:FAD:H1'2	2.02	0.41
1:B:360:GLN:HB2	1:B:390:TYR:CZ	2.56	0.41
1:D:447:VAL:CG2	1:D:496:ILE:HD11	2.47	0.41
1:F:437:SER:HA	1:F:440:MET:HB2	2.02	0.41
1:L:16:ALA:O	1:L:178[B]:HIS:HE1	2.02	0.41
1:A:293:ILE:HG12	3:A:612:FAD:C4A	2.50	0.41
1:A:343[A]:ARG:HH22	5:A:616:PO4:P	2.43	0.41
1:D:419:GLN:HG2	1:D:451:LEU:HB3	2.02	0.41
1:H:346:LEU:CD1	1:H:534:ILE:HD13	2.51	0.41
1:K:275:GLN:O	1:K:276:PHE:C	2.59	0.41
1:L:373:ASP:O	1:L:425:ARG:NH1	2.47	0.41
1:A:13:LEU:O	1:A:18:VAL:HG13	2.21	0.41
1:I:312:ILE:HG12	3:I:612:FAD:C2A	2.50	0.41
1:J:447:VAL:CG2	1:J:496:ILE:HD11	2.45	0.41
1:A:437:SER:O	1:B:441:GLY:HA3	2.20	0.41
1:C:382:THR:N	1:C:383:PRO:CD	2.83	0.41
1:H:419:GLN:HG2	1:H:451:LEU:HB3	2.03	0.41
1:I:447:VAL:CG2	1:I:496:ILE:HD11	2.46	0.41
1:I:533:ALA:C	1:I:534:ILE:HG13	2.41	0.41
1:G:13:LEU:O	1:G:18:VAL:HG13	2.20	0.41
1:G:419:GLN:HG2	1:G:451:LEU:HB3	2.02	0.41
1:L:35:SER:O	1:L:39:MET:HB2	2.21	0.41
1:B:437:SER:HA	1:B:440:MET:HB2	2.02	0.41
1:C:13:LEU:O	1:C:18:VAL:HG13	2.21	0.41
1:E:175:HIS:CD2	6:H:657:HOH:O	2.73	0.41
1:F:52:VAL:HG13	1:F:413:PRO:HB3	2.03	0.41
1:I:275:GLN:O	1:I:276:PHE:C	2.59	0.41
2:K:611:TPP:N1'	1:L:50:GLU:OE2	2.54	0.41
1:C:275:GLN:O	1:C:276:PHE:C	2.58	0.41
1:E:235:ARG:NH2	6:E:1269:HOH:O	2.44	0.41
1:E:279:ARG:NH1	1:F:106:GLU:OE2	2.53	0.41
1:I:35:SER:O	1:I:39:MET:HB2	2.20	0.41
1:J:74:CYS:HA	1:J:100:ALA:O	2.21	0.41
1:C:48:ARG:HD3	1:C:48:ARG:HA	1.85	0.40
1:D:48:ARG:HA	1:D:48:ARG:HD3	1.87	0.40
1:E:287:LYS:HE3	1:E:287:LYS:HB2	1.71	0.40
1:G:292:ASP:OD1	3:G:612:FAD:O2B	2.39	0.40
1:L:419:GLN:HG2	1:L:451:LEU:HB3	2.03	0.40
1:B:128:CYS:C	1:B:129[A]:GLU:HG2	2.41	0.40
1:C:437:SER:HA	1:C:440:MET:HB2	2.04	0.40
2:C:611:TPP:H2	2:C:611:TPP:HN42	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:TYR:CZ	1:D:129:GLU:HG3	2.55	0.40
1:D:275:GLN:O	1:D:276:PHE:C	2.59	0.40
1:H:373:ASP:O	1:H:425:ARG:NH1	2.46	0.40
1:I:254:ILE:HG12	3:I:612:FAD:C4	2.51	0.40
1:L:28[B]:SER:OG	1:L:74:CYS:SG	2.59	0.40
1:B:48:ARG:HD3	1:B:48:ARG:HA	1.85	0.40
1:C:173:THR:HG22	6:C:619:HOH:O	2.15	0.40
1:K:337:GLU:OE1	1:K:340:ARG:NH2	2.52	0.40
1:B:74:CYS:HA	1:B:100:ALA:O	2.22	0.40
1:D:35:SER:O	1:D:39:MET:HB2	2.22	0.40
1:F:419:GLN:HG2	1:F:451:LEU:HB3	2.03	0.40
1:H:264:MET:HE3	6:L:647:HOH:O	2.21	0.40
1:L:416:LEU:HD12	1:L:416:LEU:HA	1.88	0.40
1:C:419:GLN:HG2	1:C:451:LEU:HB3	2.03	0.40
1:E:74:CYS:HA	1:E:100:ALA:O	2.22	0.40
1:E:533:ALA:O	1:E:535:PRO:HD3	2.21	0.40
3:G:612:FAD:H1'1	3:G:612:FAD:H9	1.76	0.40
1:I:293:ILE:HG12	3:I:612:FAD:C4A	2.52	0.40
1:K:122[B]:ARG:HG3	1:K:122[B]:ARG:NH1	2.37	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:GLU:OE1	1:L:200:TYR:OH[4_545]	1.76	0.44
1:A:344:LYS:NZ	1:L:330:LYS:CE[4_545]	1.92	0.28

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	535/549 (97%)	513 (96%)	22 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	525/549 (96%)	505 (96%)	20 (4%)	0	100	100
1	C	524/549 (95%)	509 (97%)	14 (3%)	1 (0%)	47	68
1	D	522/549 (95%)	503 (96%)	19 (4%)	0	100	100
1	E	521/549 (95%)	504 (97%)	17 (3%)	0	100	100
1	F	520/549 (95%)	502 (96%)	18 (4%)	0	100	100
1	G	517/549 (94%)	502 (97%)	15 (3%)	0	100	100
1	H	522/549 (95%)	507 (97%)	15 (3%)	0	100	100
1	I	521/549 (95%)	506 (97%)	15 (3%)	0	100	100
1	J	524/549 (95%)	507 (97%)	17 (3%)	0	100	100
1	K	524/549 (95%)	504 (96%)	19 (4%)	1 (0%)	47	68
1	L	527/549 (96%)	509 (97%)	18 (3%)	0	100	100
All	All	6282/6588 (95%)	6071 (97%)	209 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	484	ASP
1	K	479	GLY

### 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	434/439 (99%)	411 (95%)	23 (5%)	22	43
1	B	424/439 (97%)	401 (95%)	23 (5%)	22	42
1	C	423/439 (96%)	402 (95%)	21 (5%)	24	46
1	D	421/439 (96%)	401 (95%)	20 (5%)	25	48
1	E	420/439 (96%)	399 (95%)	21 (5%)	24	46
1	F	420/439 (96%)	400 (95%)	20 (5%)	25	48
1	G	417/439 (95%)	401 (96%)	16 (4%)	33	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	422/439 (96%)	397 (94%)	25 (6%)	19	37
1	I	420/439 (96%)	399 (95%)	21 (5%)	24	46
1	J	423/439 (96%)	402 (95%)	21 (5%)	24	46
1	K	424/439 (97%)	404 (95%)	20 (5%)	26	49
1	L	426/439 (97%)	407 (96%)	19 (4%)	27	51
All	All	5074/5268 (96%)	4824 (95%)	250 (5%)	25	47

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	34	ASP
1	A	122	ARG
1	A	126	HIS
1	A	146	ARG
1	A	173	THR
1	A	184	VAL
1	A	189	GLU
1	A	231	VAL
1	A	251	THR
1	A	256	PHE
1	A	287	LYS
1	A	311	ASP
1	A	343[A]	ARG
1	A	343[B]	ARG
1	A	346	LEU
1	A	354	GLU
1	A	360	GLN
1	A	425	ARG
1	A	461[A]	SER
1	A	461[B]	SER
1	A	489	ARG
1	A	509	GLU
1	B	122	ARG
1	B	126	HIS
1	B	146	ARG
1	B	173	THR
1	B	185	THR
1	B	189	GLU
1	B	231	VAL

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Mol	Chain	Res	Type
1	B	251	THR
1	B	256	PHE
1	B	284	THR
1	B	311	ASP
1	B	314	SER
1	B	326	LYS
1	B	338	ASP
1	B	343	ARG
1	B	346	LEU
1	B	354	GLU
1	B	360	GLN
1	B	425	ARG
1	B	484	ASP
1	B	489	ARG
1	B	509	GLU
1	B	534	ILE
1	C	2	LYS
1	C	28	SER
1	C	126	HIS
1	C	146	ARG
1	C	173	THR
1	C	185	THR
1	C	199	ARG
1	C	231	VAL
1	C	251	THR
1	C	256	PHE
1	C	311	ASP
1	C	326	LYS
1	C	346	LEU
1	C	354	GLU
1	C	360	GLN
1	C	372[A]	ASP
1	C	372[B]	ASP
1	C	425	ARG
1	C	489	ARG
1	C	509	GLU
1	C	529	LYS
1	D	2	LYS
1	D	3	GLN
1	D	34	ASP
1	D	146	ARG
1	D	173	THR

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Mol	Chain	Res	Type
1	D	184	VAL
1	D	185[A]	THR
1	D	185[B]	THR
1	D	231	VAL
1	D	251	THR
1	D	256	PHE
1	D	311	ASP
1	D	338	ASP
1	D	346	LEU
1	D	354	GLU
1	D	360	GLN
1	D	425	ARG
1	D	489	ARG
1	D	509	GLU
1	D	529	LYS
1	E	122	ARG
1	E	126	HIS
1	E	146	ARG
1	E	173	THR
1	E	185	THR
1	E	189	GLU
1	E	231	VAL
1	E	251	THR
1	E	256	PHE
1	E	284	THR
1	E	287	LYS
1	E	311	ASP
1	E	340	ARG
1	E	346	LEU
1	E	354	GLU
1	E	360	GLN
1	E	425	ARG
1	E	489	ARG
1	E	509	GLU
1	E	529	LYS
1	E	531	GLU
1	F	1	MET
1	F	34	ASP
1	F	122	ARG
1	F	146	ARG
1	F	173	THR
1	F	192	ARG

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Mol	Chain	Res	Type
1	F	231	VAL
1	F	248	VAL
1	F	251	THR
1	F	256	PHE
1	F	285	ASP
1	F	287	LYS
1	F	311	ASP
1	F	346	LEU
1	F	354	GLU
1	F	360	GLN
1	F	425	ARG
1	F	489	ARG
1	F	509	GLU
1	F	531	GLU
1	G	1	MET
1	G	146	ARG
1	G	173	THR
1	G	231	VAL
1	G	251	THR
1	G	256	PHE
1	G	311	ASP
1	G	340	ARG
1	G	346	LEU
1	G	354	GLU
1	G	360	GLN
1	G	425	ARG
1	G	453	VAL
1	G	489	ARG
1	G	509	GLU
1	G	513	ARG
1	H	1	MET
1	H	2	LYS
1	H	34	ASP
1	H	126	HIS
1	H	146	ARG
1	H	173	THR
1	H	184[A]	VAL
1	H	184[B]	VAL
1	H	185	THR
1	H	189	GLU
1	H	197	LEU
1	H	231	VAL

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Mol	Chain	Res	Type
1	H	248	VAL
1	H	251	THR
1	H	256	PHE
1	H	311	ASP
1	H	326	LYS
1	H	346	LEU
1	H	354	GLU
1	H	360	GLN
1	H	425	ARG
1	H	480	THR
1	H	489	ARG
1	H	509	GLU
1	H	529	LYS
1	I	126	HIS
1	I	146	ARG
1	I	152	ARG
1	I	173	THR
1	I	184	VAL
1	I	185	THR
1	I	231	VAL
1	I	251	THR
1	I	256	PHE
1	I	311	ASP
1	I	340	ARG
1	I	346	LEU
1	I	354	GLU
1	I	360	GLN
1	I	425	ARG
1	I	453	VAL
1	I	461	SER
1	I	480	THR
1	I	489	ARG
1	I	509	GLU
1	I	529	LYS
1	J	34	ASP
1	J	126	HIS
1	J	146	ARG
1	J	173	THR
1	J	184[A]	VAL
1	J	184[B]	VAL
1	J	197	LEU
1	J	231	VAL

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Mol	Chain	Res	Type
1	J	251	THR
1	J	256	PHE
1	J	287	LYS
1	J	311	ASP
1	J	326	LYS
1	J	343	ARG
1	J	346	LEU
1	J	354	GLU
1	J	360	GLN
1	J	425	ARG
1	J	453	VAL
1	J	489	ARG
1	J	509	GLU
1	K	34	ASP
1	K	126	HIS
1	K	146	ARG
1	K	173	THR
1	K	189	GLU
1	K	231	VAL
1	K	251	THR
1	K	256	PHE
1	K	284	THR
1	K	311	ASP
1	K	338	ASP
1	K	346	LEU
1	K	354	GLU
1	K	360	GLN
1	K	372	ASP
1	K	425	ARG
1	K	481	GLU
1	K	489	ARG
1	K	509	GLU
1	K	529	LYS
1	L	38	ARG
1	L	146	ARG
1	L	173	THR
1	L	184	VAL
1	L	197	LEU
1	L	231	VAL
1	L	251	THR
1	L	256	PHE
1	L	311	ASP

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Mol	Chain	Res	Type
1	L	326	LYS
1	L	343[A]	ARG
1	L	343[B]	ARG
1	L	346	LEU
1	L	354	GLU
1	L	360	GLN
1	L	425	ARG
1	L	489	ARG
1	L	509	GLU
1	L	529	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	37	ASN
1	A	275	GLN
1	A	290	GLN
1	A	364	GLN
1	A	365	GLN
1	A	448	GLN
1	A	537	GLN
1	B	151	ASN
1	B	275	GLN
1	B	290	GLN
1	B	364	GLN
1	B	365	GLN
1	B	448	GLN
1	C	3	GLN
1	C	37	ASN
1	C	151	ASN
1	C	178	HIS
1	C	275	GLN
1	C	290	GLN
1	C	364	GLN
1	C	365	GLN
1	C	448	GLN
1	D	3	GLN
1	D	37	ASN
1	D	92	HIS
1	D	151	ASN
1	D	290	GLN

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Mol	Chain	Res	Type
1	D	364	GLN
1	D	365	GLN
1	D	448	GLN
1	E	3	GLN
1	E	37	ASN
1	E	92	HIS
1	E	151	ASN
1	E	290	GLN
1	E	364	GLN
1	E	365	GLN
1	E	448	GLN
1	F	3	GLN
1	F	151	ASN
1	F	275	GLN
1	F	290	GLN
1	F	364	GLN
1	F	365	GLN
1	F	448	GLN
1	G	3	GLN
1	G	37	ASN
1	G	151	ASN
1	G	178	HIS
1	G	275	GLN
1	G	290	GLN
1	G	364	GLN
1	G	365	GLN
1	G	448	GLN
1	H	3	GLN
1	H	113	GLN
1	H	151	ASN
1	H	275	GLN
1	H	290	GLN
1	H	364	GLN
1	H	365	GLN
1	H	448	GLN
1	I	3	GLN
1	I	37	ASN
1	I	151	ASN
1	I	178	HIS
1	I	275	GLN
1	I	290	GLN
1	I	364	GLN

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Mol	Chain	Res	Type
1	I	365	GLN
1	I	448	GLN
1	J	151	ASN
1	J	275	GLN
1	J	290	GLN
1	J	364	GLN
1	J	365	GLN
1	J	448	GLN
1	K	3	GLN
1	K	37	ASN
1	K	92	HIS
1	K	151	ASN
1	K	290	GLN
1	K	364	GLN
1	K	365	GLN
1	K	448	GLN
1	L	3	GLN
1	L	151	ASN
1	L	275	GLN
1	L	290	GLN
1	L	364	GLN
1	L	365	GLN
1	L	448	GLN

### 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](#)

Of 72 ligands modelled in this entry, 12 are monoatomic - leaving 60 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FAD	F	612	-	51,58,58	1.13	3 (5%)	60,89,89	1.90	12 (20%)
3	FAD	K	612	-	51,58,58	0.96	3 (5%)	60,89,89	1.62	12 (20%)
3	FAD	A	612	-	51,58,58	1.05	4 (7%)	60,89,89	1.71	11 (18%)
3	FAD	C	612	-	51,58,58	1.05	2 (3%)	60,89,89	2.03	15 (25%)
5	PO4	C	614	-	4,4,4	0.78	0	6,6,6	1.78	2 (33%)
5	PO4	G	616	-	4,4,4	0.65	0	6,6,6	0.68	0
5	PO4	G	614	-	4,4,4	0.88	0	6,6,6	0.72	0
5	PO4	B	615	-	4,4,4	0.95	0	6,6,6	0.66	0
5	PO4	I	614	-	4,4,4	0.85	0	6,6,6	0.84	0
5	PO4	A	619	-	4,4,4	0.81	0	6,6,6	0.48	0
5	PO4	J	614	-	4,4,4	0.77	0	6,6,6	0.90	0
5	PO4	L	614	-	4,4,4	0.71	0	6,6,6	0.54	0
5	PO4	A	618	-	4,4,4	0.78	0	6,6,6	0.81	0
5	PO4	A	617	-	4,4,4	0.86	0	6,6,6	1.30	1 (16%)
2	TPP	A	611	4	22,27,27	1.32	3 (13%)	29,40,40	3.36	10 (34%)
5	PO4	F	614	-	4,4,4	0.67	0	6,6,6	0.88	0
5	PO4	E	614	-	4,4,4	0.81	0	6,6,6	0.42	0
2	TPP	I	611	4	22,27,27	1.08	2 (9%)	29,40,40	1.96	9 (31%)
5	PO4	L	615	-	4,4,4	0.59	0	6,6,6	1.00	0
5	PO4	C	615	-	4,4,4	0.60	0	6,6,6	0.70	0
5	PO4	B	614	-	4,4,4	0.38	0	6,6,6	1.57	1 (16%)
3	FAD	G	612	-	51,58,58	1.02	2 (3%)	60,89,89	1.71	13 (21%)
5	PO4	G	615	-	4,4,4	0.91	0	6,6,6	1.05	0
2	TPP	F	611	4	22,27,27	0.98	0	29,40,40	2.61	10 (34%)
2	TPP	K	611	4	22,27,27	1.40	2 (9%)	29,40,40	2.56	10 (34%)
2	TPP	C	611	4	22,27,27	0.95	1 (4%)	29,40,40	2.29	11 (37%)
3	FAD	E	612	-	51,58,58	1.15	4 (7%)	60,89,89	1.92	12 (20%)
5	PO4	L	617	-	4,4,4	0.70	0	6,6,6	0.89	0
5	PO4	H	614	-	4,4,4	0.50	0	6,6,6	0.70	0
3	FAD	J	612	-	51,58,58	0.96	3 (5%)	60,89,89	1.74	11 (18%)
2	TPP	E	611	4	22,27,27	0.91	1 (4%)	29,40,40	2.40	10 (34%)
3	FAD	D	612	-	51,58,58	1.21	6 (11%)	60,89,89	2.00	14 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FAD	L	612	-	51,58,58	1.02	4 (7%)	60,89,89	2.28	13 (21%)
5	PO4	A	616	-	4,4,4	1.03	0	6,6,6	0.79	0
5	PO4	L	616	-	4,4,4	0.91	0	6,6,6	0.75	0
5	PO4	K	614	-	4,4,4	0.69	0	6,6,6	1.44	2 (33%)
3	FAD	B	612	-	51,58,58	1.02	3 (5%)	60,89,89	1.89	16 (26%)
5	PO4	E	615	-	4,4,4	0.72	0	6,6,6	0.78	0
5	PO4	I	615	-	4,4,4	0.75	0	6,6,6	0.85	0
5	PO4	D	616	-	4,4,4	0.45	0	6,6,6	1.21	1 (16%)
3	FAD	H	612	-	51,58,58	1.20	6 (11%)	60,89,89	2.02	13 (21%)
2	TPP	B	611	4	22,27,27	1.17	2 (9%)	29,40,40	2.39	14 (48%)
5	PO4	A	614	-	4,4,4	0.69	0	6,6,6	1.39	1 (16%)
2	TPP	D	611	4	22,27,27	1.69	3 (13%)	29,40,40	2.15	10 (34%)
5	PO4	D	614	-	4,4,4	0.85	0	6,6,6	0.80	0
5	PO4	D	617	-	4,4,4	1.05	0	6,6,6	0.89	0
5	PO4	D	620	-	4,4,4	0.53	0	6,6,6	0.63	0
5	PO4	D	619	-	4,4,4	0.67	0	6,6,6	0.53	0
2	TPP	G	611	4	22,27,27	1.07	1 (4%)	29,40,40	2.55	13 (44%)
5	PO4	D	618	-	4,4,4	0.67	0	6,6,6	0.94	0
5	PO4	F	615	-	4,4,4	0.64	0	6,6,6	0.84	0
5	PO4	H	615	-	4,4,4	0.71	0	6,6,6	0.67	0
5	PO4	D	615	-	4,4,4	0.61	0	6,6,6	1.53	1 (16%)
5	PO4	A	615	-	4,4,4	0.79	0	6,6,6	0.73	0
2	TPP	J	611	4	22,27,27	1.12	2 (9%)	29,40,40	2.56	13 (44%)
5	PO4	B	616	-	4,4,4	0.66	0	6,6,6	0.65	0
2	TPP	L	611	4	22,27,27	1.88	1 (4%)	29,40,40	2.49	11 (37%)
3	FAD	I	612	-	51,58,58	1.22	6 (11%)	60,89,89	1.71	10 (16%)
5	PO4	L	618	-	4,4,4	0.87	0	6,6,6	0.44	0
2	TPP	H	611	4	22,27,27	0.87	1 (4%)	29,40,40	2.27	11 (37%)

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	F	612	-	-	9/30/50/50	0/6/6/6
3	FAD	K	612	-	-	9/30/50/50	0/6/6/6
3	FAD	A	612	-	-	5/30/50/50	0/6/6/6
3	FAD	C	612	-	-	11/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPP	A	611	4	-	4/16/17/17	0/2/2/2
2	TPP	I	611	4	-	5/16/17/17	0/2/2/2
3	FAD	G	612	-	-	11/30/50/50	0/6/6/6
2	TPP	F	611	4	-	6/16/17/17	0/2/2/2
2	TPP	K	611	4	-	1/8/17/17	-
2	TPP	C	611	4	-	4/16/17/17	0/2/2/2
3	FAD	E	612	-	-	8/30/50/50	0/6/6/6
3	FAD	J	612	-	-	9/30/50/50	0/6/6/6
2	TPP	E	611	4	-	6/16/17/17	0/2/2/2
3	FAD	D	612	-	-	8/30/50/50	0/6/6/6
3	FAD	L	612	-	-	9/30/50/50	0/6/6/6
3	FAD	B	612	-	-	10/30/50/50	0/6/6/6
3	FAD	H	612	-	-	9/30/50/50	0/6/6/6
2	TPP	B	611	4	-	5/16/17/17	0/2/2/2
2	TPP	D	611	4	-	6/16/17/17	0/2/2/2
2	TPP	G	611	4	-	3/16/17/17	0/2/2/2
2	TPP	J	611	4	-	5/16/17/17	0/2/2/2
2	TPP	L	611	4	-	5/16/17/17	0/2/2/2
3	FAD	I	612	-	-	9/30/50/50	0/6/6/6
2	TPP	H	611	4	-	5/16/17/17	0/2/2/2

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	611	TPP	C6-C5	-8.00	1.47	1.50
2	D	611	TPP	C4-N3	-5.94	1.34	1.39
2	K	611	TPP	C6-C5	-4.08	1.49	1.50
2	A	611	TPP	C6-C5	-4.06	1.49	1.50
3	E	612	FAD	C4X-C10	3.63	1.42	1.38
3	D	612	FAD	C4X-N5	3.61	1.38	1.33
3	F	612	FAD	C4X-N5	3.51	1.38	1.33
2	G	611	TPP	C4-N3	-3.47	1.36	1.39
3	G	612	FAD	C10-N1	3.36	1.37	1.33
3	D	612	FAD	C2B-C1B	-3.24	1.48	1.53
3	E	612	FAD	C10-N1	3.23	1.37	1.33
3	I	612	FAD	C4X-C10	3.23	1.42	1.38
2	J	611	TPP	C4-N3	-3.17	1.37	1.39
3	C	612	FAD	C6-C5X	-3.16	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	612	FAD	C4X-C10	3.13	1.41	1.38
3	H	612	FAD	C10-N1	3.12	1.37	1.33
3	I	612	FAD	O4B-C1B	3.11	1.45	1.41
2	C	611	TPP	C6-C5	-3.06	1.49	1.50
2	E	611	TPP	C4-N3	-3.05	1.37	1.39
3	I	612	FAD	C10-N1	3.02	1.37	1.33
3	H	612	FAD	C4X-N5	3.01	1.37	1.33
3	F	612	FAD	C2B-C1B	-2.95	1.49	1.53
2	I	611	TPP	C4-N3	-2.94	1.37	1.39
2	D	611	TPP	C6-C5	-2.90	1.49	1.50
3	H	612	FAD	C2B-C1B	-2.90	1.49	1.53
2	K	611	TPP	C4-N3	-2.90	1.37	1.39
2	B	611	TPP	C4-N3	-2.85	1.37	1.39
3	G	612	FAD	C2A-N3A	2.76	1.36	1.32
3	I	612	FAD	C4X-N5	2.73	1.37	1.33
3	E	612	FAD	C4X-N5	2.71	1.37	1.33
3	J	612	FAD	C9A-N10	-2.69	1.34	1.38
3	I	612	FAD	C2A-N3A	2.69	1.36	1.32
3	L	612	FAD	C2B-C1B	-2.66	1.49	1.53
3	I	612	FAD	C6-C5X	-2.66	1.37	1.41
3	K	612	FAD	C4X-C10	2.65	1.41	1.38
3	H	612	FAD	O4B-C1B	2.63	1.44	1.41
3	C	612	FAD	C10-N1	2.60	1.36	1.33
3	B	612	FAD	C2A-N3A	2.56	1.36	1.32
3	L	612	FAD	C2A-N3A	2.52	1.36	1.32
3	A	612	FAD	C6-C5X	-2.52	1.37	1.41
3	D	612	FAD	O4B-C1B	2.51	1.44	1.41
2	B	611	TPP	C2'-N1'	2.47	1.38	1.34
2	J	611	TPP	C5'-C4'	-2.38	1.38	1.42
2	I	611	TPP	C2'-N1'	2.38	1.38	1.34
3	E	612	FAD	O4B-C1B	2.37	1.44	1.41
2	H	611	TPP	C4-N3	-2.35	1.37	1.39
3	D	612	FAD	C2A-N3A	2.35	1.35	1.32
3	B	612	FAD	C9A-N10	-2.35	1.35	1.38
2	A	611	TPP	C2'-N3'	2.35	1.38	1.34
3	D	612	FAD	C2-N3	-2.34	1.33	1.38
2	D	611	TPP	C4'-N3'	2.31	1.38	1.35
3	L	612	FAD	C4X-N5	2.30	1.36	1.33
3	J	612	FAD	C9A-C5X	-2.24	1.38	1.42
3	K	612	FAD	C9A-N10	-2.23	1.35	1.38
3	J	612	FAD	C10-N1	2.21	1.36	1.33
3	B	612	FAD	C4X-N5	2.09	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	612	FAD	C10-N1	2.07	1.35	1.33
3	L	612	FAD	C4X-C10	2.06	1.40	1.38
3	K	612	FAD	C10-N1	2.06	1.35	1.33
3	H	612	FAD	C4X-C10	2.04	1.40	1.38
3	A	612	FAD	O4B-C1B	2.02	1.43	1.41
3	A	612	FAD	C4X-N5	2.02	1.36	1.33
3	D	612	FAD	C2-N1	-2.01	1.34	1.38
3	H	612	FAD	C9A-N10	-2.01	1.35	1.38
2	A	611	TPP	C2'-N1'	2.00	1.37	1.34

All (293) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	611	TPP	C6-C5-C4	13.35	138.15	127.43
3	L	612	FAD	C4-N3-C2	8.94	122.69	115.14
2	F	611	TPP	C6-C5-C4	8.41	134.19	127.43
3	E	612	FAD	C4-N3-C2	8.36	122.20	115.14
3	D	612	FAD	C4-N3-C2	7.97	121.88	115.14
2	G	611	TPP	C6-C5-C4	7.74	133.64	127.43
3	H	612	FAD	C4-N3-C2	7.68	121.63	115.14
2	L	611	TPP	CM4-C4-N3	7.18	131.69	122.53
3	F	612	FAD	C4-N3-C2	7.11	121.14	115.14
3	B	612	FAD	C4-N3-C2	6.97	121.03	115.14
2	A	611	TPP	CM4-C4-N3	6.96	131.41	122.53
2	E	611	TPP	C6-C5-C4	6.90	132.97	127.43
3	C	612	FAD	C4-N3-C2	6.69	120.79	115.14
2	J	611	TPP	C6-C5-C4	6.65	132.77	127.43
3	L	612	FAD	C10-C4X-N5	-6.41	116.82	121.26
3	I	612	FAD	C4-N3-C2	6.31	120.47	115.14
2	K	611	TPP	C6-C5-C4	6.24	132.44	127.43
3	G	612	FAD	C4-N3-C2	6.18	120.36	115.14
2	C	611	TPP	CM4-C4-N3	6.02	130.21	122.53
3	C	612	FAD	N3A-C2A-N1A	-5.95	119.37	128.68
3	J	612	FAD	C4-N3-C2	5.93	120.14	115.14
2	K	611	TPP	CM4-C4-N3	5.72	129.82	122.53
3	C	612	FAD	C10-C4X-N5	-5.71	117.31	121.26
3	A	612	FAD	N3A-C2A-N1A	-5.68	119.80	128.68
3	L	612	FAD	C1'-N10-C9A	5.41	122.55	118.29
3	E	612	FAD	N3A-C2A-N1A	-5.21	120.54	128.68
2	E	611	TPP	C5'-C7'-N3	-5.20	104.62	113.28
2	B	611	TPP	C5'-C7'-N3	-5.18	104.65	113.28
3	L	612	FAD	N3A-C2A-N1A	-5.14	120.65	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	611	TPP	C6-C5-C4	5.05	131.48	127.43
2	L	611	TPP	CM4-C4-C5	-4.99	116.68	127.60
2	J	611	TPP	CM2-C2'-N1'	4.96	122.59	117.14
2	A	611	TPP	CM4-C4-C5	-4.87	116.94	127.60
3	K	612	FAD	C10-C4X-N5	-4.87	117.89	121.26
3	F	612	FAD	C5X-C9A-N10	4.82	121.21	117.72
3	H	612	FAD	C1'-N10-C9A	4.73	122.02	118.29
2	J	611	TPP	CM4-C4-N3	4.73	128.56	122.53
3	B	612	FAD	C10-C4X-N5	-4.70	118.00	121.26
3	H	612	FAD	N3A-C2A-N1A	-4.70	121.34	128.68
3	A	612	FAD	C1'-N10-C9A	4.63	121.93	118.29
3	G	612	FAD	N3A-C2A-N1A	-4.61	121.48	128.68
2	H	611	TPP	C5'-C7'-N3	-4.57	105.67	113.28
3	I	612	FAD	N3A-C2A-N1A	-4.54	121.59	128.68
2	I	611	TPP	C6-C5-C4	4.53	131.06	127.43
3	J	612	FAD	N3A-C2A-N1A	-4.52	121.62	128.68
3	A	612	FAD	C4-N3-C2	4.51	118.95	115.14
3	F	612	FAD	N3A-C2A-N1A	-4.49	121.66	128.68
3	D	612	FAD	N3A-C2A-N1A	-4.47	121.69	128.68
3	H	612	FAD	C1B-N9A-C4A	-4.46	118.80	126.64
2	K	611	TPP	C6'-N1'-C2'	4.45	123.53	115.96
3	F	612	FAD	C4-C4X-C10	-4.44	117.01	119.95
3	H	612	FAD	C4-C4X-N5	4.44	123.68	118.60
2	C	611	TPP	C5'-C7'-N3	-4.37	106.01	113.28
2	H	611	TPP	CM4-C4-N3	4.29	127.99	122.53
2	B	611	TPP	CM4-C4-N3	4.28	127.99	122.53
2	D	611	TPP	CM4-C4-N3	4.28	127.98	122.53
2	K	611	TPP	C5'-C7'-N3	-4.27	106.17	113.28
3	D	612	FAD	C10-C4X-N5	-4.25	118.32	121.26
2	H	611	TPP	C6-C5-C4	4.23	130.83	127.43
3	L	612	FAD	C9A-N10-C10	-4.23	116.37	121.91
2	E	611	TPP	CM4-C4-N3	4.22	127.91	122.53
2	D	611	TPP	C6'-N1'-C2'	4.15	123.03	115.96
3	K	612	FAD	N3A-C2A-N1A	-4.14	122.21	128.68
3	L	612	FAD	C4-C4X-N5	4.11	123.30	118.60
2	F	611	TPP	CM4-C4-N3	4.11	127.77	122.53
2	D	611	TPP	CM2-C2'-N3'	4.09	123.54	117.15
3	A	612	FAD	C10-C4X-N5	-4.09	118.43	121.26
3	J	612	FAD	C1'-N10-C9A	4.09	121.51	118.29
3	G	612	FAD	C10-C4X-N5	-4.07	118.44	121.26
2	F	611	TPP	C5'-C7'-N3	-4.05	106.53	113.28
2	B	611	TPP	C6'-N1'-C2'	4.02	122.81	115.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	612	FAD	C4-C4X-C10	-4.00	117.31	119.95
2	G	611	TPP	CM4-C4-N3	3.98	127.61	122.53
3	B	612	FAD	N3A-C2A-N1A	-3.98	122.46	128.68
3	K	612	FAD	C1'-N10-C9A	3.96	121.41	118.29
3	L	612	FAD	C4X-C4-N3	-3.94	118.05	123.43
3	D	612	FAD	C4-C4X-N5	3.94	123.10	118.60
2	H	611	TPP	C6'-N1'-C2'	3.90	122.60	115.96
3	E	612	FAD	C5X-C9A-N10	3.89	120.54	117.72
3	C	612	FAD	C4X-C4-N3	-3.89	118.11	123.43
3	I	612	FAD	C4X-C4-N3	-3.85	118.17	123.43
2	C	611	TPP	CM4-C4-C5	-3.77	119.35	127.60
2	B	611	TPP	N1'-C2'-N3'	-3.76	119.06	125.54
3	F	612	FAD	C9A-N10-C10	-3.76	116.99	121.91
2	L	611	TPP	C6'-N1'-C2'	3.74	122.33	115.96
2	A	611	TPP	C5'-C7'-N3	-3.74	107.05	113.28
3	K	612	FAD	C9A-N10-C10	-3.73	117.02	121.91
3	H	612	FAD	C1'-N10-C10	-3.73	115.07	118.41
3	D	612	FAD	C9A-N10-C10	-3.73	117.03	121.91
2	F	611	TPP	CM2-C2'-N1'	3.72	121.23	117.14
2	L	611	TPP	C6-C5-C4	3.70	130.40	127.43
2	J	611	TPP	CM4-C4-C5	-3.69	119.53	127.60
3	J	612	FAD	C10-C4X-N5	-3.69	118.71	121.26
2	J	611	TPP	C5'-C6'-N1'	-3.66	117.72	123.82
3	D	612	FAD	C5X-C9A-N10	3.66	120.36	117.72
2	L	611	TPP	C5'-C7'-N3	-3.65	107.20	113.28
2	C	611	TPP	C6-C5-C4	3.62	130.34	127.43
2	I	611	TPP	C6'-C5'-C4'	3.62	120.65	115.72
3	C	612	FAD	C1'-N10-C9A	3.61	121.14	118.29
2	K	611	TPP	C5'-C6'-N1'	-3.60	117.82	123.82
3	B	612	FAD	C4X-C4-N3	-3.58	118.53	123.43
2	G	611	TPP	N1'-C2'-N3'	-3.58	119.38	125.54
3	B	612	FAD	C1'-N10-C9A	3.57	121.10	118.29
3	D	612	FAD	C4X-C4-N3	-3.57	118.55	123.43
3	C	612	FAD	C4X-N5-C5X	3.56	120.33	116.77
3	D	612	FAD	O4B-C1B-C2B	-3.56	101.73	106.93
2	E	611	TPP	C6'-N1'-C2'	3.54	121.98	115.96
2	D	611	TPP	C5'-C7'-N3	-3.52	107.42	113.28
2	F	611	TPP	CM4-C4-C5	-3.50	119.96	127.60
2	G	611	TPP	C5'-C7'-N3	-3.49	107.46	113.28
2	H	611	TPP	N1'-C2'-N3'	-3.49	119.54	125.54
2	E	611	TPP	CM4-C4-C5	-3.48	119.99	127.60
2	J	611	TPP	C6'-N1'-C2'	3.45	121.83	115.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	612	FAD	O4'-C4'-C5'	-3.43	102.20	109.92
2	G	611	TPP	O3B-PB-O2B	3.43	120.75	107.64
3	D	612	FAD	C1'-N10-C9A	3.42	120.98	118.29
3	K	612	FAD	C4-C4X-N5	3.40	122.48	118.60
3	J	612	FAD	C4-C4X-N5	3.37	122.45	118.60
2	K	611	TPP	C7'-N3-C2	-3.37	119.27	125.35
2	D	611	TPP	C5'-C6'-N1'	-3.31	118.31	123.82
3	I	612	FAD	C1'-N10-C9A	3.30	120.89	118.29
2	K	611	TPP	N1'-C2'-N3'	-3.29	119.87	125.54
2	I	611	TPP	CM4-C4-N3	3.29	126.72	122.53
3	B	612	FAD	C4-C4X-N5	3.28	122.34	118.60
3	E	612	FAD	C4X-C4-N3	-3.26	118.97	123.43
3	K	612	FAD	C4-N3-C2	3.26	117.89	115.14
2	F	611	TPP	C2'-N3'-C4'	3.26	123.16	118.08
3	H	612	FAD	C10-C4X-N5	-3.25	119.01	121.26
2	J	611	TPP	C5'-C7'-N3	-3.23	107.91	113.28
2	L	611	TPP	N1'-C2'-N3'	-3.22	119.99	125.54
2	G	611	TPP	C6'-N1'-C2'	3.22	121.45	115.96
3	G	612	FAD	O2P-P-O1P	3.21	128.10	112.24
2	K	611	TPP	CM4-C4-C5	-3.16	120.70	127.60
2	G	611	TPP	CM4-C4-C5	-3.14	120.74	127.60
2	H	611	TPP	CM4-C4-C5	-3.12	120.78	127.60
2	A	611	TPP	C7'-N3-C2	-3.11	119.73	125.35
3	F	612	FAD	C1'-N10-C10	3.08	121.17	118.41
2	L	611	TPP	CM2-C2'-N1'	3.08	120.53	117.14
2	C	611	TPP	PA-O3A-PB	-3.08	122.26	132.83
3	E	612	FAD	C9A-N10-C10	-3.07	117.89	121.91
2	H	611	TPP	CM2-C2'-N3'	3.07	121.94	117.15
3	I	612	FAD	C10-C4X-N5	-3.06	119.14	121.26
2	K	611	TPP	C6'-C5'-C4'	3.06	119.88	115.72
3	C	612	FAD	C4-C4X-N5	3.06	122.09	118.60
3	A	612	FAD	C4-C4X-N5	3.04	122.07	118.60
3	I	612	FAD	C9A-N10-C10	-3.03	117.94	121.91
2	F	611	TPP	N1'-C2'-N3'	-3.03	120.33	125.54
2	I	611	TPP	CM2-C2'-N1'	3.03	120.47	117.14
2	F	611	TPP	PA-O3A-PB	-3.02	122.45	132.83
3	A	612	FAD	C1'-C2'-C3'	3.00	118.17	109.79
2	L	611	TPP	C5'-C6'-N1'	-2.99	118.84	123.82
3	I	612	FAD	C5X-C9A-N10	2.98	119.87	117.72
5	B	614	PO4	O4-P-O2	2.93	117.38	107.97
3	I	612	FAD	C4A-C5A-N7A	-2.93	106.34	109.40
3	E	612	FAD	C1'-N10-C9A	2.93	120.60	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	611	TPP	N1'-C2'-N3'	-2.92	120.51	125.54
2	J	611	TPP	PA-O3A-PB	-2.92	122.82	132.83
2	B	611	TPP	CM4-C4-C5	-2.88	121.31	127.60
2	B	611	TPP	CM2-C2'-N1'	2.87	120.29	117.14
2	I	611	TPP	C5'-C7'-N3	-2.86	108.52	113.28
3	G	612	FAD	C9A-N10-C10	-2.86	118.17	121.91
2	C	611	TPP	C7'-N3-C2	-2.85	120.19	125.35
3	E	612	FAD	C4-C4X-N5	2.83	121.84	118.60
3	B	612	FAD	O2P-P-O1P	2.82	126.18	112.24
5	C	614	PO4	O4-P-O1	2.81	121.20	110.89
2	I	611	TPP	C5'-C6'-N1'	-2.81	119.14	123.82
2	J	611	TPP	N1'-C2'-N3'	-2.81	120.71	125.54
3	F	612	FAD	C1'-C2'-C3'	2.78	117.55	109.79
5	D	615	PO4	O3-P-O2	2.77	116.86	107.97
3	K	612	FAD	O2P-P-O1P	2.76	125.87	112.24
3	L	612	FAD	C1'-C2'-C3'	2.75	117.49	109.79
2	C	611	TPP	C6'-N1'-C2'	2.75	120.65	115.96
2	E	611	TPP	N1'-C2'-N3'	-2.74	120.82	125.54
3	G	612	FAD	C4-C4X-N5	2.74	121.72	118.60
2	F	611	TPP	O3B-PB-O2B	2.73	118.08	107.64
2	E	611	TPP	C5'-C6'-N1'	-2.73	119.27	123.82
2	J	611	TPP	C7'-N3-C2	-2.73	120.42	125.35
2	G	611	TPP	O3B-PB-O3A	-2.73	95.49	104.64
3	E	612	FAD	C5'-C4'-C3'	-2.73	106.94	112.20
3	A	612	FAD	O3B-C3B-C4B	-2.72	103.19	111.05
3	C	612	FAD	C7-C6-C5X	-2.71	117.38	121.22
3	B	612	FAD	C4X-N5-C5X	2.71	119.48	116.77
2	A	611	TPP	C6'-N1'-C2'	2.70	120.56	115.96
2	H	611	TPP	C5'-C6'-N1'	-2.70	119.32	123.82
2	B	611	TPP	C7'-N3-C2	-2.70	120.48	125.35
3	L	612	FAD	C9A-C5X-N5	-2.69	118.16	122.36
3	H	612	FAD	C5'-C4'-C3'	-2.69	107.01	112.20
2	I	611	TPP	CM4-C4-C5	-2.68	121.74	127.60
3	B	612	FAD	O4B-C1B-C2B	-2.66	103.04	106.93
3	J	612	FAD	O2P-P-O1P	2.65	125.36	112.24
2	D	611	TPP	C6'-C5'-C4'	2.64	119.32	115.72
2	A	611	TPP	N1'-C2'-N3'	-2.64	121.00	125.54
3	F	612	FAD	C1B-N9A-C4A	-2.64	122.01	126.64
3	F	612	FAD	O2P-P-O1P	2.63	125.24	112.24
3	J	612	FAD	C4X-C4-N3	-2.62	119.84	123.43
3	E	612	FAD	C1'-C2'-C3'	2.59	117.03	109.79
3	C	612	FAD	C6-C5X-C9A	2.59	122.44	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	612	FAD	O5B-C5B-C4B	-2.59	100.09	108.99
2	A	611	TPP	PA-O3A-PB	-2.57	124.02	132.83
2	C	611	TPP	C7'-C5'-C6'	-2.56	115.81	120.69
2	B	611	TPP	C5'-C6'-N1'	-2.55	119.58	123.82
3	L	612	FAD	O2'-C2'-C1'	-2.53	103.50	109.59
2	E	611	TPP	PA-O3A-PB	-2.53	124.14	132.83
5	A	617	PO4	O3-P-O2	2.53	116.08	107.97
2	K	611	TPP	CM2-C2'-N3'	2.51	121.08	117.15
3	A	612	FAD	C9A-N10-C10	-2.51	118.62	121.91
2	B	611	TPP	C6'-C5'-C4'	2.49	119.11	115.72
2	D	611	TPP	CM4-C4-C5	-2.49	122.15	127.60
2	I	611	TPP	PA-O3A-PB	-2.48	124.31	132.83
3	C	612	FAD	O4B-C1B-C2B	-2.48	103.30	106.93
3	J	612	FAD	C1'-C2'-C3'	2.48	116.71	109.79
2	B	611	TPP	O2B-PB-O1B	2.47	120.36	110.68
2	J	611	TPP	C6'-C5'-C4'	2.46	119.06	115.72
5	A	614	PO4	O2-P-O1	2.43	119.80	110.89
3	E	612	FAD	C1B-N9A-C4A	-2.43	122.38	126.64
2	D	611	TPP	C7'-C5'-C6'	-2.42	116.06	120.69
3	K	612	FAD	C4A-C5A-N7A	-2.42	106.88	109.40
3	F	612	FAD	O4B-C1B-C2B	-2.41	103.40	106.93
2	G	611	TPP	C2'-N3'-C4'	2.41	121.84	118.08
2	G	611	TPP	CM2-C2'-N1'	2.41	119.79	117.14
3	F	612	FAD	C4-C4X-N5	2.40	121.34	118.60
3	H	612	FAD	C4A-C5A-N7A	-2.39	106.91	109.40
3	I	612	FAD	C1B-N9A-C4A	-2.39	122.45	126.64
2	H	611	TPP	PA-O3A-PB	-2.38	124.64	132.83
2	E	611	TPP	CM2-C2'-N1'	2.38	119.75	117.14
3	B	612	FAD	O3'-C3'-C2'	-2.38	103.07	108.81
3	K	612	FAD	C5X-C9A-N10	2.37	119.44	117.72
3	B	612	FAD	C3B-C2B-C1B	2.37	104.54	100.98
3	D	612	FAD	C1'-C2'-C3'	2.37	116.40	109.79
3	G	612	FAD	C1'-C2'-C3'	2.36	116.39	109.79
3	D	612	FAD	C5'-C4'-C3'	-2.36	107.64	112.20
2	G	611	TPP	CM2-C2'-N3'	2.35	120.83	117.15
2	F	611	TPP	C5-C4-N3	2.35	112.27	107.57
3	G	612	FAD	O5'-C5'-C4'	-2.34	103.12	109.36
2	A	611	TPP	O3B-PB-O1B	2.34	119.83	110.68
3	E	612	FAD	C4-C4X-C10	-2.33	118.41	119.95
2	I	611	TPP	C6'-N1'-C2'	2.32	119.91	115.96
2	A	611	TPP	C6'-C5'-C4'	2.32	118.87	115.72
2	J	611	TPP	O3B-PB-O3A	-2.31	96.87	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	612	FAD	O4B-C1B-C2B	-2.30	103.56	106.93
3	L	612	FAD	C1B-N9A-C4A	-2.30	122.60	126.64
2	E	611	TPP	C5-C4-N3	2.26	112.10	107.57
3	J	612	FAD	P-O3P-PA	-2.26	125.06	132.83
3	C	612	FAD	C8M-C8-C7	-2.26	116.11	120.74
3	B	612	FAD	C9A-C5X-N5	-2.25	118.84	122.36
3	A	612	FAD	C4X-C4-N3	-2.25	120.36	123.43
5	D	616	PO4	O3-P-O1	-2.24	102.68	110.89
3	G	612	FAD	C9A-C5X-N5	-2.24	118.86	122.36
3	H	612	FAD	C4X-C4-N3	-2.23	120.38	123.43
3	G	612	FAD	C1B-N9A-C4A	-2.23	122.72	126.64
3	C	612	FAD	C1'-N10-C10	-2.23	116.41	118.41
2	B	611	TPP	CM2-C2'-N3'	2.23	120.63	117.15
5	K	614	PO4	O4-P-O1	-2.21	102.79	110.89
2	L	611	TPP	C7'-N3-C2	-2.21	121.36	125.35
3	L	612	FAD	C6-C5X-N5	2.20	121.47	119.05
3	G	612	FAD	C4X-C4-N3	-2.20	120.43	123.43
3	K	612	FAD	C1'-C2'-C3'	2.19	115.90	109.79
2	C	611	TPP	N1'-C2'-N3'	-2.19	121.78	125.54
3	K	612	FAD	O5B-C5B-C4B	-2.18	101.48	108.99
3	E	612	FAD	C10-C4X-N5	-2.17	119.76	121.26
2	J	611	TPP	C5-C4-N3	2.17	111.91	107.57
2	H	611	TPP	C7'-C5'-C6'	-2.16	116.56	120.69
2	C	611	TPP	C5'-C6'-N1'	-2.15	120.23	123.82
3	B	612	FAD	N6A-C6A-N1A	2.15	123.03	118.57
2	L	611	TPP	C6'-C5'-C4'	2.15	118.64	115.72
3	H	612	FAD	C9A-N10-C10	-2.14	119.11	121.91
3	B	612	FAD	C5X-C9A-N10	2.13	119.26	117.72
2	B	611	TPP	C7'-C5'-C6'	-2.13	116.62	120.69
2	B	611	TPP	PA-O3A-PB	-2.13	125.52	132.83
3	J	612	FAD	C5X-C9A-N10	2.13	119.26	117.72
3	I	612	FAD	C4'-C3'-C2'	-2.12	108.95	113.36
3	J	612	FAD	C9A-C5X-N5	-2.12	119.04	122.36
3	L	612	FAD	O2P-P-O1P	2.11	122.66	112.24
3	D	612	FAD	C9A-C5X-N5	-2.10	119.08	122.36
3	D	612	FAD	O2B-C2B-C1B	-2.10	103.10	110.85
3	A	612	FAD	C4X-N5-C5X	2.10	118.87	116.77
3	C	612	FAD	O2P-P-O1P	2.09	122.57	112.24
3	B	612	FAD	C9A-N10-C10	-2.09	119.18	121.91
3	B	612	FAD	O3B-C3B-C4B	-2.08	105.04	111.05
2	G	611	TPP	O2A-PA-O7	2.07	117.36	107.75
2	C	611	TPP	C5'-C4'-N4'	2.06	125.11	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	612	FAD	C4-C4X-C10	-2.06	118.58	119.95
5	K	614	PO4	O3-P-O1	2.06	118.43	110.89
3	F	612	FAD	C1'-N10-C9A	2.06	119.91	118.29
3	G	612	FAD	O5B-PA-O1A	2.06	117.11	109.07
3	K	612	FAD	C4X-C4-N3	-2.06	120.62	123.43
5	C	614	PO4	O4-P-O2	-2.05	101.40	107.97
2	G	611	TPP	C5-C4-N3	2.04	111.65	107.57
2	H	611	TPP	O3B-PB-O1B	2.03	118.61	110.68
2	L	611	TPP	C5-C4-N3	2.03	111.62	107.57
2	D	611	TPP	N4'-C4'-N3'	2.02	119.89	117.03
3	H	612	FAD	O3'-C3'-C2'	-2.02	103.94	108.81
3	C	612	FAD	C4A-C5A-N7A	-2.01	107.30	109.40

There are no chirality outliers.

All (162) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	611	TPP	C5-C6-C7-O7
2	A	611	TPP	PA-O3A-PB-O3B
2	B	611	TPP	C4-C5-C6-C7
2	B	611	TPP	C5-C6-C7-O7
2	B	611	TPP	C7-O7-PA-O1A
2	B	611	TPP	PA-O3A-PB-O3B
2	C	611	TPP	C5-C6-C7-O7
2	D	611	TPP	C4-C5-C6-C7
2	D	611	TPP	C5-C6-C7-O7
2	D	611	TPP	PA-O3A-PB-O3B
2	E	611	TPP	C5-C6-C7-O7
2	E	611	TPP	C7-O7-PA-O1A
2	E	611	TPP	PA-O3A-PB-O3B
2	F	611	TPP	C4-C5-C6-C7
2	F	611	TPP	C5-C6-C7-O7
2	F	611	TPP	C7-O7-PA-O1A
2	G	611	TPP	C4-C5-C6-C7
2	G	611	TPP	C5-C6-C7-O7
2	H	611	TPP	C5-C6-C7-O7
2	H	611	TPP	C7-O7-PA-O1A
2	H	611	TPP	C7-O7-PA-O3A
2	H	611	TPP	PA-O3A-PB-O3B
2	I	611	TPP	C5-C6-C7-O7
2	I	611	TPP	C7-O7-PA-O1A
2	I	611	TPP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
2	J	611	TPP	C5-C6-C7-O7
2	J	611	TPP	C7-O7-PA-O1A
2	L	611	TPP	C5-C6-C7-O7
2	L	611	TPP	PA-O3A-PB-O3B
3	A	612	FAD	C5B-O5B-PA-O1A
3	A	612	FAD	C5B-O5B-PA-O2A
3	A	612	FAD	C2'-C1'-N10-C9A
3	B	612	FAD	C5B-O5B-PA-O2A
3	B	612	FAD	C5B-O5B-PA-O3P
3	B	612	FAD	P-O3P-PA-O5B
3	B	612	FAD	C2'-C1'-N10-C9A
3	C	612	FAD	C5B-O5B-PA-O1A
3	C	612	FAD	C5B-O5B-PA-O2A
3	C	612	FAD	C5B-O5B-PA-O3P
3	C	612	FAD	C2'-C1'-N10-C9A
3	D	612	FAD	C5B-O5B-PA-O1A
3	D	612	FAD	C5B-O5B-PA-O2A
3	D	612	FAD	C5B-O5B-PA-O3P
3	D	612	FAD	C2'-C1'-N10-C9A
3	E	612	FAD	C5B-O5B-PA-O1A
3	E	612	FAD	C5B-O5B-PA-O2A
3	E	612	FAD	C2'-C1'-N10-C9A
3	E	612	FAD	C3'-C4'-C5'-O5'
3	E	612	FAD	O4'-C4'-C5'-O5'
3	F	612	FAD	C5B-O5B-PA-O1A
3	F	612	FAD	C5B-O5B-PA-O2A
3	F	612	FAD	C2'-C1'-N10-C9A
3	F	612	FAD	C5'-O5'-P-O3P
3	G	612	FAD	C5B-O5B-PA-O1A
3	G	612	FAD	C5B-O5B-PA-O2A
3	G	612	FAD	P-O3P-PA-O5B
3	G	612	FAD	C2'-C1'-N10-C9A
3	G	612	FAD	O4'-C4'-C5'-O5'
3	H	612	FAD	C5B-O5B-PA-O1A
3	H	612	FAD	C5B-O5B-PA-O2A
3	H	612	FAD	C2'-C1'-N10-C9A
3	I	612	FAD	C5B-O5B-PA-O2A
3	I	612	FAD	C5B-O5B-PA-O3P
3	I	612	FAD	O4B-C4B-C5B-O5B
3	I	612	FAD	C2'-C1'-N10-C9A
3	J	612	FAD	C5B-O5B-PA-O2A
3	J	612	FAD	C5B-O5B-PA-O3P

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Mol	Chain	Res	Type	Atoms
3	J	612	FAD	C2'-C1'-N10-C9A
3	J	612	FAD	C5'-O5'-P-O3P
3	K	612	FAD	C5B-O5B-PA-O2A
3	K	612	FAD	C5B-O5B-PA-O3P
3	K	612	FAD	O4B-C4B-C5B-O5B
3	K	612	FAD	C2'-C1'-N10-C9A
3	L	612	FAD	C5B-O5B-PA-O1A
3	L	612	FAD	C5B-O5B-PA-O2A
3	L	612	FAD	C5B-O5B-PA-O3P
3	L	612	FAD	C2'-C1'-N10-C9A
3	B	612	FAD	O4B-C4B-C5B-O5B
3	I	612	FAD	C3B-C4B-C5B-O5B
3	K	612	FAD	C3B-C4B-C5B-O5B
3	G	612	FAD	O3'-C3'-C4'-C5'
3	G	612	FAD	C2'-C3'-C4'-C5'
3	B	612	FAD	C3B-C4B-C5B-O5B
3	J	612	FAD	O4B-C4B-C5B-O5B
3	B	612	FAD	O4'-C4'-C5'-O5'
3	C	612	FAD	O4'-C4'-C5'-O5'
3	I	612	FAD	O4'-C4'-C5'-O5'
3	K	612	FAD	O4'-C4'-C5'-O5'
3	L	612	FAD	O4'-C4'-C5'-O5'
3	B	612	FAD	O3'-C3'-C4'-C5'
3	C	612	FAD	C3B-C4B-C5B-O5B
3	B	612	FAD	C3'-C4'-C5'-O5'
3	C	612	FAD	C3'-C4'-C5'-O5'
3	G	612	FAD	C3'-C4'-C5'-O5'
3	I	612	FAD	C3'-C4'-C5'-O5'
3	K	612	FAD	C3'-C4'-C5'-O5'
3	L	612	FAD	C3'-C4'-C5'-O5'
3	C	612	FAD	P-O3P-PA-O5B
3	D	612	FAD	P-O3P-PA-O5B
3	F	612	FAD	P-O3P-PA-O5B
3	H	612	FAD	P-O3P-PA-O5B
3	I	612	FAD	P-O3P-PA-O5B
3	L	612	FAD	P-O3P-PA-O5B
3	C	612	FAD	O4B-C4B-C5B-O5B
3	H	612	FAD	O4B-C4B-C5B-O5B
2	F	611	TPP	PA-O3A-PB-O1B
2	K	611	TPP	C5-C6-C7-O7
2	B	611	TPP	C7-O7-PA-O3A
2	D	611	TPP	C7-O7-PA-O3A

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Mol	Chain	Res	Type	Atoms
2	E	611	TPP	C7-O7-PA-O3A
2	F	611	TPP	C7-O7-PA-O3A
3	D	612	FAD	C5'-O5'-P-O3P
3	E	612	FAD	C5B-O5B-PA-O3P
3	F	612	FAD	C5B-O5B-PA-O3P
3	G	612	FAD	C5B-O5B-PA-O3P
3	K	612	FAD	C5'-O5'-P-O3P
3	H	612	FAD	C3'-C4'-C5'-O5'
3	J	612	FAD	C5B-O5B-PA-O1A
2	E	611	TPP	C4-C5-C6-C7
2	I	611	TPP	C4-C5-C6-C7
2	L	611	TPP	C4-C5-C6-C7
3	J	612	FAD	C3B-C4B-C5B-O5B
3	C	612	FAD	O3'-C3'-C4'-O4'
3	D	612	FAD	O4B-C4B-C5B-O5B
3	C	612	FAD	O3'-C3'-C4'-C5'
3	B	612	FAD	O3'-C3'-C4'-O4'
3	I	612	FAD	O3'-C3'-C4'-C5'
3	L	612	FAD	O4B-C4B-C5B-O5B
2	C	611	TPP	PA-O3A-PB-O1B
3	E	612	FAD	O2'-C2'-C3'-C4'
3	D	612	FAD	C3B-C4B-C5B-O5B
3	G	612	FAD	O4B-C4B-C5B-O5B
2	A	611	TPP	PA-O3A-PB-O1B
2	D	611	TPP	PA-O3A-PB-O1B
2	E	611	TPP	PA-O3A-PB-O1B
2	H	611	TPP	PA-O3A-PB-O1B
2	J	611	TPP	PA-O3A-PB-O1B
3	H	612	FAD	O4'-C4'-C5'-O5'
2	A	611	TPP	PA-O3A-PB-O2B
2	C	611	TPP	PA-O3A-PB-O2B
2	C	611	TPP	PA-O3A-PB-O3B
2	D	611	TPP	PA-O3A-PB-O2B
2	F	611	TPP	PA-O3A-PB-O2B
2	G	611	TPP	PA-O3A-PB-O2B
2	I	611	TPP	PA-O3A-PB-O2B
2	J	611	TPP	PA-O3A-PB-O2B
2	J	611	TPP	PA-O3A-PB-O3B
2	L	611	TPP	PA-O3A-PB-O2B
3	A	612	FAD	C5B-O5B-PA-O3P
3	H	612	FAD	C5B-O5B-PA-O3P
3	E	612	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	F	612	FAD	O4B-C4B-C5B-O5B
3	L	612	FAD	C3B-C4B-C5B-O5B
2	L	611	TPP	C7-O7-PA-O1A
3	F	612	FAD	C5'-O5'-P-O1P
3	J	612	FAD	C5'-O5'-P-O1P
3	K	612	FAD	C5'-O5'-P-O1P
3	A	612	FAD	O4B-C4B-C5B-O5B
3	F	612	FAD	C3B-C4B-C5B-O5B
3	G	612	FAD	C3B-C4B-C5B-O5B
3	H	612	FAD	C3B-C4B-C5B-O5B
3	J	612	FAD	O4'-C4'-C5'-O5'

There are no ring outliers.

39 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	612	FAD	4	0
3	K	612	FAD	2	0
3	A	612	FAD	1	0
3	C	612	FAD	1	0
5	I	614	PO4	1	0
5	A	619	PO4	3	0
5	A	618	PO4	2	0
5	A	617	PO4	1	0
2	A	611	TPP	3	0
5	F	614	PO4	1	0
5	E	614	PO4	1	0
2	I	611	TPP	3	0
5	B	614	PO4	1	0
3	G	612	FAD	4	0
2	F	611	TPP	2	0
2	K	611	TPP	6	0
2	C	611	TPP	2	0
3	E	612	FAD	5	0
5	L	617	PO4	1	0
3	J	612	FAD	4	0
2	E	611	TPP	2	0
3	D	612	FAD	3	0
3	L	612	FAD	2	0
5	A	616	PO4	2	0
5	L	616	PO4	1	0
5	K	614	PO4	1	0

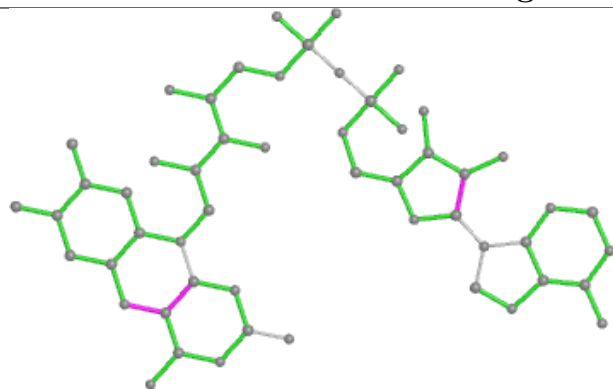
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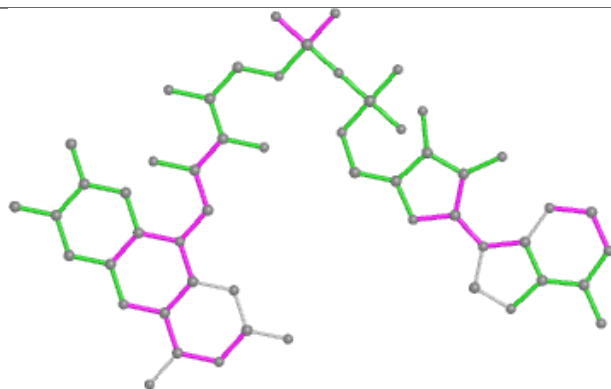
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	612	FAD	3	0
3	H	612	FAD	2	0
2	B	611	TPP	1	0
2	D	611	TPP	1	0
5	D	614	PO4	1	0
2	G	611	TPP	2	0
5	D	618	PO4	1	0
5	H	615	PO4	1	0
5	D	615	PO4	1	0
2	J	611	TPP	2	0
2	L	611	TPP	4	0
3	I	612	FAD	6	0
2	H	611	TPP	2	0

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.

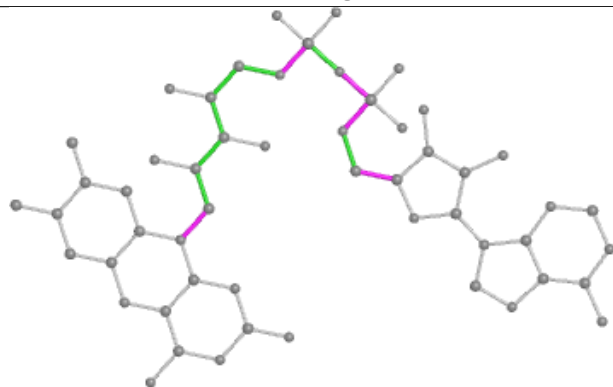
## Ligand FAD F 612



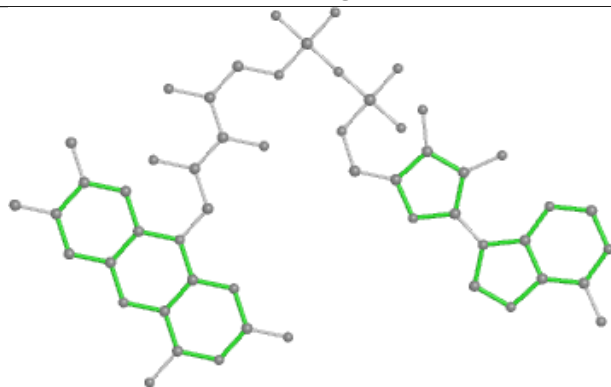
Bond lengths



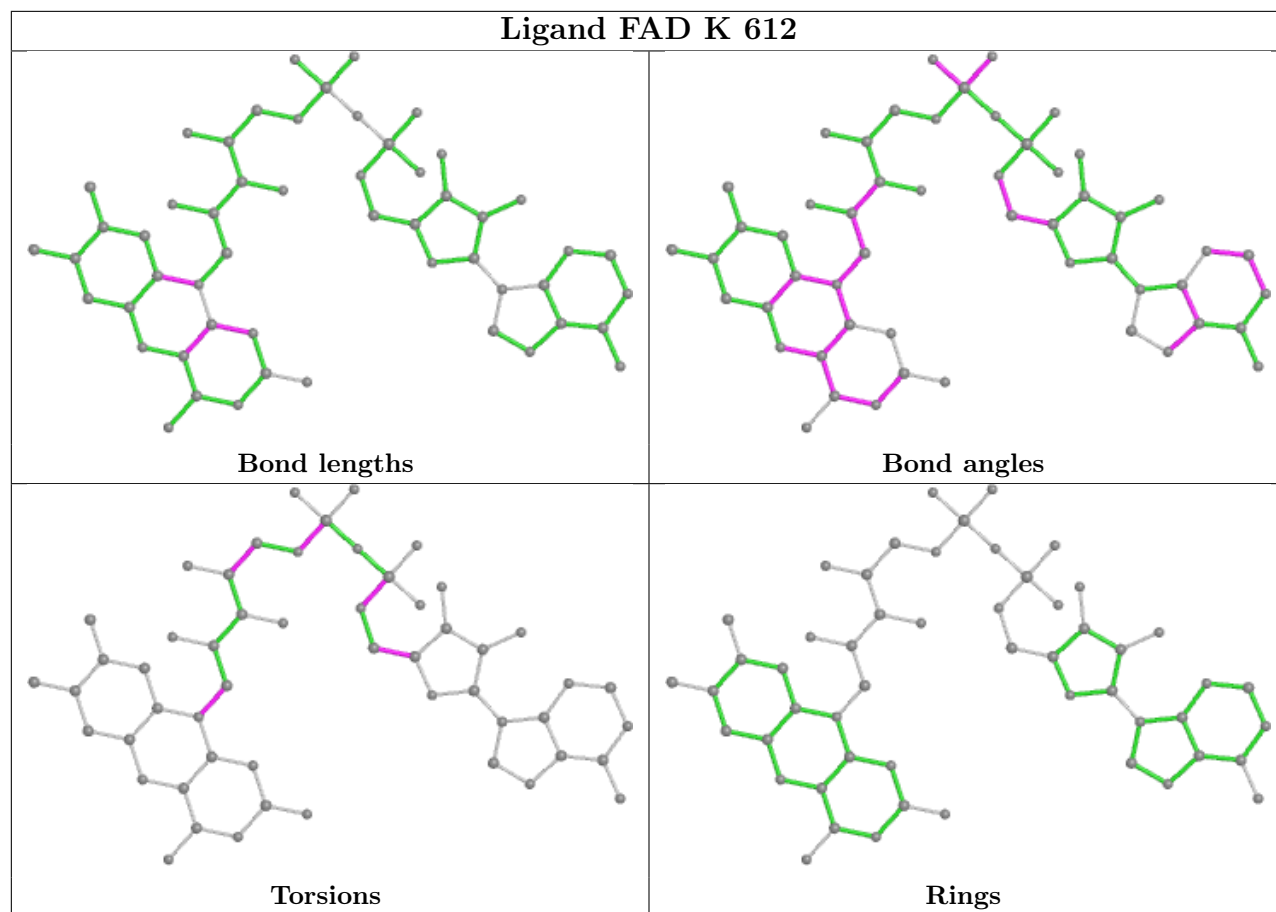
Bond angles



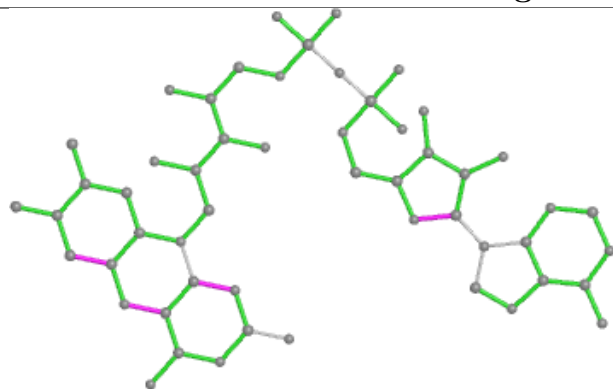
Torsions



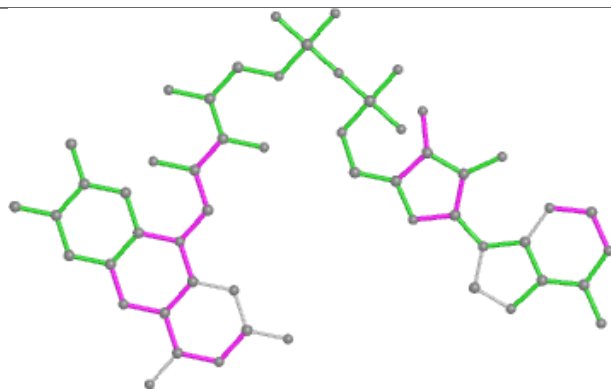
Rings



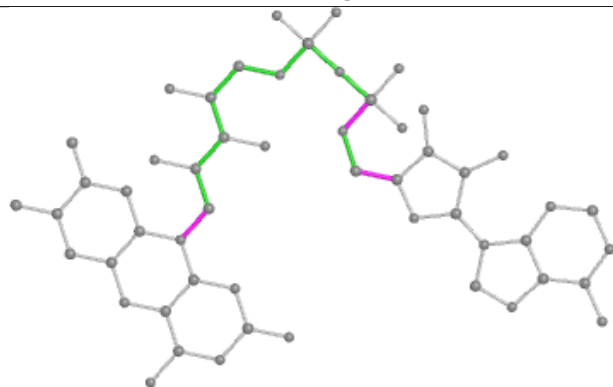
## Ligand FAD A 612



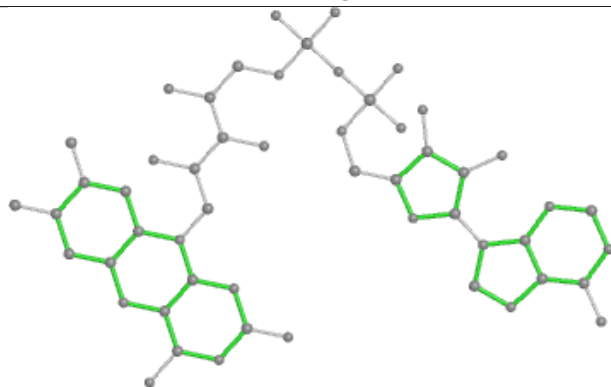
Bond lengths



Bond angles

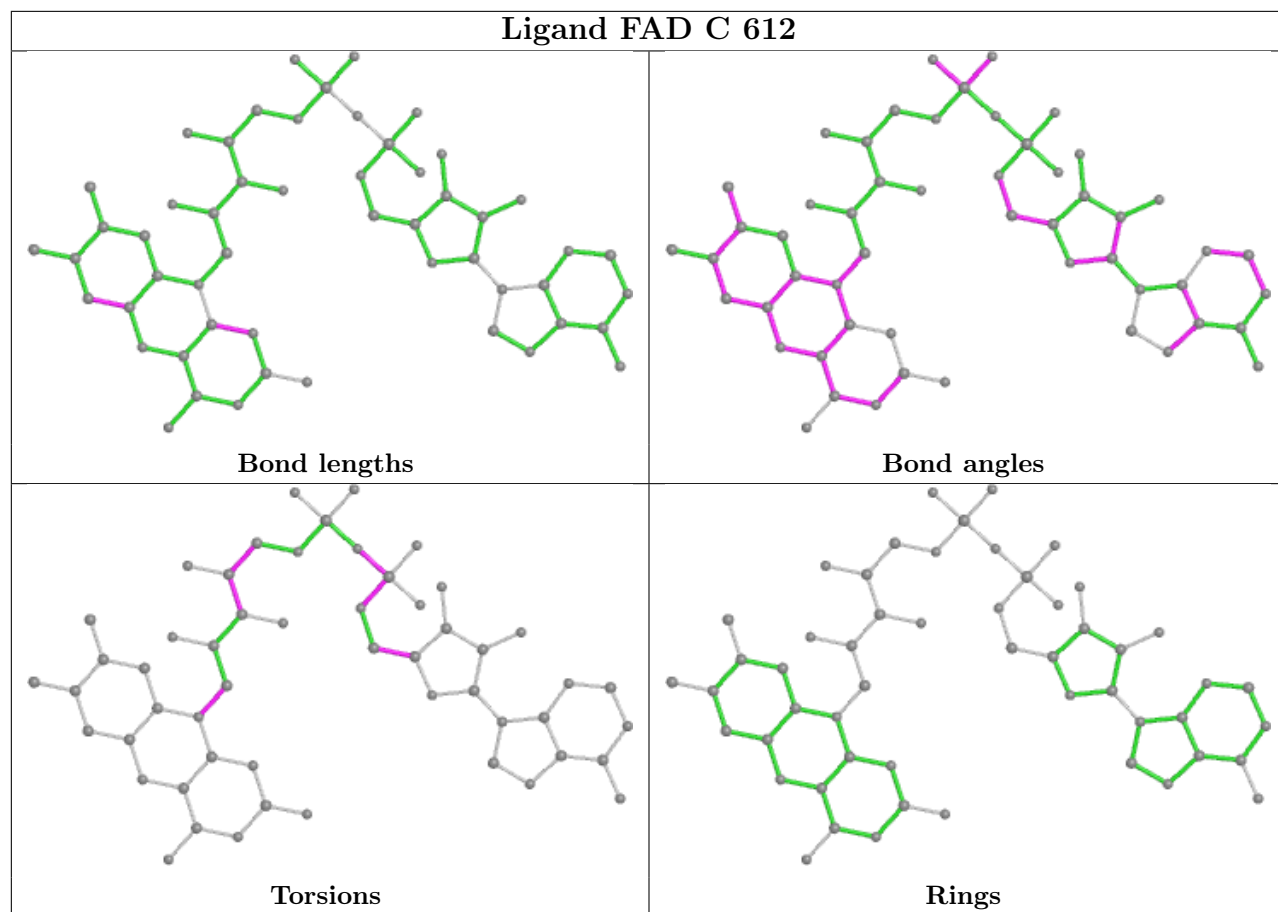


Torsions

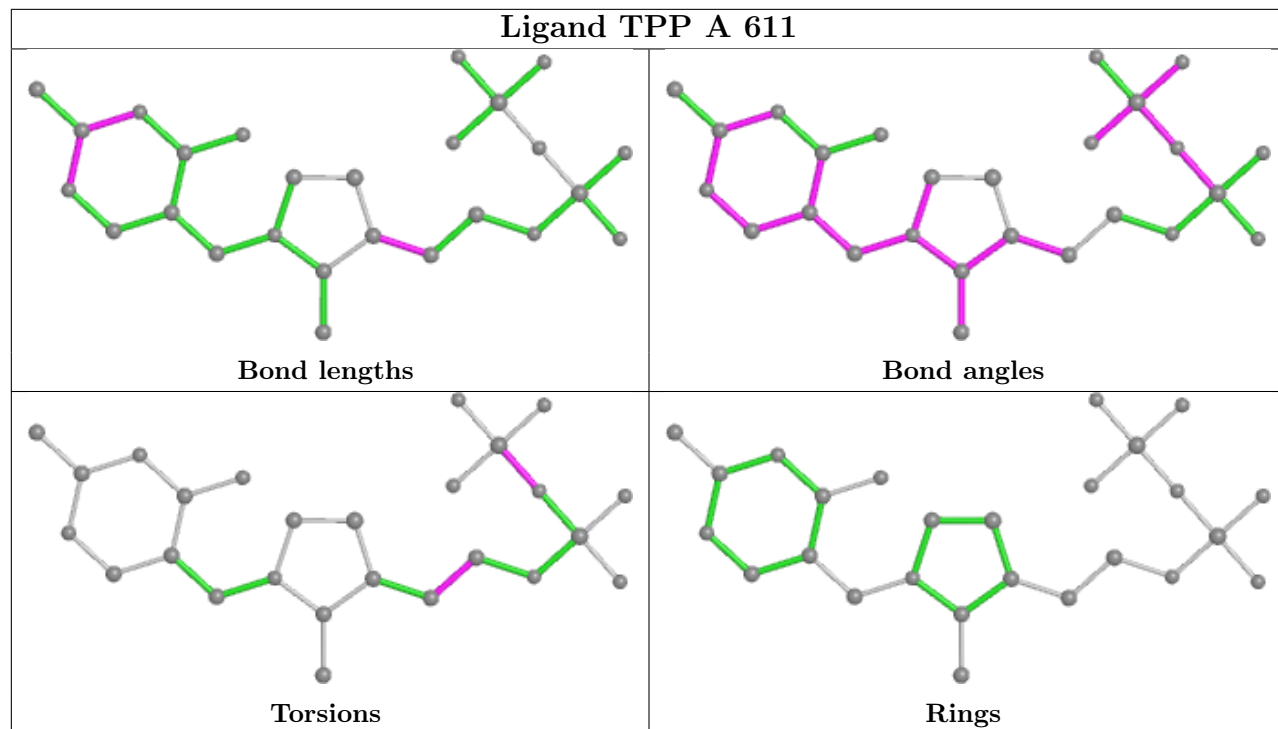


Rings

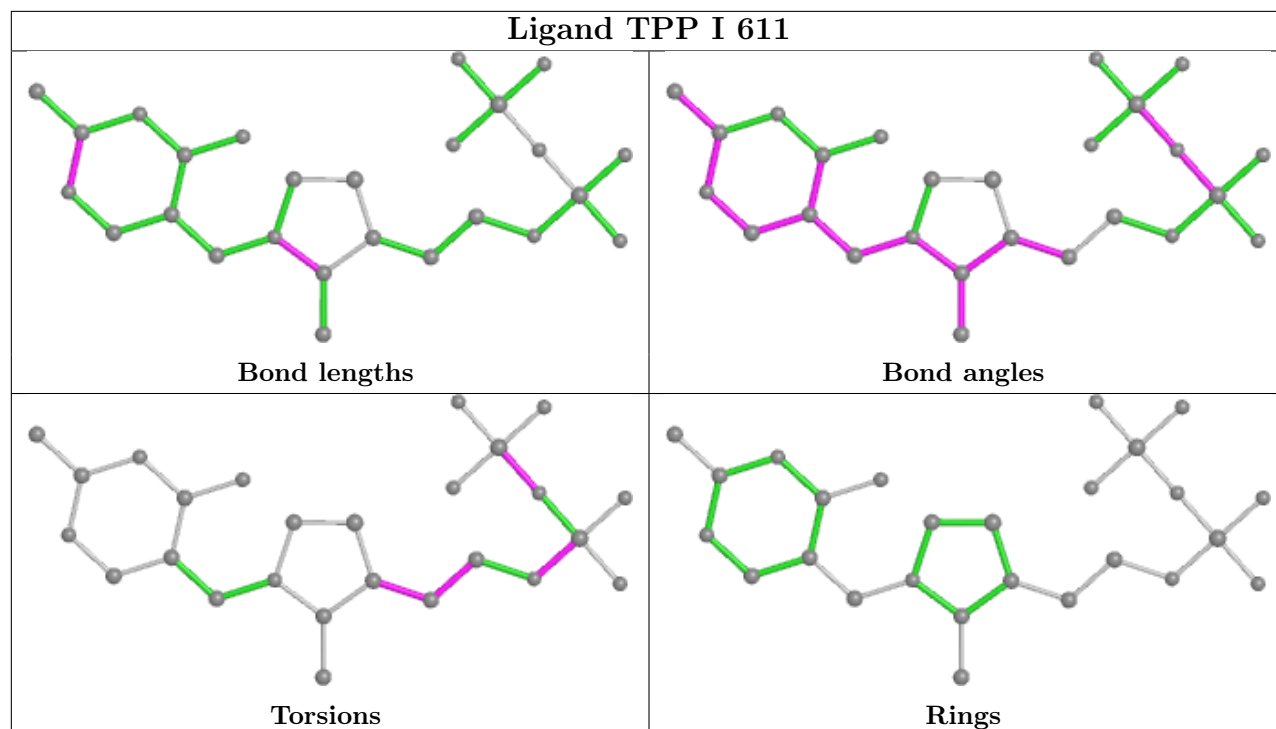
## Ligand FAD C 612



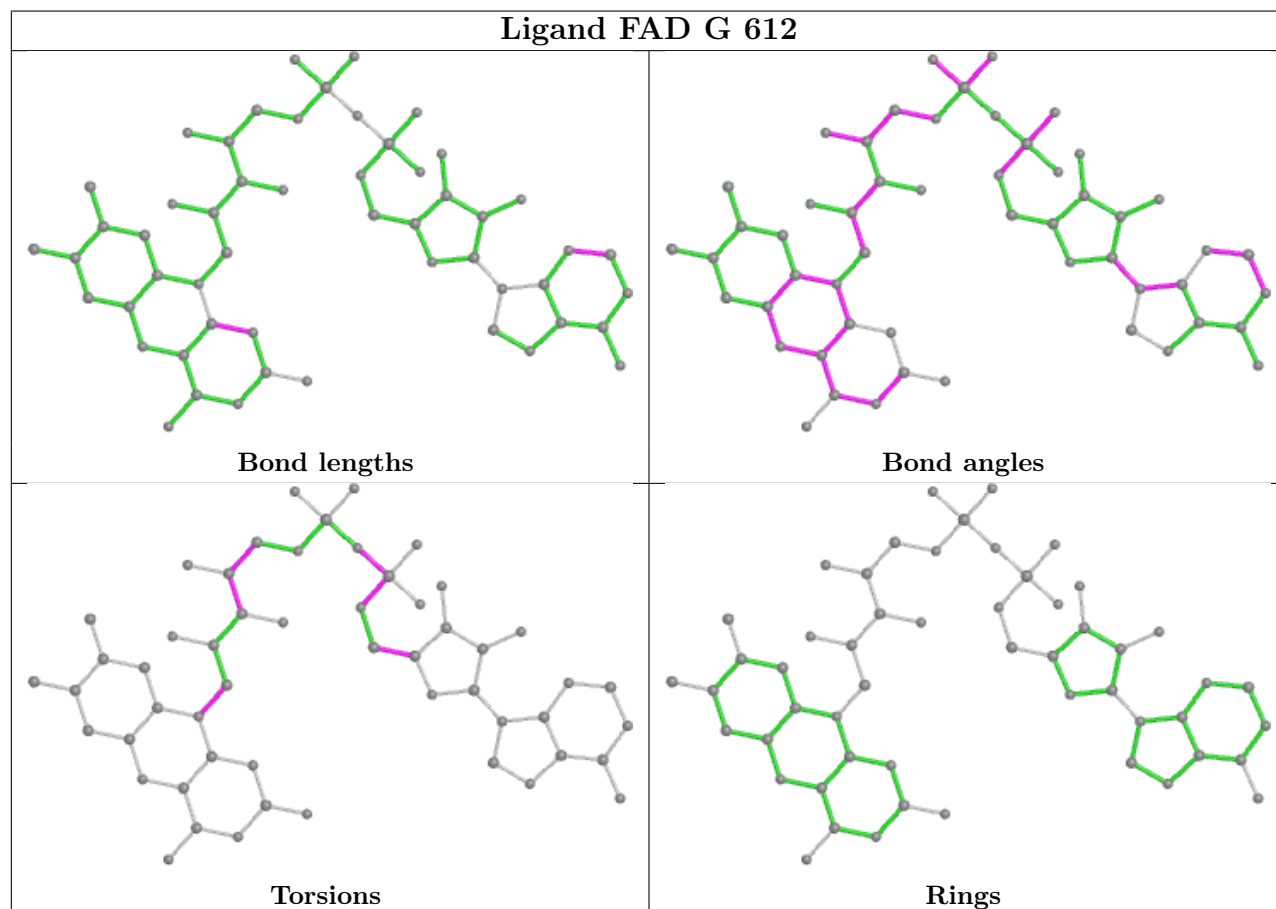
## Ligand TPP A 611



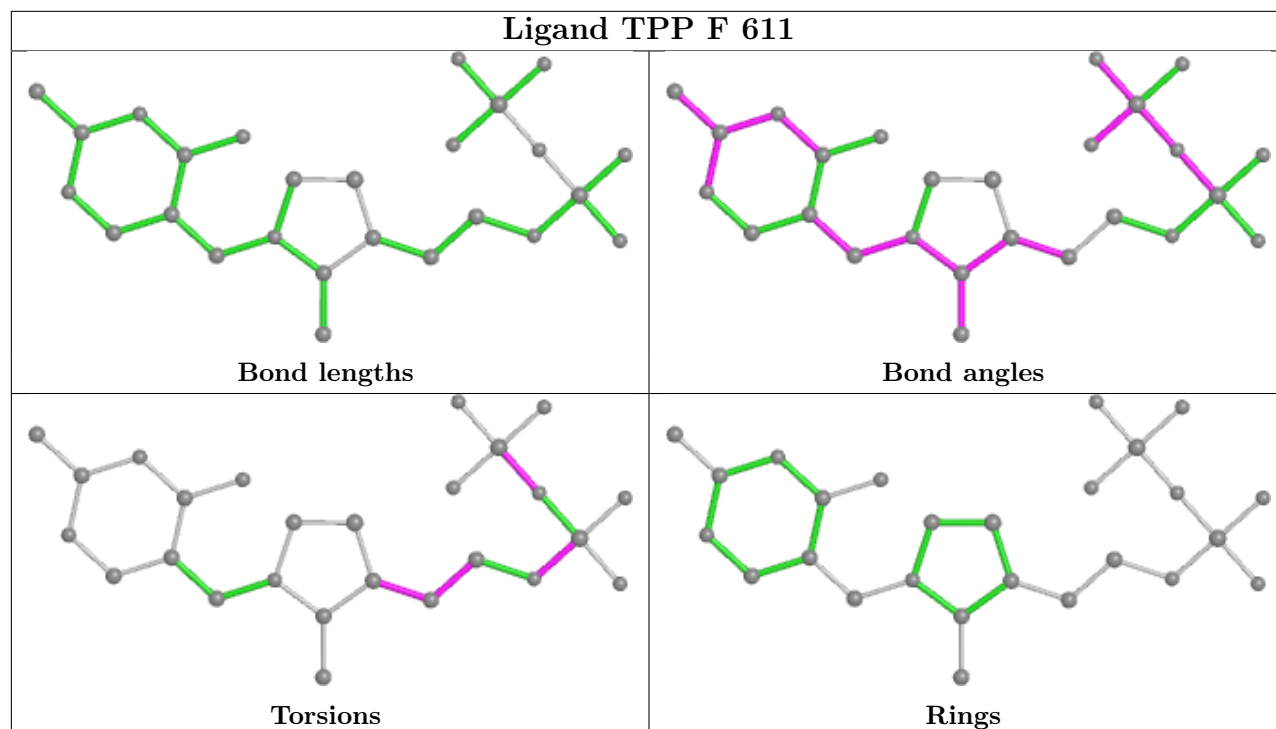
## Ligand TPP I 611



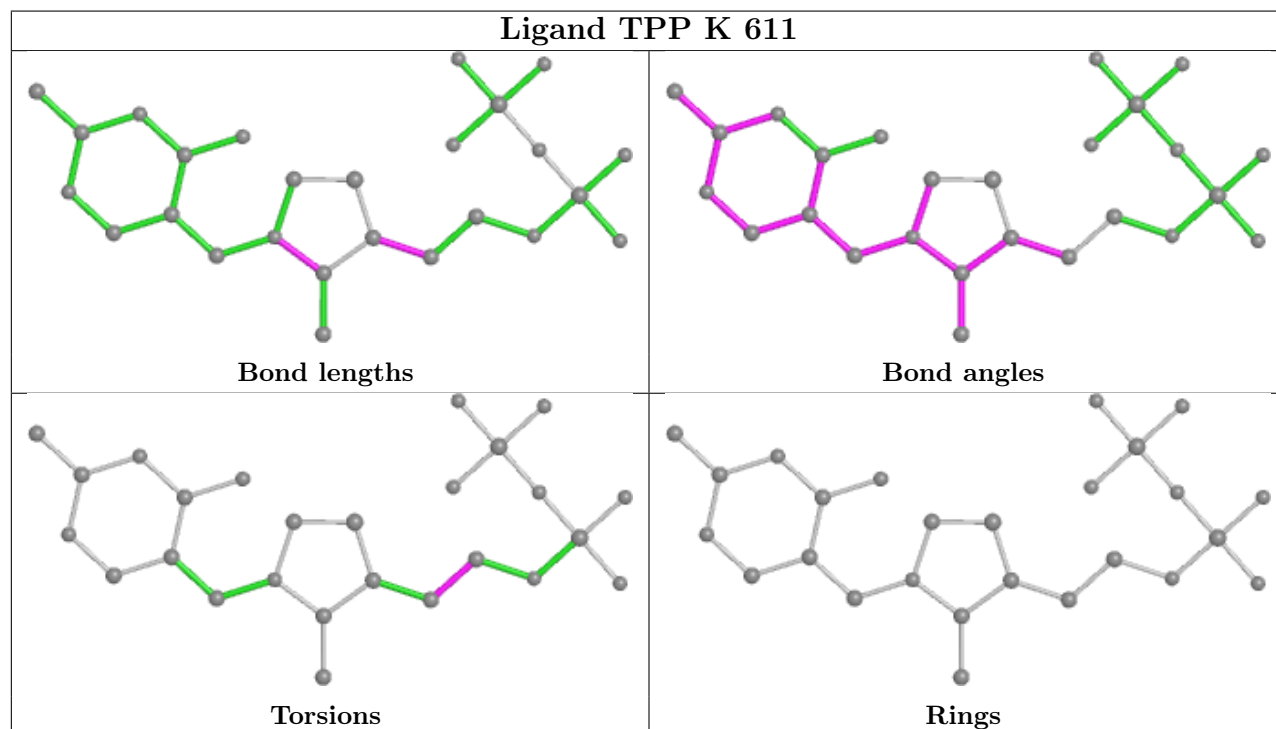
## Ligand FAD G 612



## Ligand TPP F 611

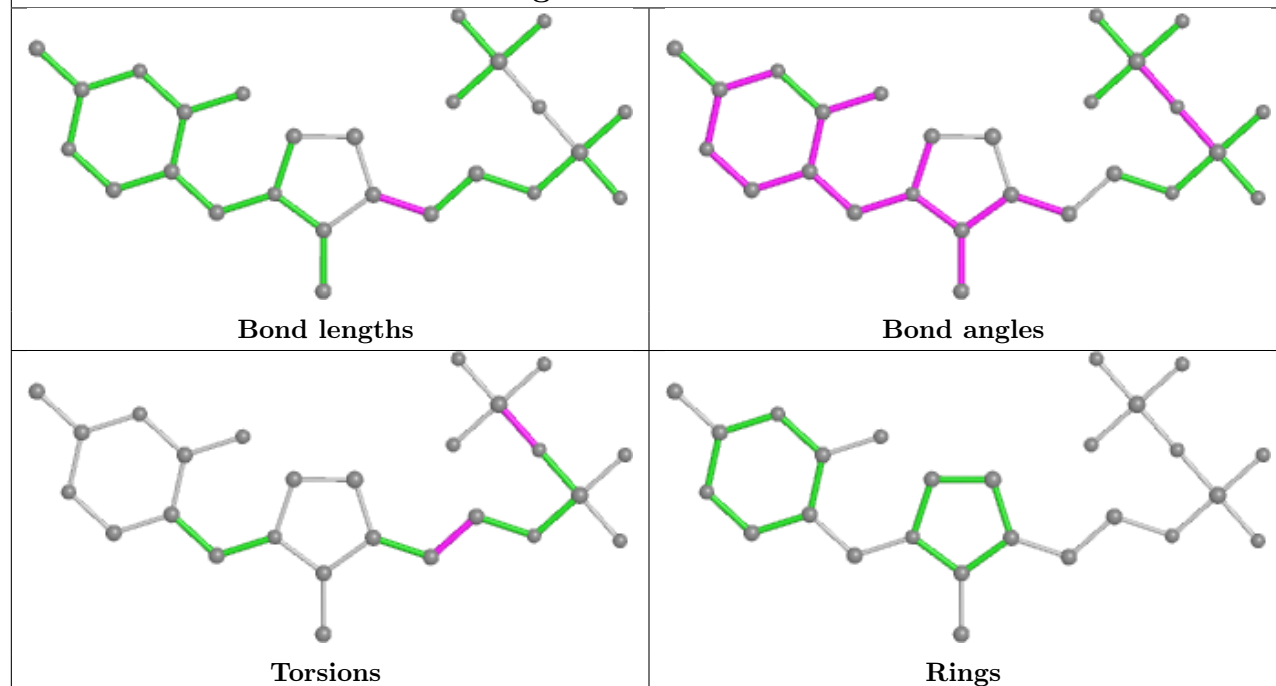


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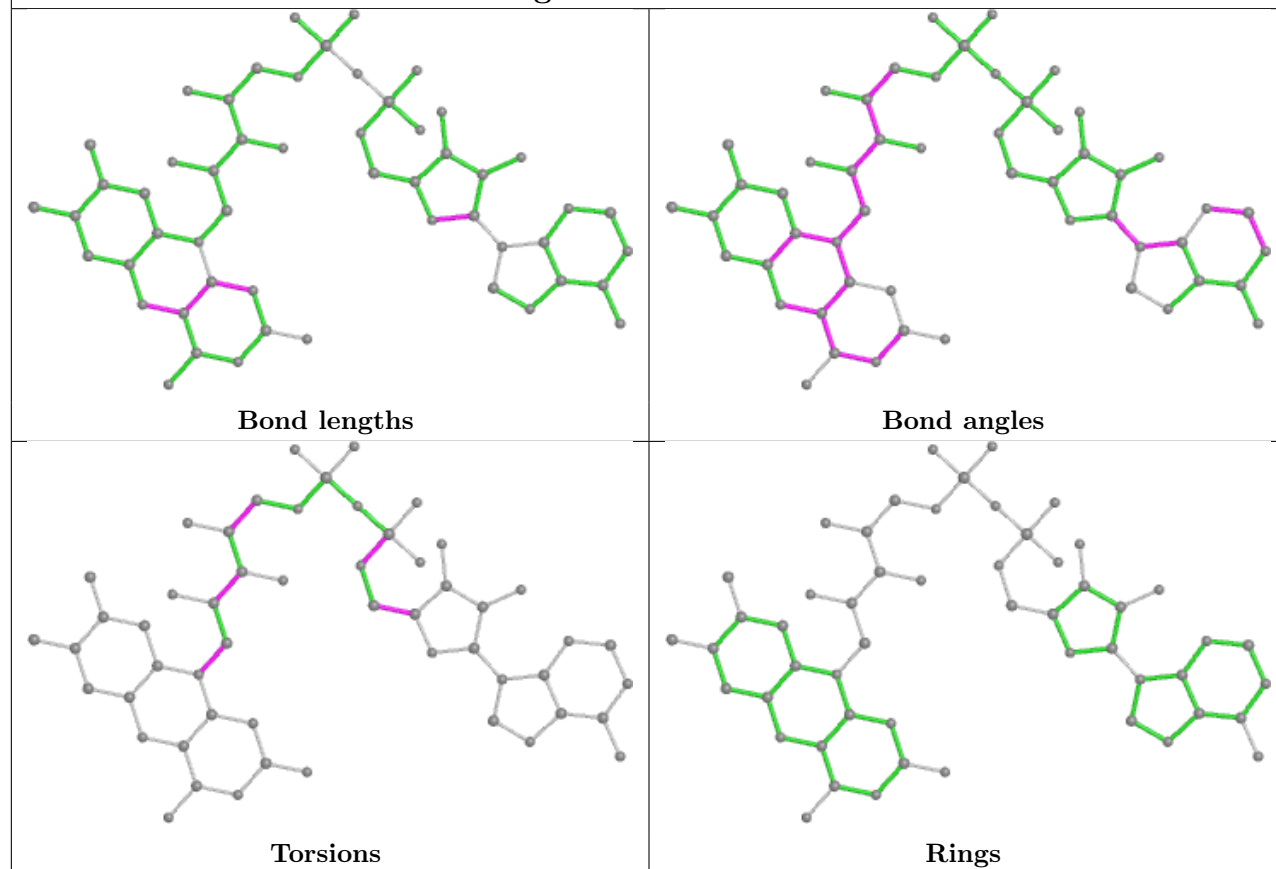




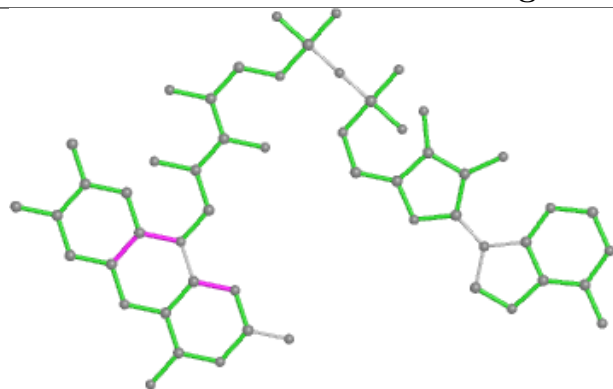
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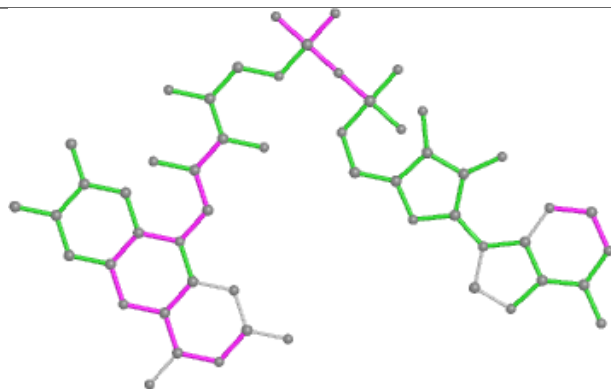
## Ligand FAD E 612



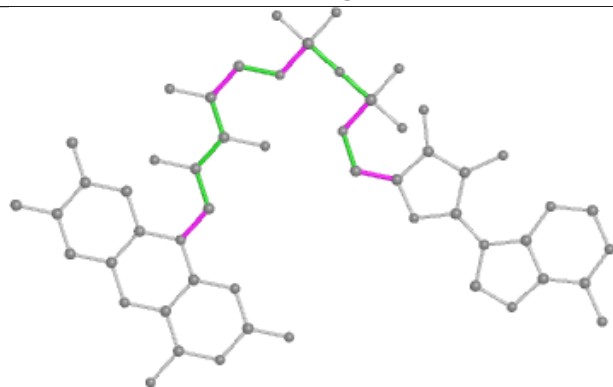
## Ligand FAD J 612



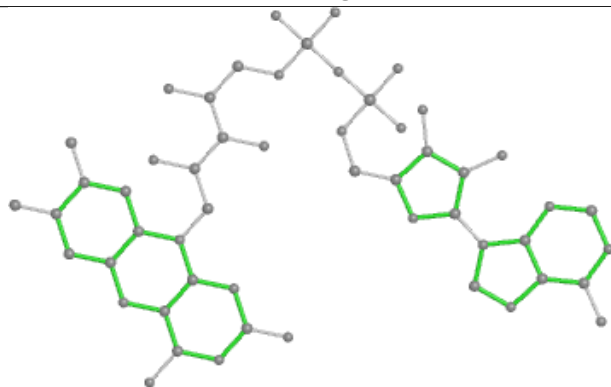
Bond lengths



Bond angles

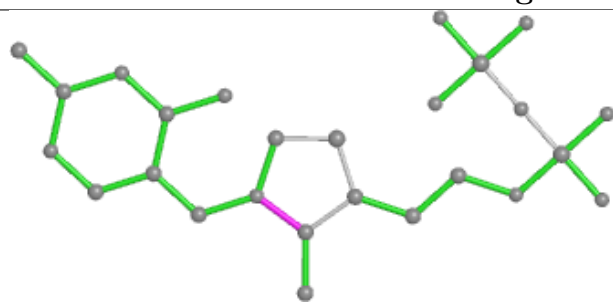


Torsions

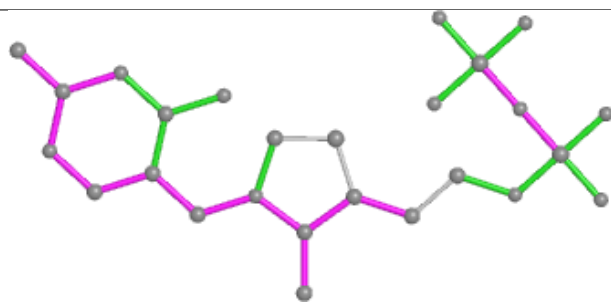


Rings

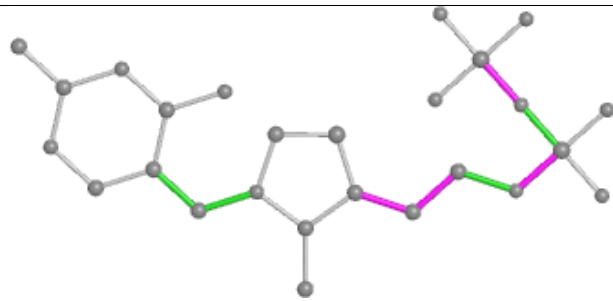
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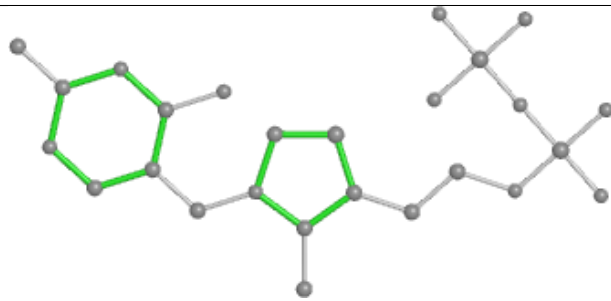
Bond lengths



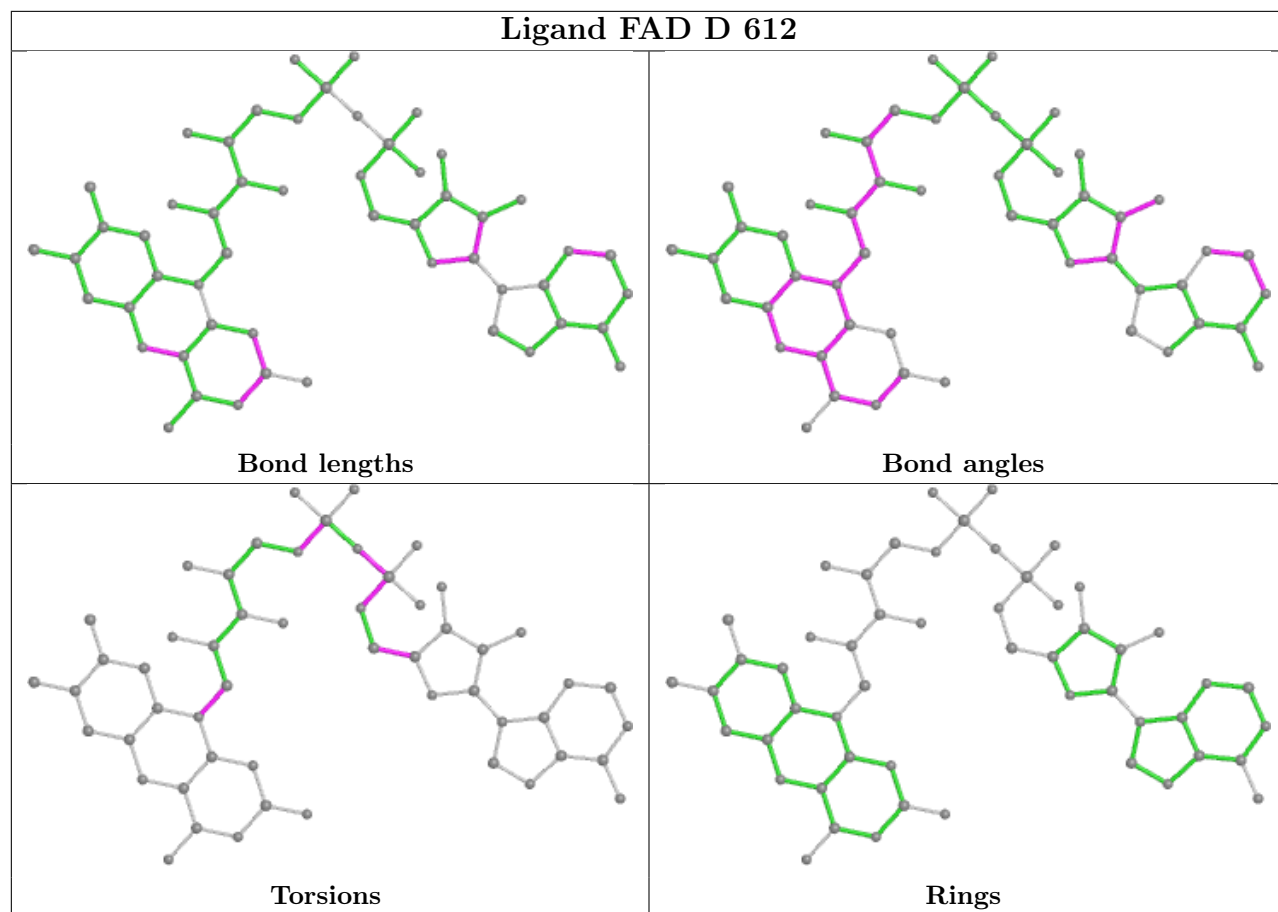
Bond angles



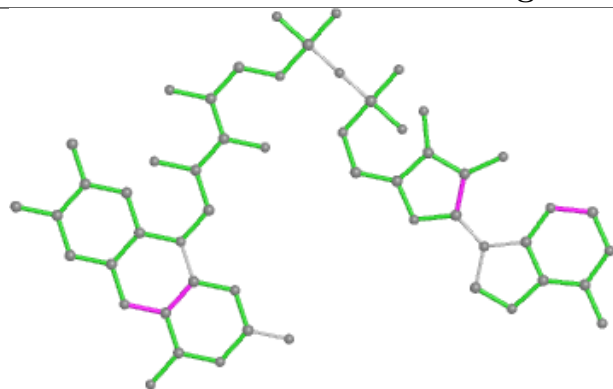
Torsions



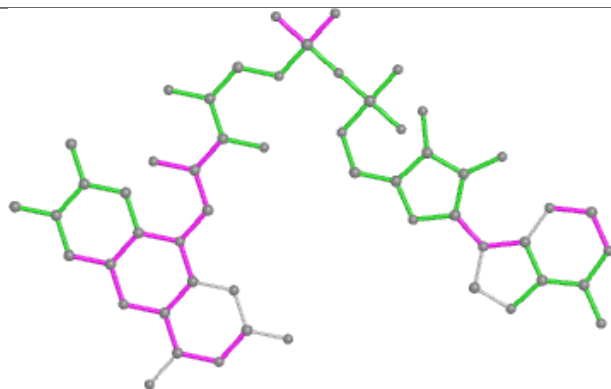
Rings



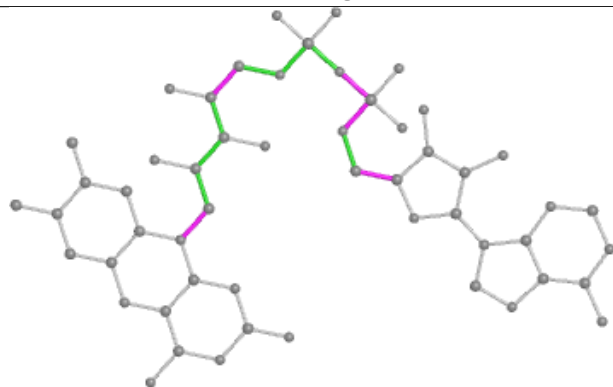
## Ligand FAD L 612



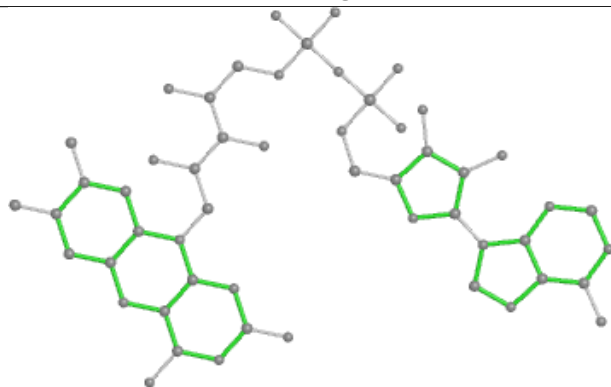
Bond lengths



Bond angles

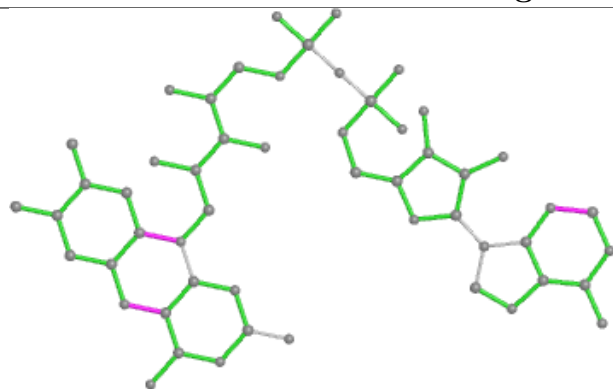


Torsions

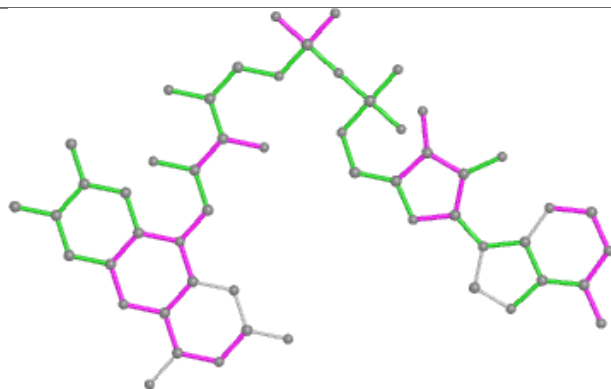


Rings

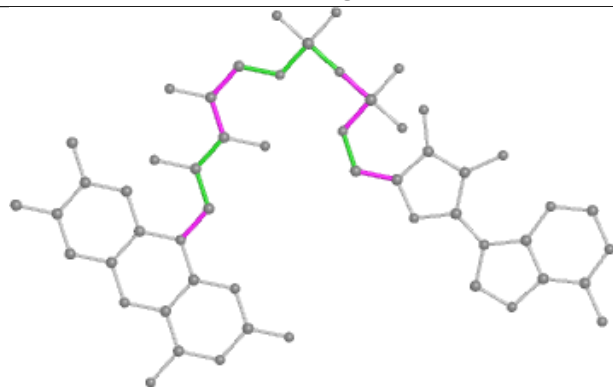
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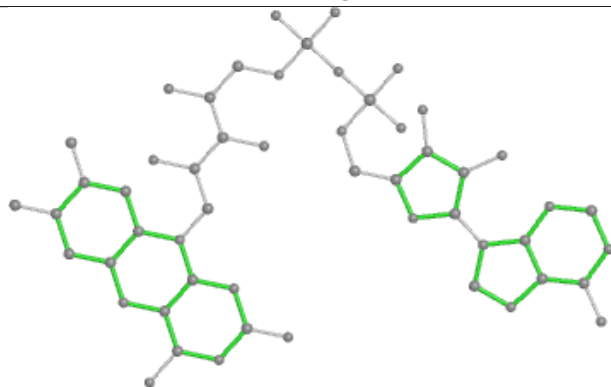
Bond lengths



Bond angles

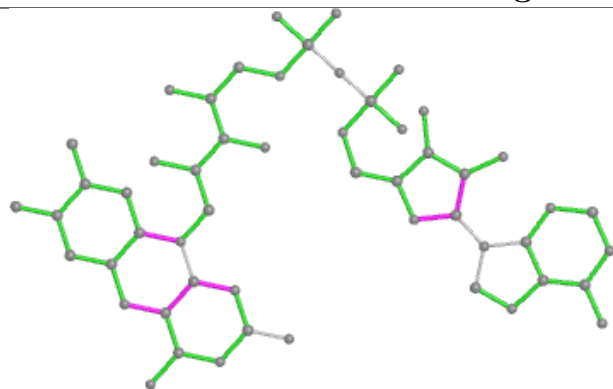


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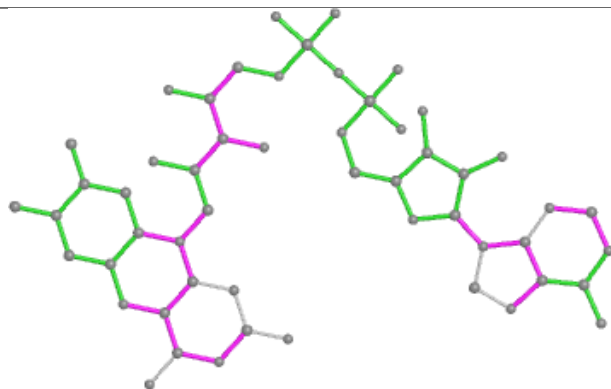


Rings

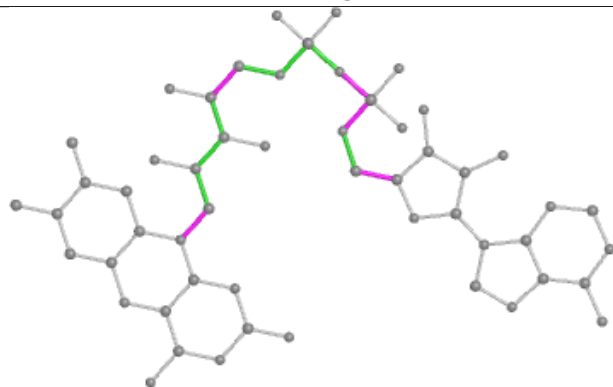
## Ligand FAD H 612



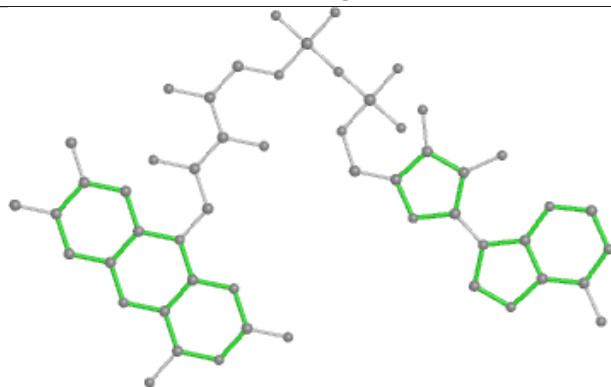
Bond lengths



Bond angles

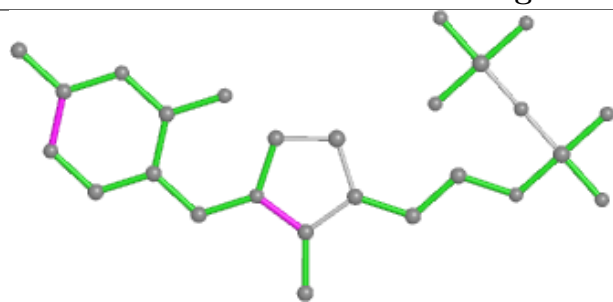


Torsions

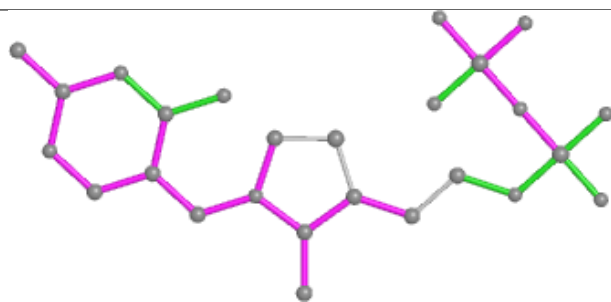


Rings

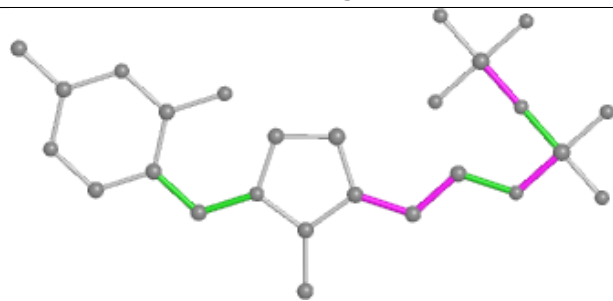
## Ligand TPP B 611



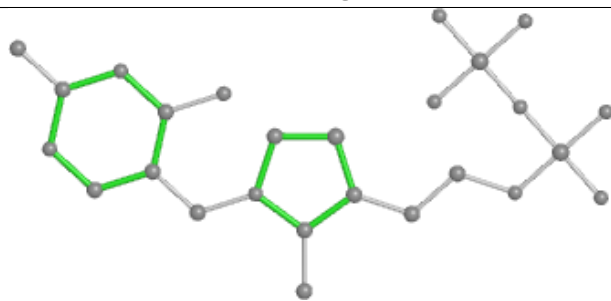
Bond lengths



Bond angles

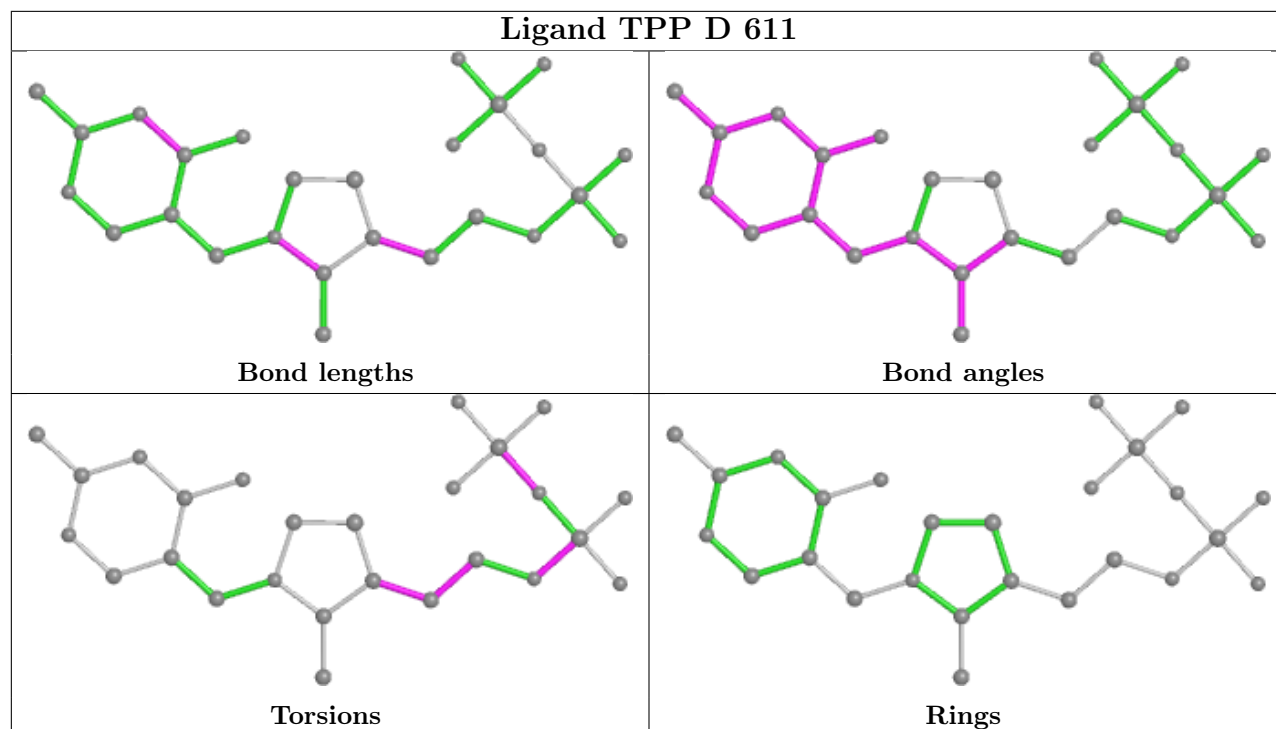


Torsions

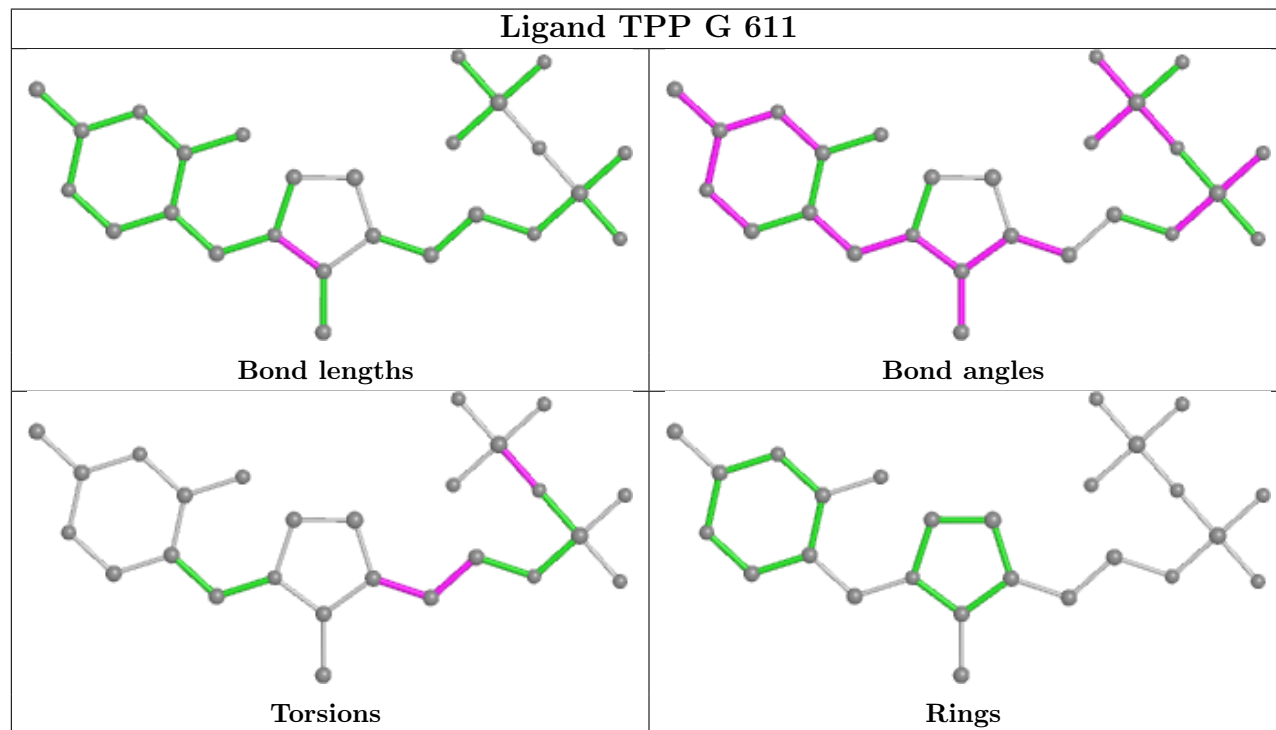


Rings

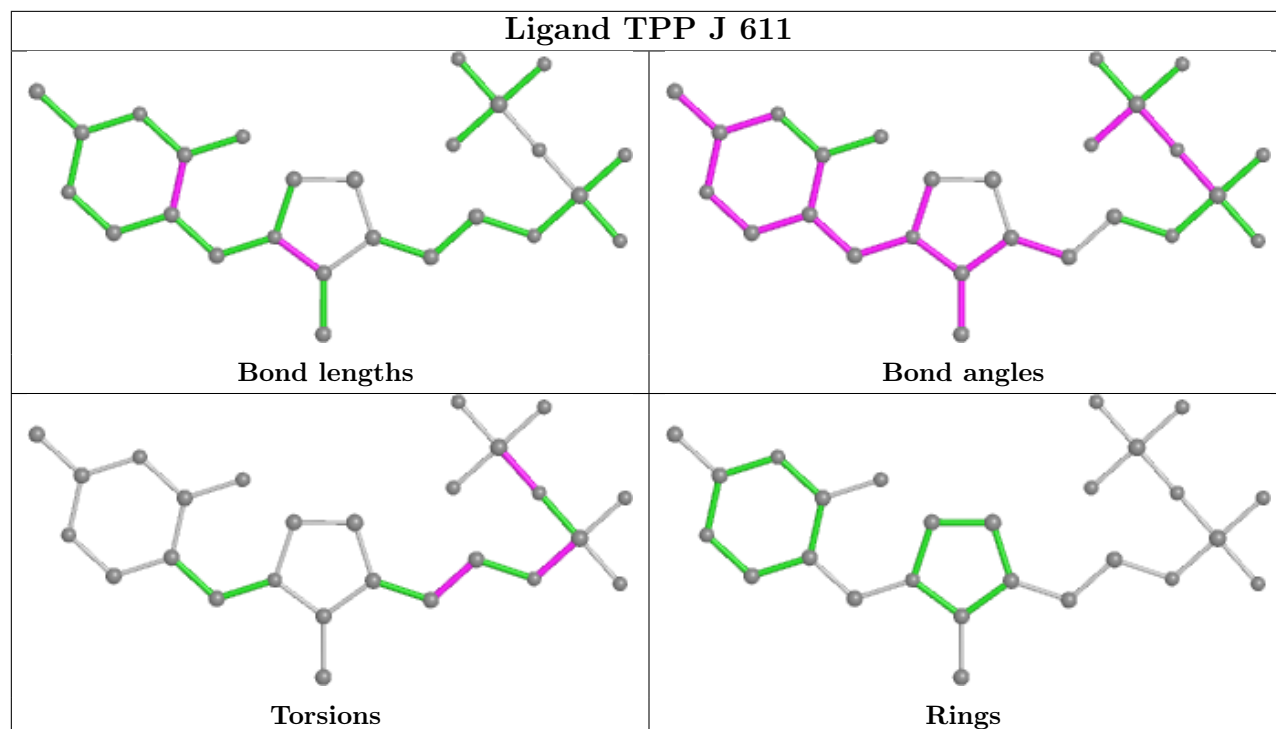
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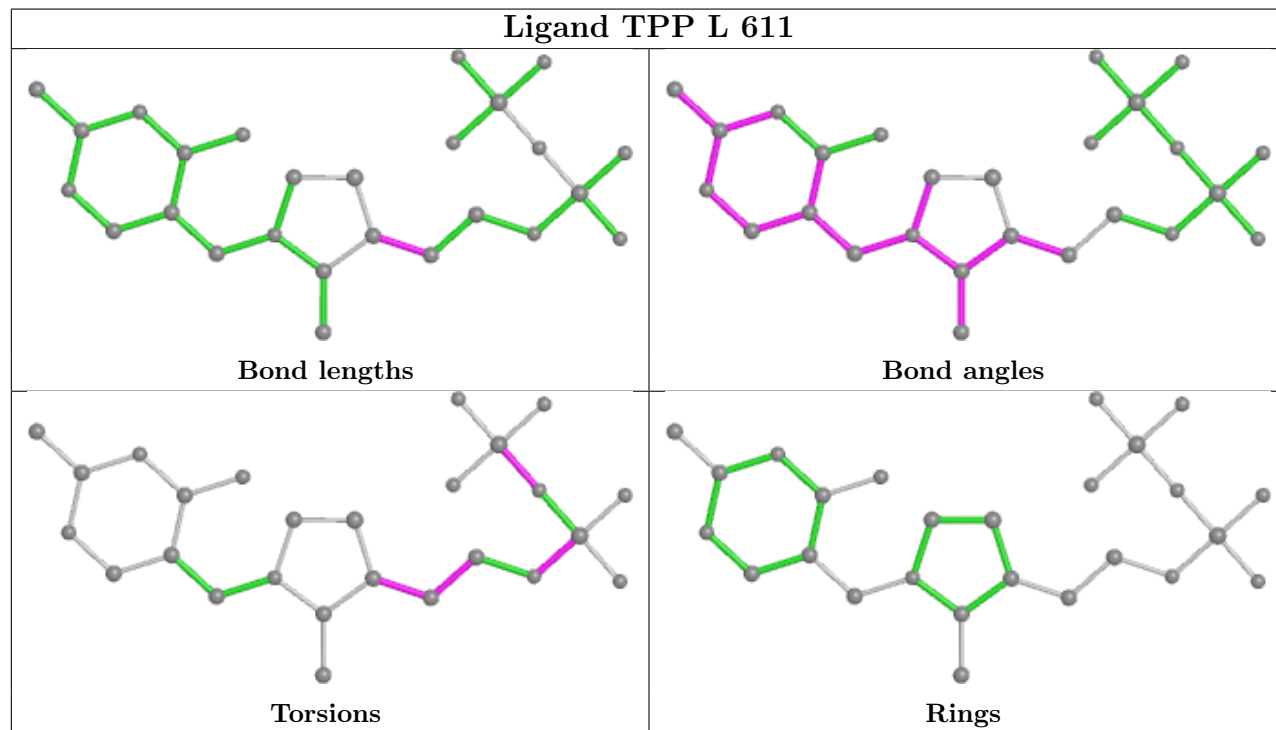
## Ligand TPP G 611



## Ligand TPP J 611

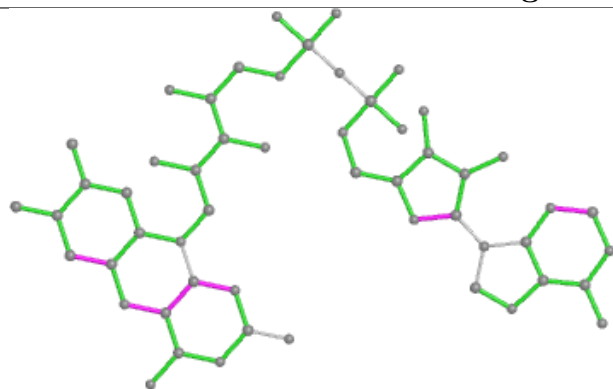


## Ligand TPP L 611

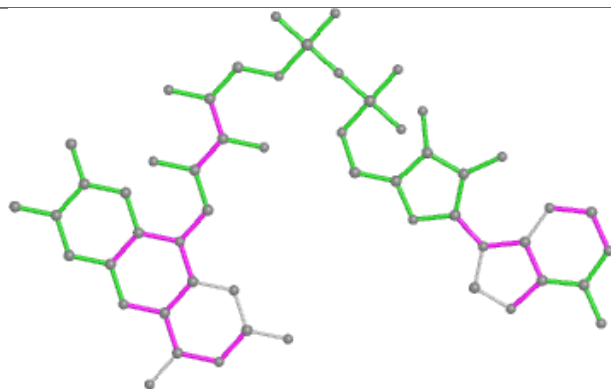




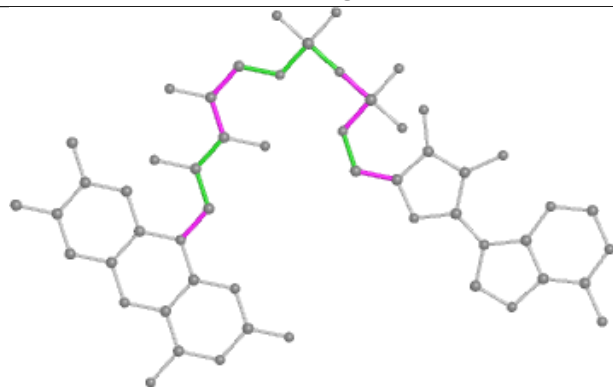
## Ligand FAD I 612



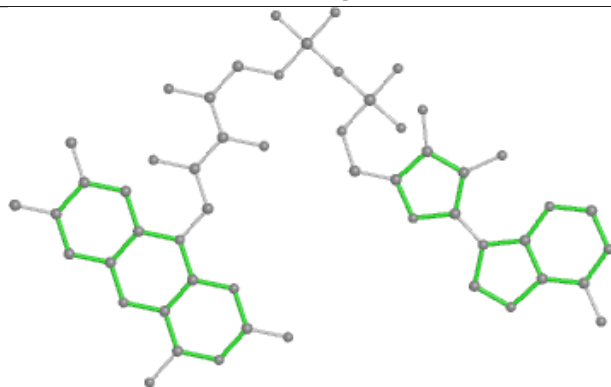
Bond lengths



Bond angles

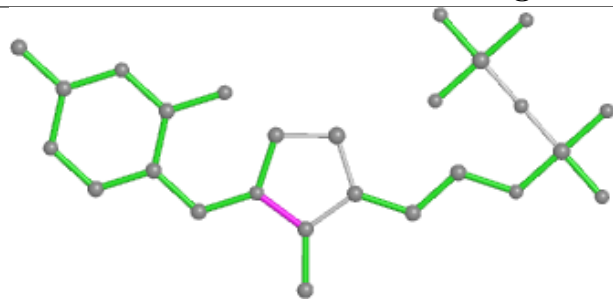


Torsions

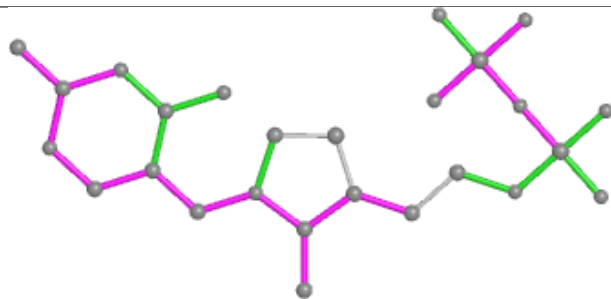


Rings

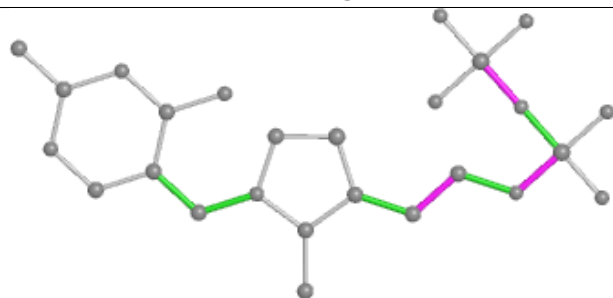
## Ligand TPP H 611



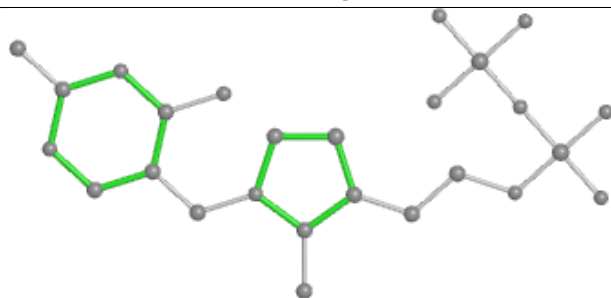
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	527/549 (95%)	-0.13	17 (3%)	47	51	37, 50, 73, 115	10 (1%)
1	B	524/549 (95%)	-0.05	22 (4%)	36	39	39, 60, 92, 128	11 (2%)
1	C	522/549 (95%)	-0.09	24 (4%)	32	34	39, 57, 84, 124	10 (1%)
1	D	520/549 (94%)	-0.09	17 (3%)	46	50	39, 54, 78, 94	10 (1%)
1	E	522/549 (95%)	0.07	26 (4%)	28	30	45, 70, 110, 169	8 (1%)
1	F	521/549 (94%)	0.02	26 (4%)	28	30	48, 71, 103, 143	9 (1%)
1	G	519/549 (94%)	0.09	34 (6%)	18	19	46, 71, 104, 137	8 (1%)
1	H	522/549 (95%)	-0.07	22 (4%)	36	39	45, 62, 96, 147	8 (1%)
1	I	523/549 (95%)	0.01	26 (4%)	28	30	44, 64, 98, 137	10 (1%)
1	J	522/549 (95%)	0.06	27 (5%)	27	29	42, 66, 98, 132	10 (1%)
1	K	523/549 (95%)	-0.06	23 (4%)	34	37	39, 55, 81, 118	10 (1%)
1	L	523/549 (95%)	-0.24	13 (2%)	57	61	38, 51, 75, 119	10 (1%)
All	All	6268/6588 (95%)	-0.04	277 (4%)	34	37	37, 60, 96, 169	114 (1%)

All (277) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	534	ILE	6.8
1	J	465	PHE	6.8
1	J	466	VAL	6.7
1	F	1	MET	6.2
1	H	535	PRO	6.1
1	J	1	MET	6.0
1	K	463	LEU	6.0
1	K	535	PRO	5.9
1	F	463	LEU	5.7
1	D	466	VAL	5.6
1	F	462	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	536	PRO	5.6
1	J	533	ALA	5.4
1	E	479	GLY	5.3
1	I	1	MET	5.3
1	L	466	VAL	5.3
1	E	534	ILE	5.2
1	D	465	PHE	5.2
1	H	479	GLY	5.2
1	I	535	PRO	5.1
1	J	532	LEU	5.0
1	A	1	MET	5.0
1	K	355	LYS	5.0
1	E	464	GLY	5.0
1	K	465	PHE	5.0
1	E	535	PRO	4.9
1	C	465	PHE	4.9
1	B	466	VAL	4.8
1	L	465	PHE	4.8
1	F	481	GLU	4.7
1	K	482	LEU	4.7
1	A	466	VAL	4.6
1	F	464	GLY	4.6
1	K	1	MET	4.6
1	K	533	ALA	4.6
1	H	536	PRO	4.6
1	J	355	LYS	4.5
1	I	465	PHE	4.4
1	L	200	TYR	4.4
1	C	479	GLY	4.4
1	G	479	GLY	4.4
1	F	479	GLY	4.4
1	I	534	ILE	4.3
1	B	465	PHE	4.3
1	E	1	MET	4.2
1	A	2	LYS	4.2
1	I	482	LEU	4.2
1	B	478	ASP	4.1
1	F	534	ILE	4.1
1	J	200	TYR	4.1
1	J	463	LEU	4.1
1	I	481	GLU	4.0
1	G	532	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	I	533	ALA	3.9
1	C	355	LYS	3.8
1	K	2	LYS	3.8
1	I	463	LEU	3.8
1	K	462	VAL	3.8
1	A	539	LYS	3.7
1	K	534	ILE	3.7
1	H	463	LEU	3.7
1	J	534	ILE	3.7
1	L	535	PRO	3.7
1	G	355	LYS	3.7
1	A	200	TYR	3.7
1	H	482	LEU	3.6
1	F	2	LYS	3.6
1	G	354	GLU	3.6
1	G	533	ALA	3.6
1	G	341	ASP	3.5
1	F	355	LYS	3.5
1	D	533	ALA	3.5
1	E	533	ALA	3.5
1	C	38	ARG	3.5
1	C	285	ASP	3.5
1	G	531	GLU	3.5
1	A	462	VAL	3.5
1	G	462	VAL	3.5
1	B	535	PRO	3.5
1	G	464	GLY	3.5
1	D	38	ARG	3.5
1	C	480	THR	3.4
1	H	533	ALA	3.4
1	C	533	ALA	3.4
1	H	481	GLU	3.3
1	B	481	GLU	3.3
1	E	2	LYS	3.3
1	G	38	ARG	3.3
1	L	464	GLY	3.3
1	F	27	ASP	3.3
1	B	27	ASP	3.2
1	G	200	TYR	3.2
1	J	349	LEU	3.2
1	K	354	GLU	3.2
1	F	533	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	38	ARG	3.2
1	L	463	LEU	3.2
1	F	535	PRO	3.2
1	K	484	ASP	3.2
1	F	354	GLU	3.2
1	C	200	TYR	3.2
1	L	534	ILE	3.1
1	D	206	LEU	3.1
1	F	484	ASP	3.1
1	B	340	ARG	3.1
1	G	27	ASP	3.1
1	D	463	LEU	3.1
1	G	463	LEU	3.0
1	A	285	ASP	3.0
1	C	27	ASP	3.0
1	I	355	LYS	3.0
1	B	482	LEU	3.0
1	D	37	ASN	3.0
1	I	2	LYS	3.0
1	J	348	ASP	3.0
1	C	284	THR	3.0
1	E	463	LEU	3.0
1	J	482	LEU	3.0
1	B	37	ASN	3.0
1	G	280	ALA	3.0
1	G	484	ASP	3.0
1	K	38	ARG	2.9
1	E	356	ALA	2.9
1	J	38[A]	ARG	2.9
1	A	465	PHE	2.9
1	K	270	VAL	2.9
1	E	450	LYS	2.9
1	G	2	LYS	2.9
1	I	464	GLY	2.9
1	G	40	GLY	2.8
1	H	531	GLU	2.8
1	I	285	ASP	2.8
1	C	354	GLU	2.8
1	G	344	LYS	2.8
1	H	355	LYS	2.8
1	E	518	ASP	2.8
1	F	480	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	1	MET	2.8
1	A	463	LEU	2.8
1	C	463	LEU	2.8
1	H	532	LEU	2.8
1	J	464	GLY	2.8
1	B	330	LYS	2.8
1	I	462	VAL	2.8
1	G	481	GLU	2.8
1	G	480	THR	2.8
1	I	260	PHE	2.8
1	D	482	LEU	2.8
1	H	354	GLU	2.7
1	J	462	VAL	2.7
1	L	533	ALA	2.7
1	B	260	PHE	2.7
1	I	200	TYR	2.7
1	F	352	PRO	2.7
1	E	337	GLU	2.7
1	H	429	ALA	2.7
1	B	171	GLY	2.7
1	I	330	LYS	2.7
1	C	462	VAL	2.7
1	A	284	THR	2.7
1	J	479	GLY	2.6
1	L	479	GLY	2.6
1	B	344	LYS	2.6
1	A	479	GLY	2.6
1	J	354	GLU	2.6
1	L	481	GLU	2.6
1	B	450	LYS	2.6
1	H	330	LYS	2.6
1	D	518	ASP	2.6
1	E	429	ALA	2.6
1	J	284	THR	2.6
1	B	531	GLU	2.6
1	J	285	ASP	2.6
1	F	482	LEU	2.6
1	F	170	GLU	2.6
1	C	466	VAL	2.5
1	I	354	GLU	2.5
1	D	205	ALA	2.5
1	G	431	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	455	ILE	2.5
1	F	518	ASP	2.5
1	J	484	ASP	2.5
1	E	529	LYS	2.5
1	K	464	GLY	2.5
1	F	260	PHE	2.5
1	G	199	ARG	2.5
1	J	531	GLU	2.5
1	A	328	ASP	2.5
1	E	484	ASP	2.5
1	J	518	ASP	2.5
1	E	331	PHE	2.5
1	H	1	MET	2.5
1	G	285	ASP	2.5
1	I	284	THR	2.5
1	J	2	LYS	2.4
1	I	40	GLY	2.4
1	I	479	GLY	2.4
1	B	355	LYS	2.4
1	H	348	ASP	2.4
1	K	531	GLU	2.4
1	B	38	ARG	2.4
1	F	344	LYS	2.4
1	C	429	ALA	2.4
1	D	271	LEU	2.4
1	F	348	ASP	2.4
1	K	341	ASP	2.4
1	I	38	ARG	2.4
1	J	327	ALA	2.4
1	I	37	ASN	2.4
1	J	517	ILE	2.4
1	F	368	HIS	2.4
1	I	230	ILE	2.4
1	I	372	ASP	2.4
1	H	484	ASP	2.3
1	D	270	VAL	2.3
1	H	347	ASP	2.3
1	H	412	MET	2.3
1	L	39	MET	2.3
1	F	171	GLY	2.3
1	C	34	ASP	2.3
1	J	344	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	34	ASP	2.3
1	G	482	LEU	2.3
1	A	411	ALA	2.3
1	F	531	GLU	2.3
1	D	355	LYS	2.2
1	C	37	ASN	2.2
1	K	479	GLY	2.2
1	K	289	ILE	2.2
1	B	200	TYR	2.2
1	K	265	ASN	2.2
1	G	461	SER	2.2
1	H	424	GLU	2.2
1	F	349	LEU	2.2
1	B	317	ARG	2.2
1	H	455	ILE	2.2
1	E	171	GLY	2.2
1	I	348	ASP	2.2
1	K	27	ASP	2.2
1	B	1	MET	2.2
1	A	208	CYS	2.2
1	G	483	HIS	2.2
1	E	355	LYS	2.2
1	K	411	ALA	2.2
1	E	340	ARG	2.2
1	E	344	LYS	2.1
1	E	516	SER	2.2
1	L	355	LYS	2.1
1	C	324	GLU	2.1
1	G	265	ASN	2.1
1	A	206	LEU	2.1
1	J	25	THR	2.1
1	D	272	LEU	2.1
1	E	482	LEU	2.1
1	I	206	LEU	2.1
1	A	518	ASP	2.1
1	C	464	GLY	2.1
1	G	345	GLY	2.1
1	G	377	THR	2.1
1	C	260	PHE	2.1
1	C	482	LEU	2.1
1	B	337	GLU	2.1
1	C	531	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	430	MET	2.1
1	A	484	ASP	2.1
1	E	34	ASP	2.1
1	H	349	LEU	2.1
1	G	450	LYS	2.1
1	G	518	ASP	2.0
1	K	518	ASP	2.0
1	C	534	ILE	2.0
1	D	200	TYR	2.0
1	E	455	ILE	2.0
1	D	532	LEU	2.0
1	G	41	THR	2.0
1	L	462	VAL	2.0
1	B	285	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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(Å <sup>2</sup> )	Q<0.9
5	PO4	D	616	5/5	0.61	0.45	67,67,69,69	5
5	PO4	C	615	5/5	0.69	0.33	72,73,73,74	5
4	MG	F	613	1/1	0.70	0.08	76,76,76,76	0
4	MG	G	613	1/1	0.70	0.10	67,67,67,67	0
4	MG	E	613	1/1	0.72	0.07	70,70,70,70	0
4	MG	K	613	1/1	0.76	0.19	50,50,50,50	0
4	MG	L	613	1/1	0.76	0.12	47,47,47,47	0
5	PO4	A	615	5/5	0.77	0.30	62,62,64,66	5
5	PO4	H	614	5/5	0.79	0.28	98,99,99,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	B	613	1/1	0.80	0.12	55,55,55,55	0
5	PO4	A	619	5/5	0.81	0.32	72,73,74,74	5
5	PO4	E	615	5/5	0.81	0.25	73,73,74,74	5
4	MG	J	613	1/1	0.81	0.13	72,72,72,72	0
4	MG	D	613	1/1	0.82	0.16	57,57,57,57	0
5	PO4	B	616	5/5	0.82	0.41	71,71,72,73	5
4	MG	C	613	1/1	0.82	0.12	63,63,63,63	0
5	PO4	B	615	5/5	0.84	0.22	71,71,72,72	5
5	PO4	A	617	5/5	0.84	0.21	66,67,68,68	5
4	MG	A	613	1/1	0.85	0.11	52,52,52,52	0
5	PO4	L	617	5/5	0.85	0.24	58,58,60,61	5
5	PO4	D	620	5/5	0.86	0.27	51,53,54,55	5
5	PO4	A	616	5/5	0.86	0.31	56,57,58,58	5
5	PO4	I	614	5/5	0.87	0.15	68,68,68,69	5
5	PO4	L	615	5/5	0.88	0.32	91,92,93,93	0
5	PO4	D	619	5/5	0.89	0.18	68,69,69,70	5
5	PO4	L	614	5/5	0.89	0.20	97,97,98,98	0
5	PO4	G	616	5/5	0.89	0.20	71,71,71,72	5
5	PO4	D	618	5/5	0.89	0.21	67,68,69,69	5
5	PO4	D	614	5/5	0.90	0.21	68,68,69,69	5
5	PO4	D	617	5/5	0.91	0.26	61,61,62,62	5
5	PO4	F	615	5/5	0.91	0.21	61,61,62,64	5
5	PO4	L	618	5/5	0.91	0.20	63,63,64,65	5
4	MG	I	613	1/1	0.92	0.08	62,62,62,62	0
5	PO4	A	618	5/5	0.93	0.13	56,56,57,57	5
4	MG	H	613	1/1	0.93	0.07	59,59,59,59	0
5	PO4	J	614	5/5	0.94	0.15	89,89,90,91	0
5	PO4	C	614	5/5	0.94	0.12	73,74,75,77	0
5	PO4	G	614	5/5	0.94	0.20	65,65,66,66	5
5	PO4	G	615	5/5	0.94	0.16	84,85,86,86	0
5	PO4	I	615	5/5	0.94	0.15	91,91,92,93	0
5	PO4	K	614	5/5	0.95	0.19	69,72,72,73	0
2	TPP	E	611	26/26	0.95	0.13	59,65,67,69	0
5	PO4	E	614	5/5	0.95	0.13	96,96,97,98	0
2	TPP	G	611	26/26	0.95	0.14	56,59,62,63	0
5	PO4	F	614	5/5	0.95	0.13	91,91,92,93	0
3	FAD	G	612	53/53	0.96	0.11	52,57,64,64	0
2	TPP	J	611	26/26	0.96	0.11	48,61,63,65	0
5	PO4	D	615	5/5	0.96	0.15	73,73,74,75	0
5	PO4	B	614	5/5	0.96	0.16	69,70,72,73	0
3	FAD	F	612	53/53	0.97	0.09	50,55,59,63	0
2	TPP	F	611	26/26	0.97	0.11	50,61,63,65	0

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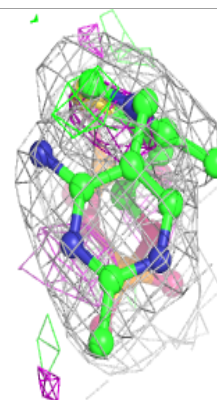
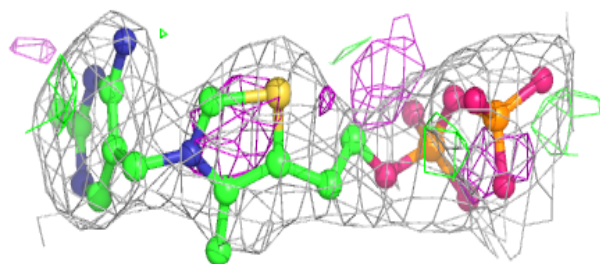
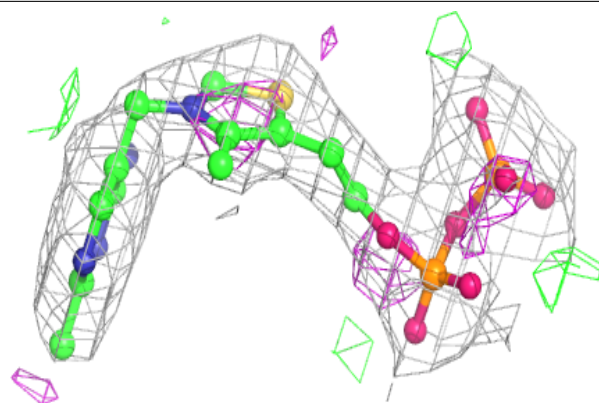
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FAD	I	612	53/53	0.97	0.10	45,49,53,57	0
3	FAD	J	612	53/53	0.97	0.10	47,52,57,60	0
3	FAD	K	612	53/53	0.97	0.10	40,45,52,55	0
5	PO4	H	615	5/5	0.97	0.11	82,83,84,85	0
5	PO4	A	614	5/5	0.97	0.11	70,70,72,73	0
2	TPP	C	611	26/26	0.97	0.11	43,49,53,54	0
2	TPP	I	611	26/26	0.97	0.11	44,56,58,60	0
2	TPP	B	611	26/26	0.97	0.10	42,50,54,58	0
2	TPP	L	611	26/26	0.97	0.10	43,46,49,50	0
3	FAD	C	612	53/53	0.97	0.10	38,46,50,53	0
3	FAD	D	612	53/53	0.97	0.11	39,43,48,49	0
3	FAD	E	612	53/53	0.97	0.10	53,57,63,65	0
3	FAD	L	612	53/53	0.98	0.10	40,45,47,50	0
2	TPP	K	611	26/26	0.98	0.10	39,45,48,50	0
2	TPP	H	611	26/26	0.98	0.09	55,58,60,63	0
3	FAD	A	612	53/53	0.98	0.10	36,41,44,45	0
3	FAD	H	612	53/53	0.98	0.09	45,49,53,54	0
3	FAD	B	612	53/53	0.98	0.09	43,47,52,52	0
2	TPP	D	611	26/26	0.98	0.11	42,48,51,51	0
2	TPP	A	611	26/26	0.98	0.10	39,46,49,50	0
5	PO4	L	616	5/5	0.99	0.10	67,67,68,69	0

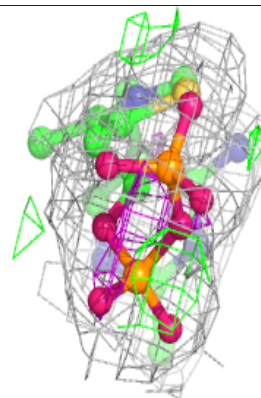
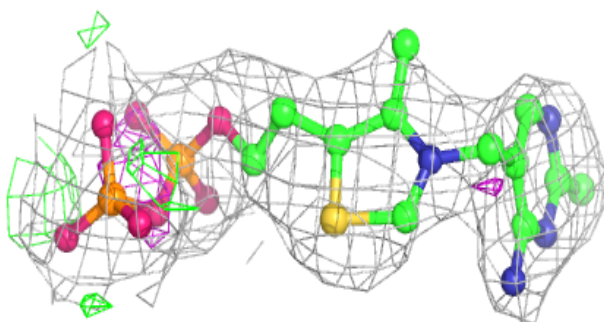
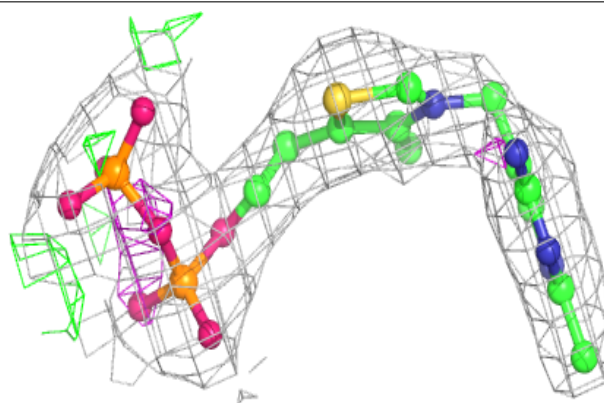
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TPP E 611:**

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

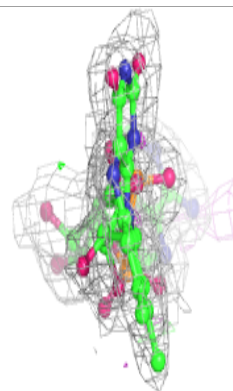
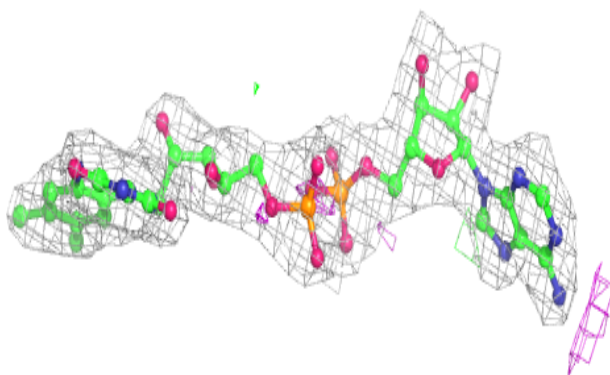
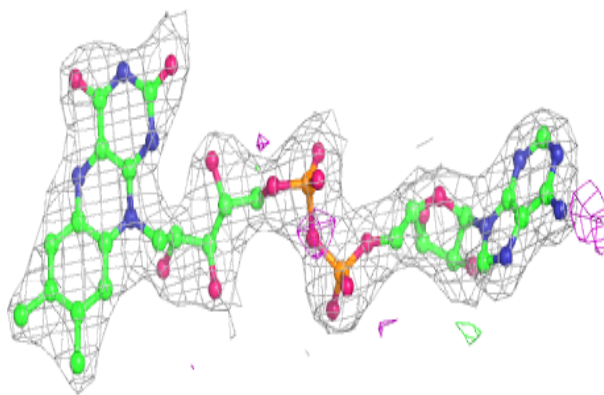
**Electron density around TPP G 611:**

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

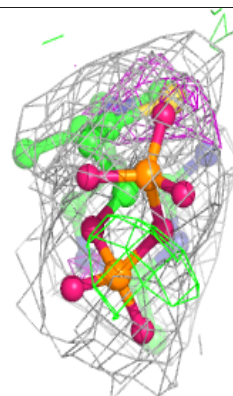
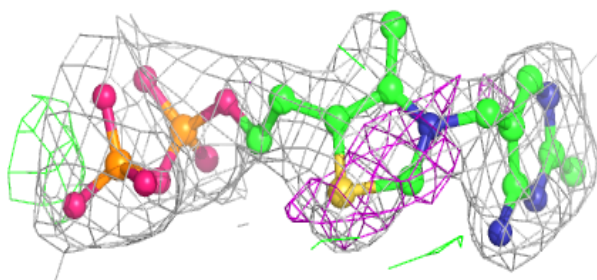
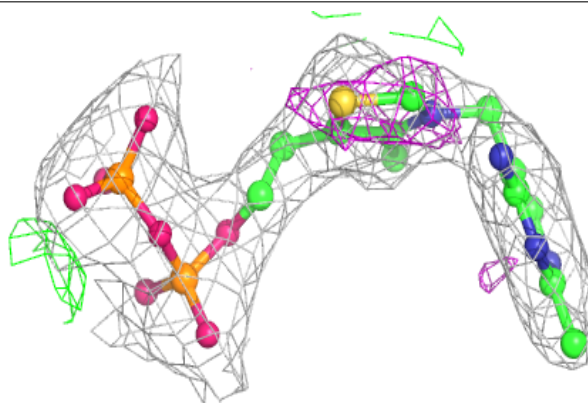


**Electron density around FAD G 612:**

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

**Electron density around TPP J 611:**

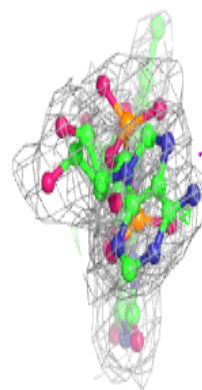
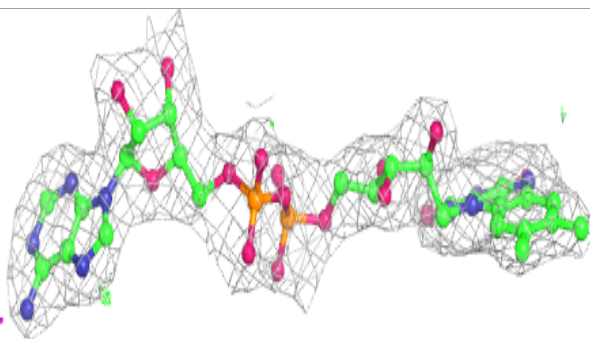
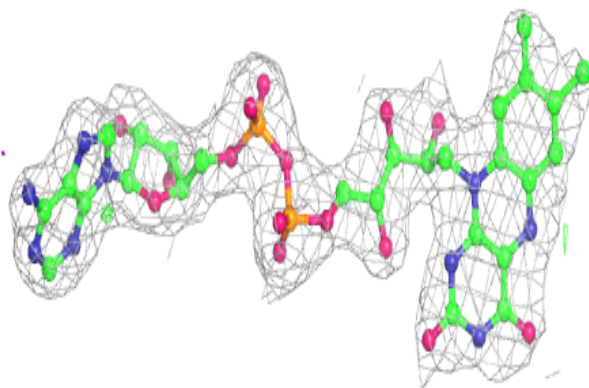
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



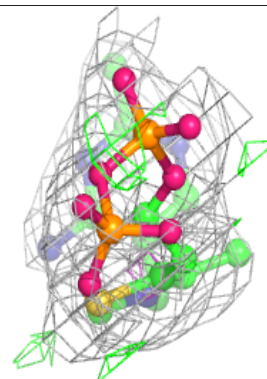
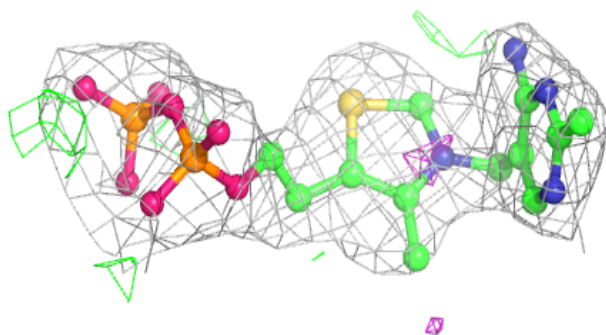
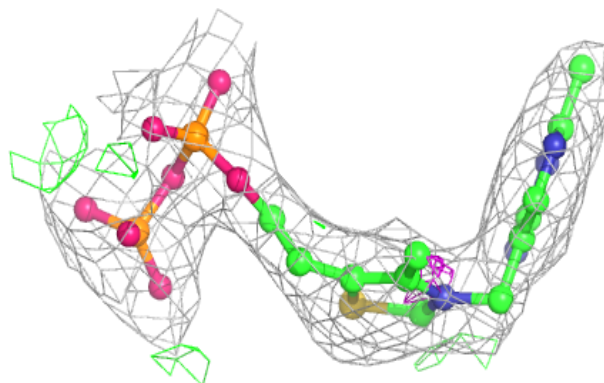


**Electron density around FAD F 612:**

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

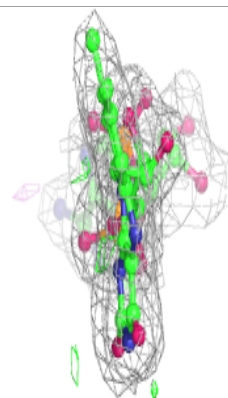
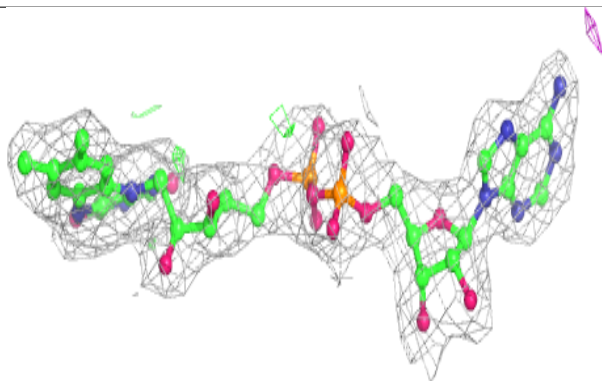
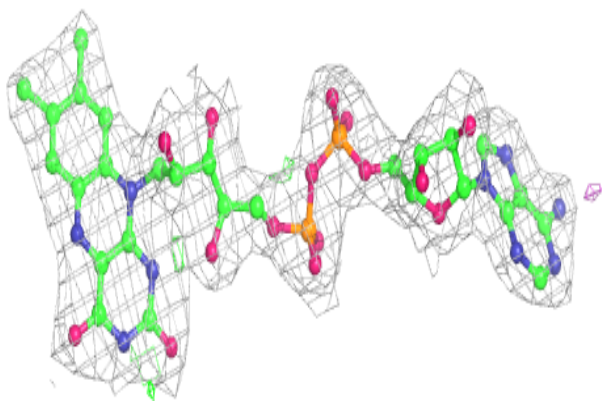
**Electron density around TPP F 611:**

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

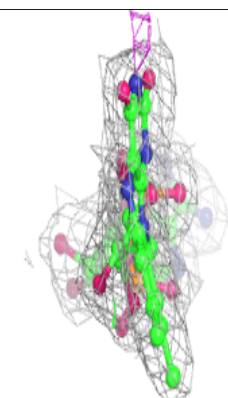
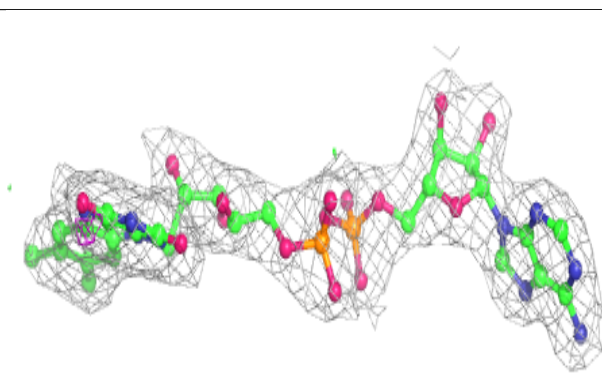
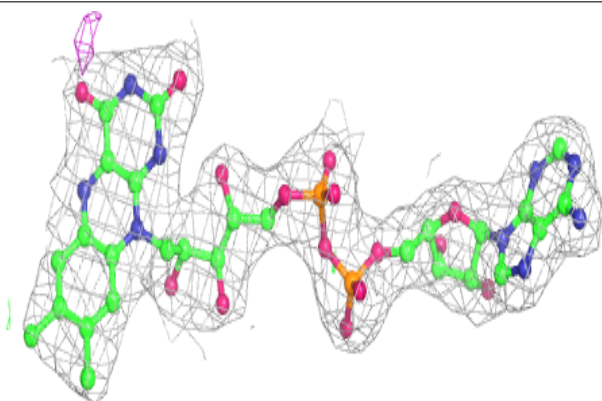


**Electron density around FAD I 612:**

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

**Electron density around FAD J 612:**

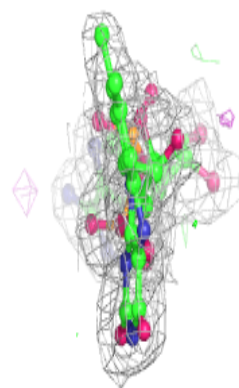
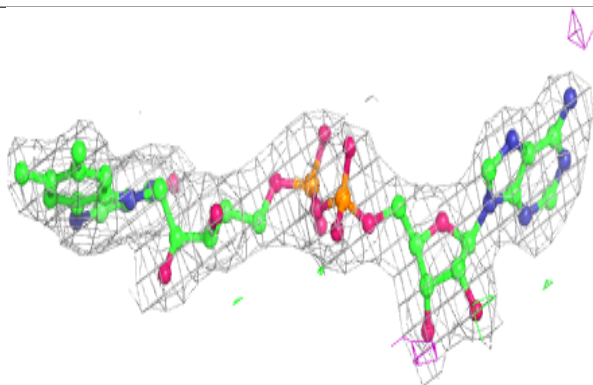
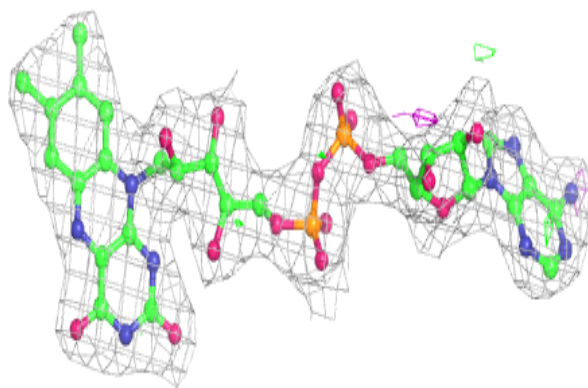
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



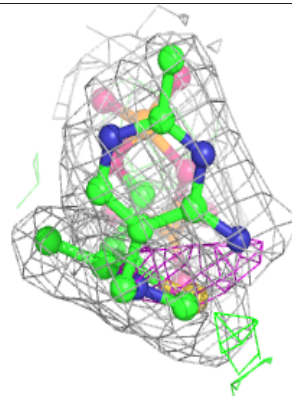
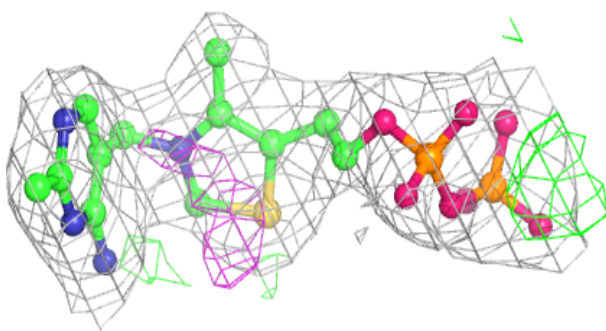
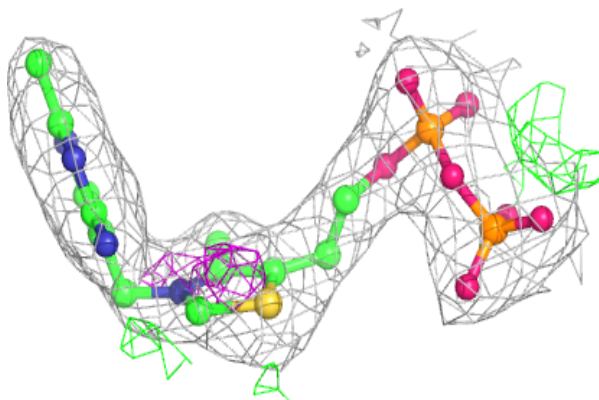


**Electron density around FAD K 612:**

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

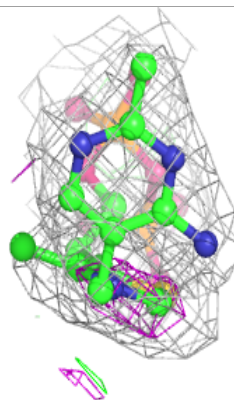
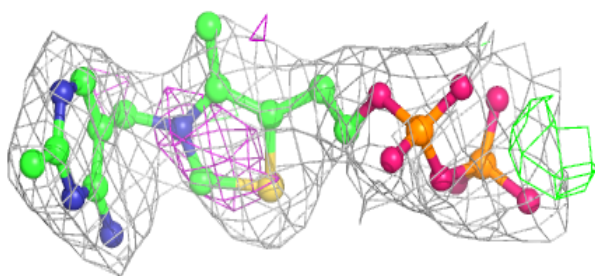
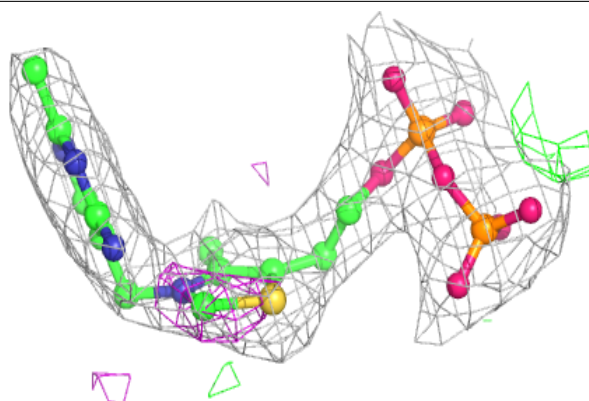
**Electron density around TPP C 611:**

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

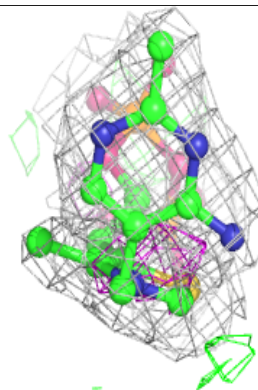
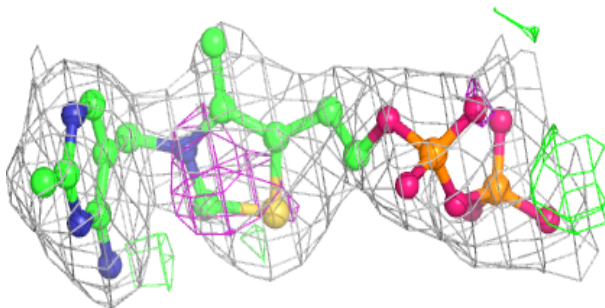
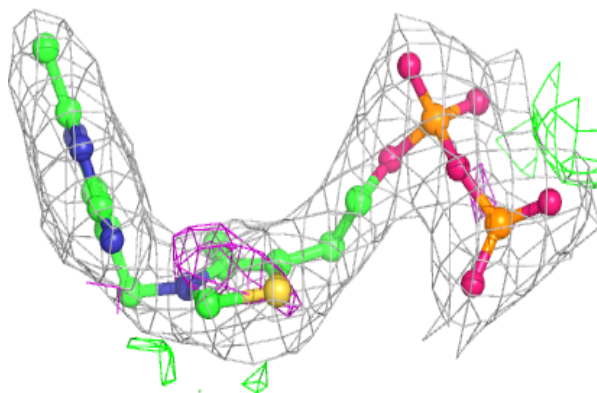


**Electron density around TPP I 611:**

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

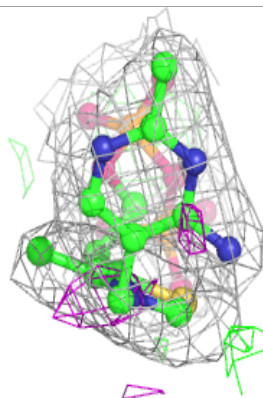
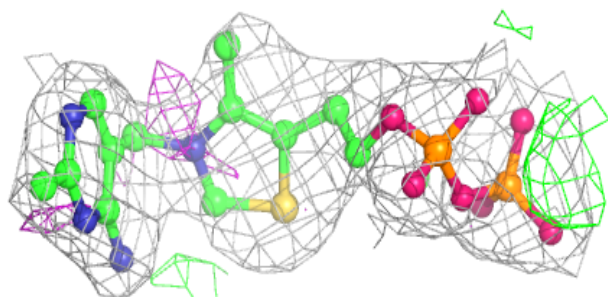
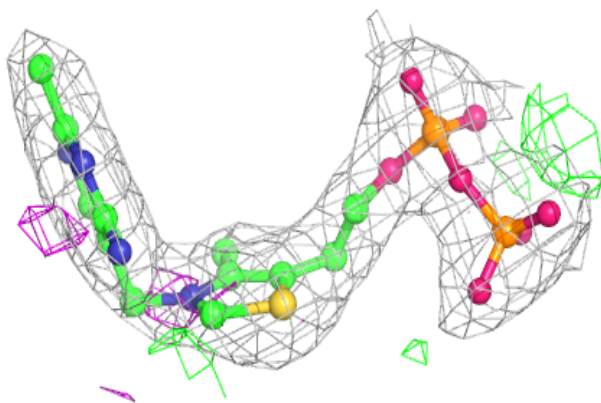
**Electron density around TPP B 611:**

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

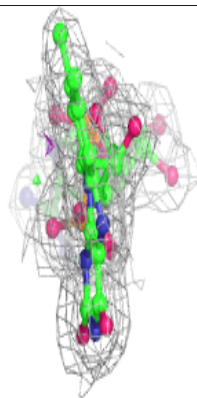
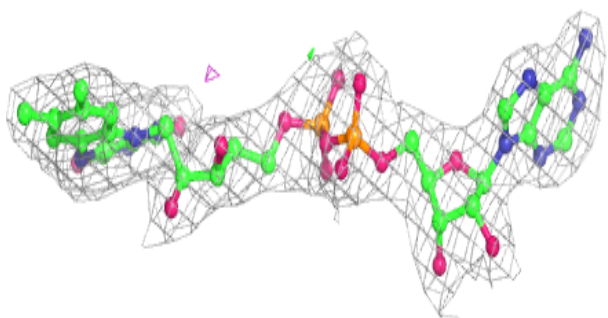
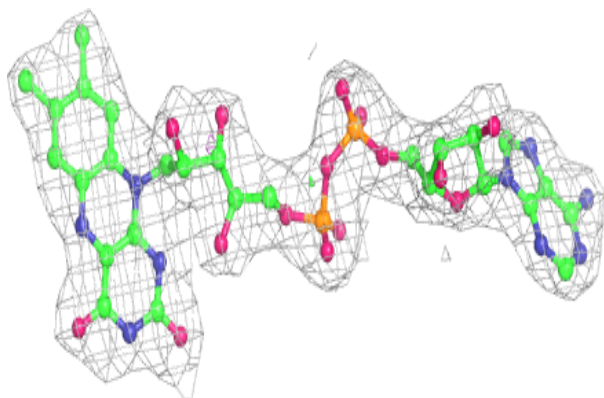


**Electron density around TPP L 611:**

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

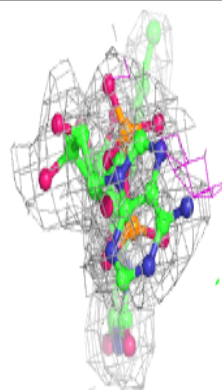
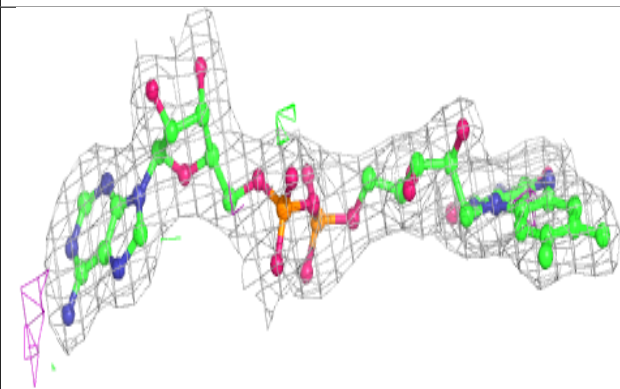
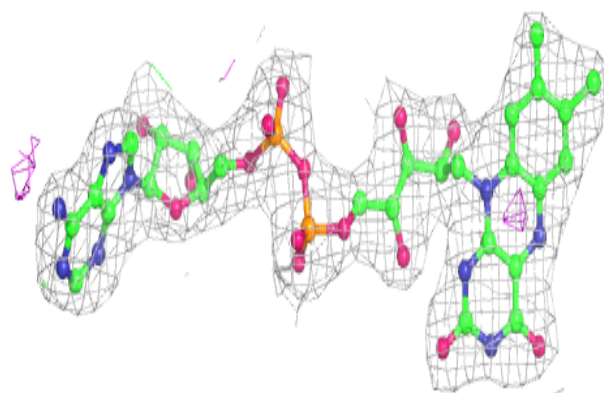
**Electron density around FAD C 612:**

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

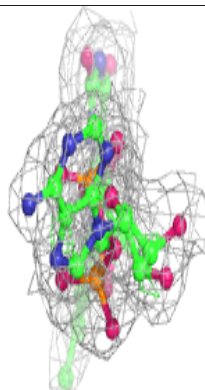
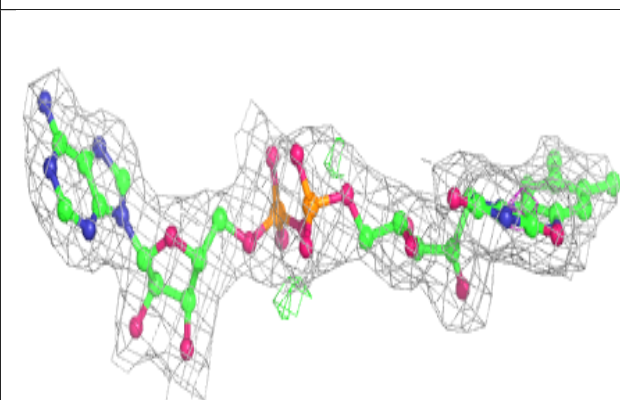
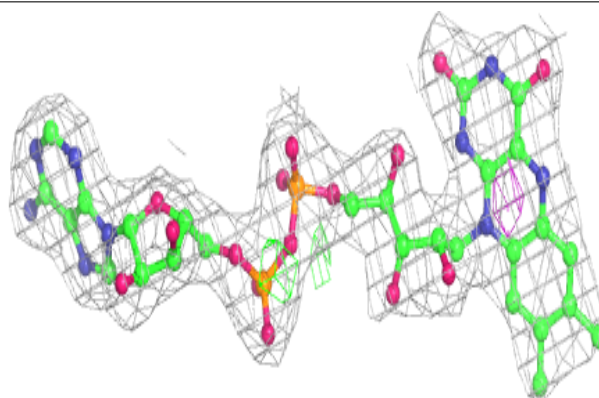


**Electron density around FAD D 612:**

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

**Electron density around FAD E 612:**

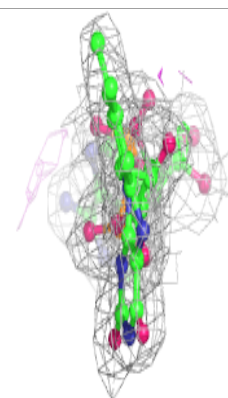
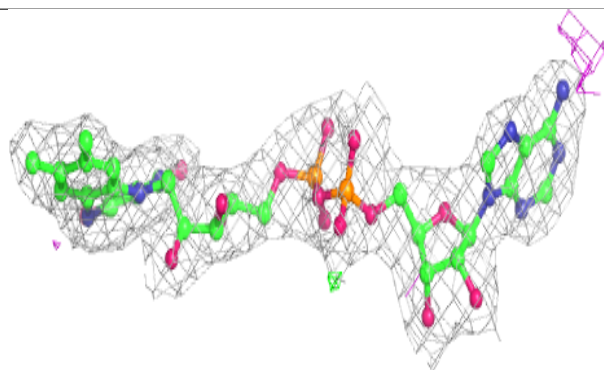
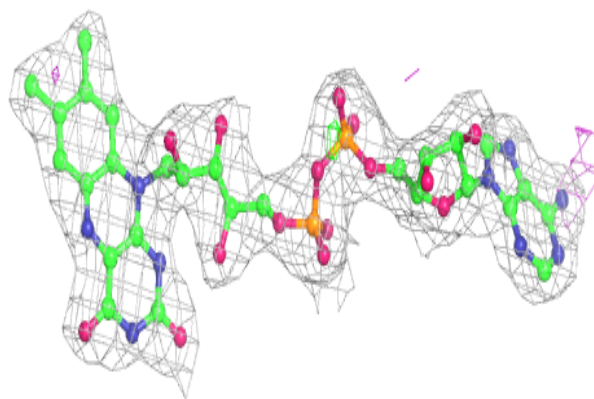
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



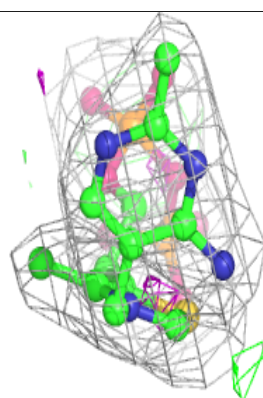
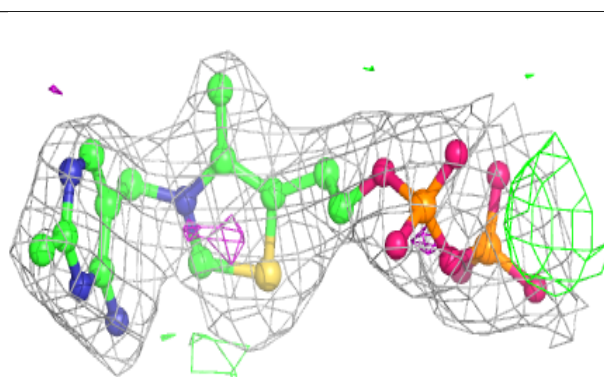
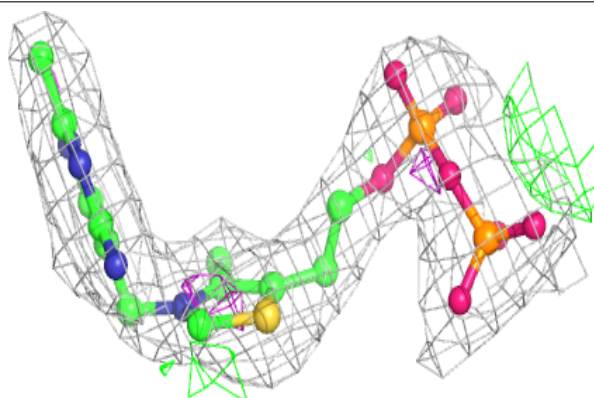


**Electron density around FAD L 612:**

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

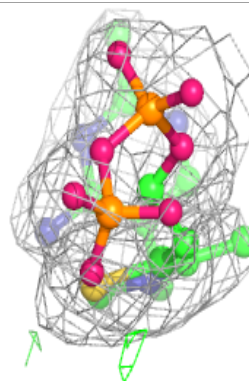
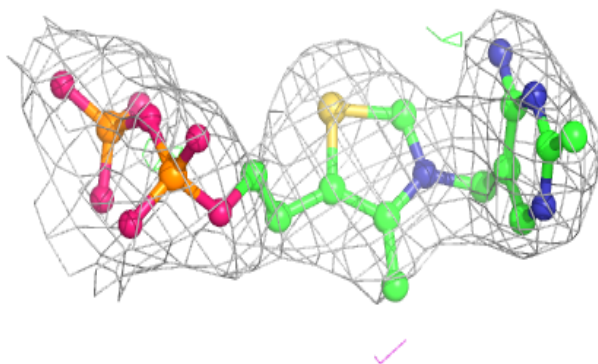
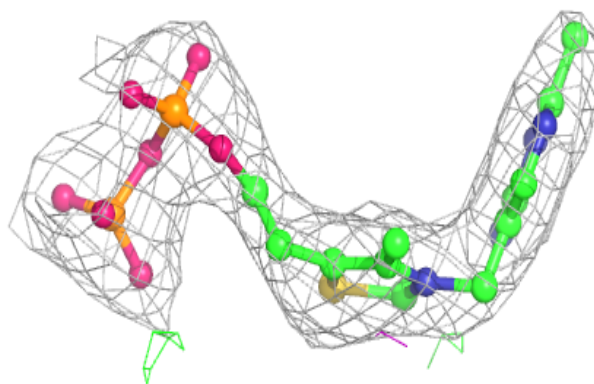
**Electron density around TPP K 611:**

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

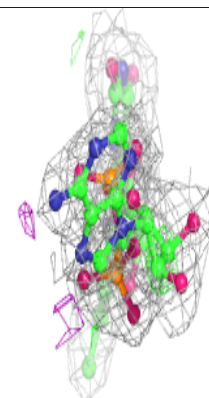
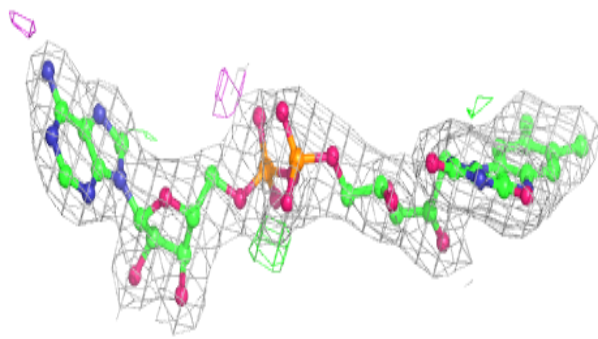
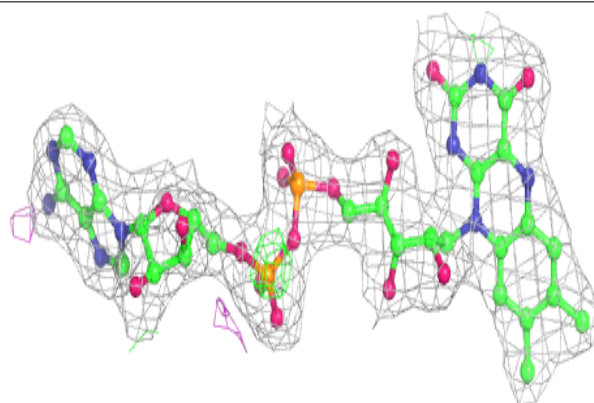


**Electron density around TPP H 611:**

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

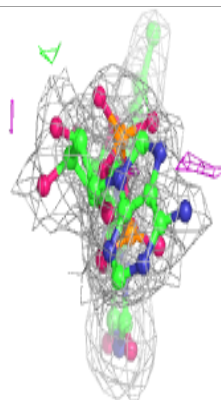
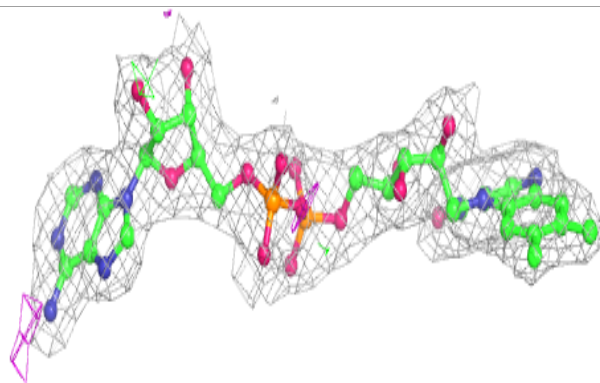
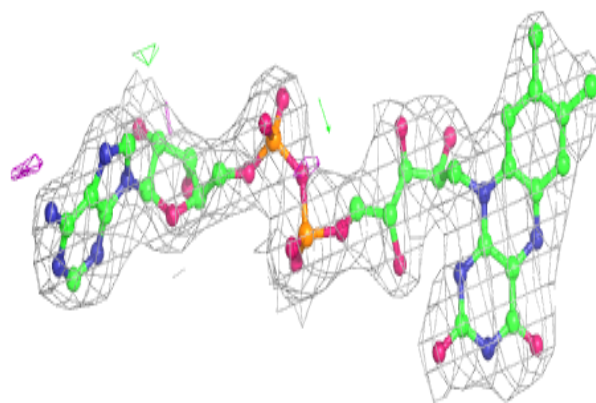
**Electron density around FAD A 612:**

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

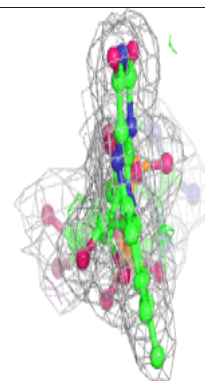
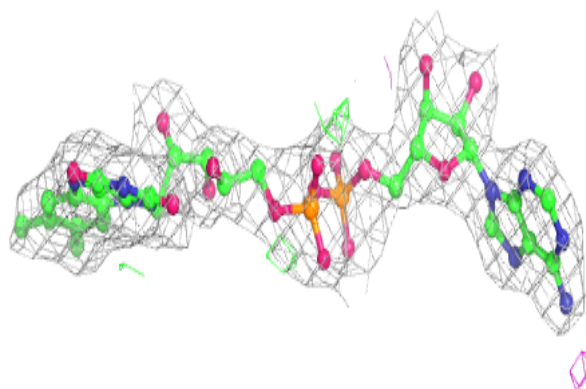
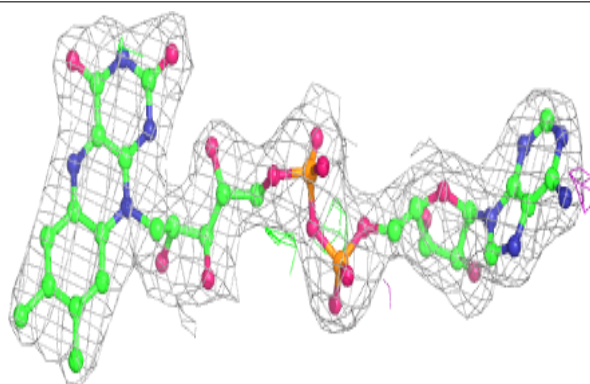


**Electron density around FAD H 612:**

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

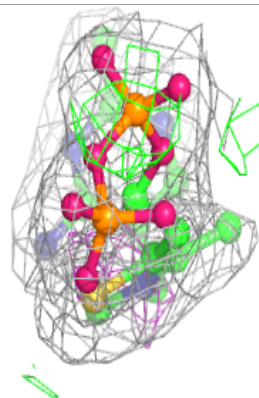
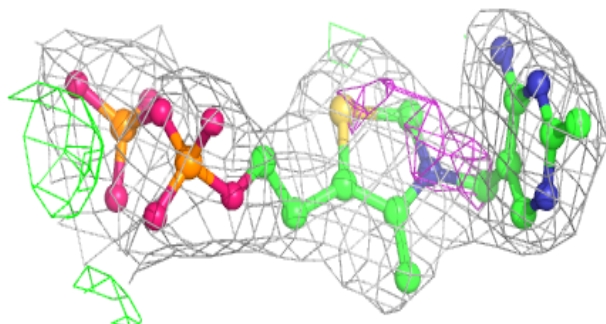
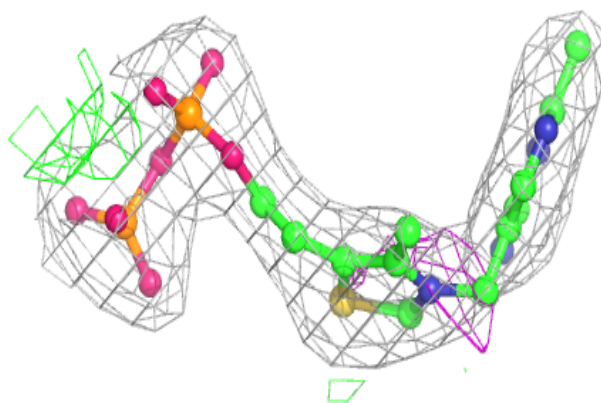
**Electron density around FAD B 612:**

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

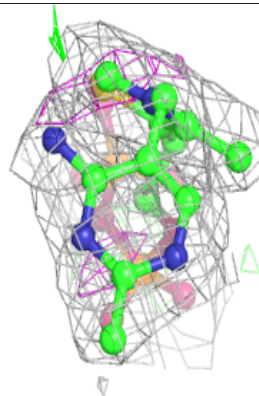
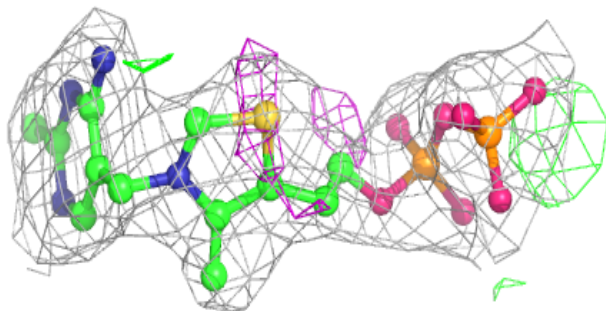
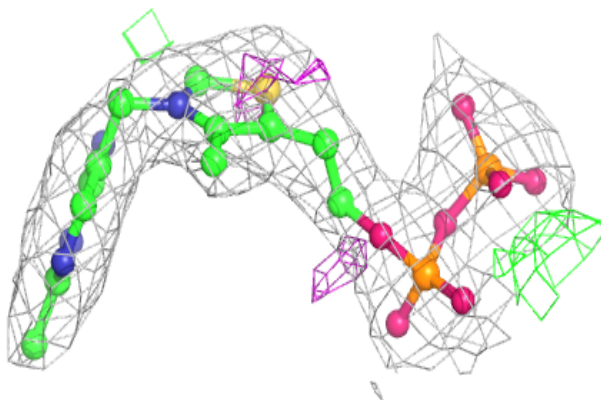


**Electron density around TPP D 611:**

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

**Electron density around TPP A 611:**

$2mF_o-DF_c$  (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.