Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2021 – 04:57 PM EDT

PDB ID	:	2PAN
Title	:	Crystal structure of E. coli glyoxylate carboligase
Authors	:	Kaplun, A.; Chipman, D.M.; Barak, Z.; Vyazmensky, M.; Shaanan, B.
Deposited on	:	2007-03-27
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

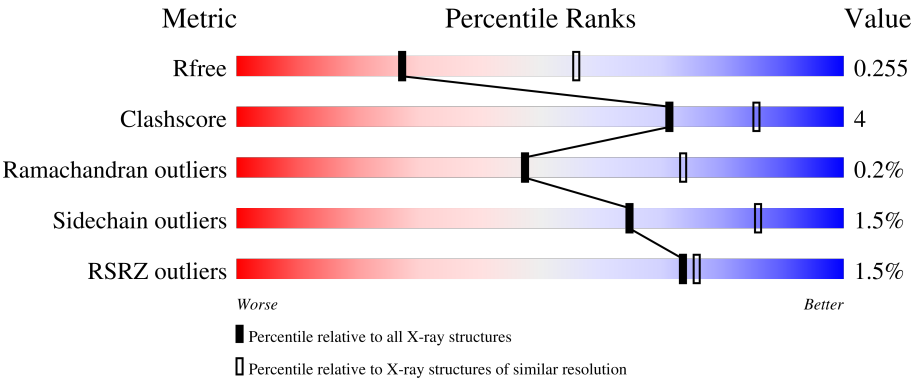
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.22
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	616	86% 9% .
1	B	616	87% 8% .
1	C	616	% 88% 8% .
1	D	616	% 87% 9% .
1	E	616	4% 89% 7% .

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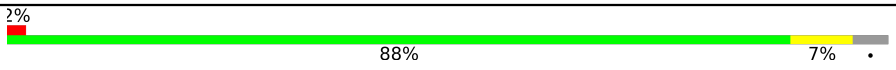
Mol	Chain	Length	Quality of chain
1	F	616	

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	DTT	C	901	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 28107 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 Glyoxylate carboligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	592	Total	C	N	O	S	Se	0	0	0
			4530	2870	792	834	12	22			
1	B	592	Total	C	N	O	S	Se	0	0	0
			4530	2870	792	834	12	22			
1	C	592	Total	C	N	O	S	Se	0	0	0
			4530	2870	792	834	12	22			
1	D	592	Total	C	N	O	S	Se	0	0	0
			4530	2870	792	834	12	22			
1	E	592	Total	C	N	O	S	Se	0	0	0
			4530	2870	792	834	12	22			
1	F	592	Total	C	N	O	S	Se	0	0	0
			4530	2870	792	834	12	22			

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	expression tag	UNP P0AEP7
A	-21	GLY	-	expression tag	UNP P0AEP7
A	-20	SER	-	expression tag	UNP P0AEP7
A	-19	SER	-	expression tag	UNP P0AEP7
A	-18	HIS	-	expression tag	UNP P0AEP7
A	-17	HIS	-	expression tag	UNP P0AEP7
A	-16	HIS	-	expression tag	UNP P0AEP7
A	-15	HIS	-	expression tag	UNP P0AEP7
A	-14	HIS	-	expression tag	UNP P0AEP7
A	-13	HIS	-	expression tag	UNP P0AEP7
A	-12	SER	-	expression tag	UNP P0AEP7
A	-11	SER	-	expression tag	UNP P0AEP7
A	-10	GLY	-	expression tag	UNP P0AEP7
A	-9	LEU	-	expression tag	UNP P0AEP7
A	-8	VAL	-	expression tag	UNP P0AEP7
A	-7	PRO	-	expression tag	UNP P0AEP7
A	-6	ARG	-	expression tag	UNP P0AEP7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP P0AEP7
A	-4	SER	-	expression tag	UNP P0AEP7
A	-3	HIS	-	expression tag	UNP P0AEP7
A	-2	MSE	-	expression tag	UNP P0AEP7
A	-1	ALA	-	expression tag	UNP P0AEP7
A	0	SER	-	expression tag	UNP P0AEP7
B	-22	MSE	-	expression tag	UNP P0AEP7
B	-21	GLY	-	expression tag	UNP P0AEP7
B	-20	SER	-	expression tag	UNP P0AEP7
B	-19	SER	-	expression tag	UNP P0AEP7
B	-18	HIS	-	expression tag	UNP P0AEP7
B	-17	HIS	-	expression tag	UNP P0AEP7
B	-16	HIS	-	expression tag	UNP P0AEP7
B	-15	HIS	-	expression tag	UNP P0AEP7
B	-14	HIS	-	expression tag	UNP P0AEP7
B	-13	HIS	-	expression tag	UNP P0AEP7
B	-12	SER	-	expression tag	UNP P0AEP7
B	-11	SER	-	expression tag	UNP P0AEP7
B	-10	GLY	-	expression tag	UNP P0AEP7
B	-9	LEU	-	expression tag	UNP P0AEP7
B	-8	VAL	-	expression tag	UNP P0AEP7
B	-7	PRO	-	expression tag	UNP P0AEP7
B	-6	ARG	-	expression tag	UNP P0AEP7
B	-5	GLY	-	expression tag	UNP P0AEP7
B	-4	SER	-	expression tag	UNP P0AEP7
B	-3	HIS	-	expression tag	UNP P0AEP7
B	-2	MSE	-	expression tag	UNP P0AEP7
B	-1	ALA	-	expression tag	UNP P0AEP7
B	0	SER	-	expression tag	UNP P0AEP7
C	-22	MSE	-	expression tag	UNP P0AEP7
C	-21	GLY	-	expression tag	UNP P0AEP7
C	-20	SER	-	expression tag	UNP P0AEP7
C	-19	SER	-	expression tag	UNP P0AEP7
C	-18	HIS	-	expression tag	UNP P0AEP7
C	-17	HIS	-	expression tag	UNP P0AEP7
C	-16	HIS	-	expression tag	UNP P0AEP7
C	-15	HIS	-	expression tag	UNP P0AEP7
C	-14	HIS	-	expression tag	UNP P0AEP7
C	-13	HIS	-	expression tag	UNP P0AEP7
C	-12	SER	-	expression tag	UNP P0AEP7
C	-11	SER	-	expression tag	UNP P0AEP7
C	-10	GLY	-	expression tag	UNP P0AEP7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	LEU	-	expression tag	UNP P0AEP7
C	-8	VAL	-	expression tag	UNP P0AEP7
C	-7	PRO	-	expression tag	UNP P0AEP7
C	-6	ARG	-	expression tag	UNP P0AEP7
C	-5	GLY	-	expression tag	UNP P0AEP7
C	-4	SER	-	expression tag	UNP P0AEP7
C	-3	HIS	-	expression tag	UNP P0AEP7
C	-2	MSE	-	expression tag	UNP P0AEP7
C	-1	ALA	-	expression tag	UNP P0AEP7
C	0	SER	-	expression tag	UNP P0AEP7
D	-22	MSE	-	expression tag	UNP P0AEP7
D	-21	GLY	-	expression tag	UNP P0AEP7
D	-20	SER	-	expression tag	UNP P0AEP7
D	-19	SER	-	expression tag	UNP P0AEP7
D	-18	HIS	-	expression tag	UNP P0AEP7
D	-17	HIS	-	expression tag	UNP P0AEP7
D	-16	HIS	-	expression tag	UNP P0AEP7
D	-15	HIS	-	expression tag	UNP P0AEP7
D	-14	HIS	-	expression tag	UNP P0AEP7
D	-13	HIS	-	expression tag	UNP P0AEP7
D	-12	SER	-	expression tag	UNP P0AEP7
D	-11	SER	-	expression tag	UNP P0AEP7
D	-10	GLY	-	expression tag	UNP P0AEP7
D	-9	LEU	-	expression tag	UNP P0AEP7
D	-8	VAL	-	expression tag	UNP P0AEP7
D	-7	PRO	-	expression tag	UNP P0AEP7
D	-6	ARG	-	expression tag	UNP P0AEP7
D	-5	GLY	-	expression tag	UNP P0AEP7
D	-4	SER	-	expression tag	UNP P0AEP7
D	-3	HIS	-	expression tag	UNP P0AEP7
D	-2	MSE	-	expression tag	UNP P0AEP7
D	-1	ALA	-	expression tag	UNP P0AEP7
D	0	SER	-	expression tag	UNP P0AEP7
E	-22	MSE	-	expression tag	UNP P0AEP7
E	-21	GLY	-	expression tag	UNP P0AEP7
E	-20	SER	-	expression tag	UNP P0AEP7
E	-19	SER	-	expression tag	UNP P0AEP7
E	-18	HIS	-	expression tag	UNP P0AEP7
E	-17	HIS	-	expression tag	UNP P0AEP7
E	-16	HIS	-	expression tag	UNP P0AEP7
E	-15	HIS	-	expression tag	UNP P0AEP7
E	-14	HIS	-	expression tag	UNP P0AEP7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-13	HIS	-	expression tag	UNP P0AEP7
E	-12	SER	-	expression tag	UNP P0AEP7
E	-11	SER	-	expression tag	UNP P0AEP7
E	-10	GLY	-	expression tag	UNP P0AEP7
E	-9	LEU	-	expression tag	UNP P0AEP7
E	-8	VAL	-	expression tag	UNP P0AEP7
E	-7	PRO	-	expression tag	UNP P0AEP7
E	-6	ARG	-	expression tag	UNP P0AEP7
E	-5	GLY	-	expression tag	UNP P0AEP7
E	-4	SER	-	expression tag	UNP P0AEP7
E	-3	HIS	-	expression tag	UNP P0AEP7
E	-2	MSE	-	expression tag	UNP P0AEP7
E	-1	ALA	-	expression tag	UNP P0AEP7
E	0	SER	-	expression tag	UNP P0AEP7
F	-22	MSE	-	expression tag	UNP P0AEP7
F	-21	GLY	-	expression tag	UNP P0AEP7
F	-20	SER	-	expression tag	UNP P0AEP7
F	-19	SER	-	expression tag	UNP P0AEP7
F	-18	HIS	-	expression tag	UNP P0AEP7
F	-17	HIS	-	expression tag	UNP P0AEP7
F	-16	HIS	-	expression tag	UNP P0AEP7
F	-15	HIS	-	expression tag	UNP P0AEP7
F	-14	HIS	-	expression tag	UNP P0AEP7
F	-13	HIS	-	expression tag	UNP P0AEP7
F	-12	SER	-	expression tag	UNP P0AEP7
F	-11	SER	-	expression tag	UNP P0AEP7
F	-10	GLY	-	expression tag	UNP P0AEP7
F	-9	LEU	-	expression tag	UNP P0AEP7
F	-8	VAL	-	expression tag	UNP P0AEP7
F	-7	PRO	-	expression tag	UNP P0AEP7
F	-6	ARG	-	expression tag	UNP P0AEP7
F	-5	GLY	-	expression tag	UNP P0AEP7
F	-4	SER	-	expression tag	UNP P0AEP7
F	-3	HIS	-	expression tag	UNP P0AEP7
F	-2	MSE	-	expression tag	UNP P0AEP7
F	-1	ALA	-	expression tag	UNP P0AEP7
F	0	SER	-	expression tag	UNP P0AEP7

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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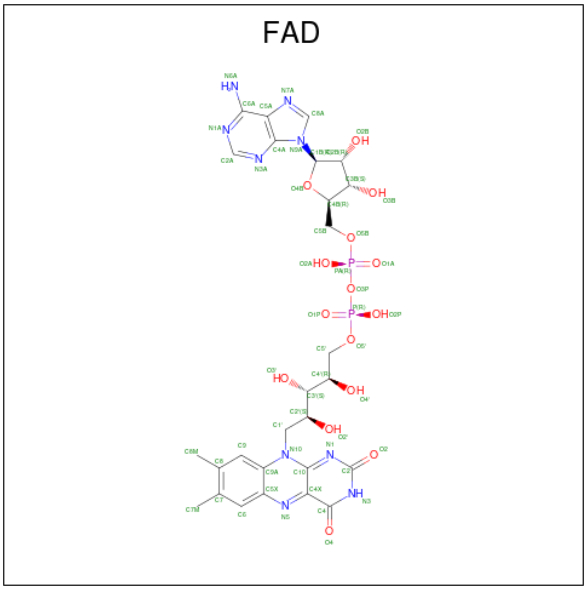
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

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

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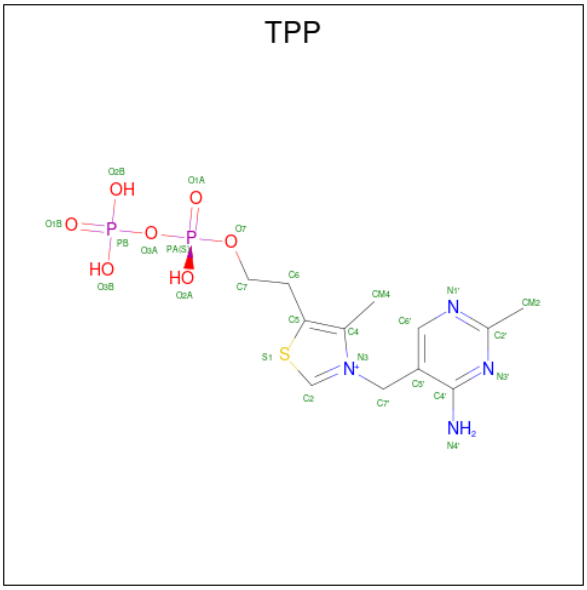
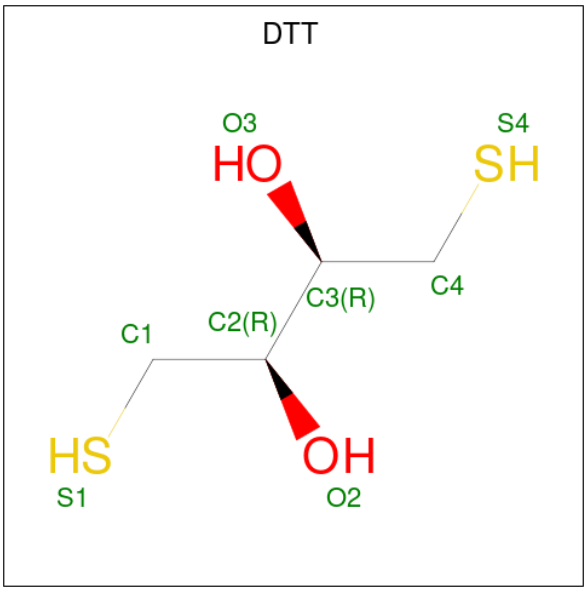
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C N O P 53 27 9 15 2	0	0
3	F	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 4 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



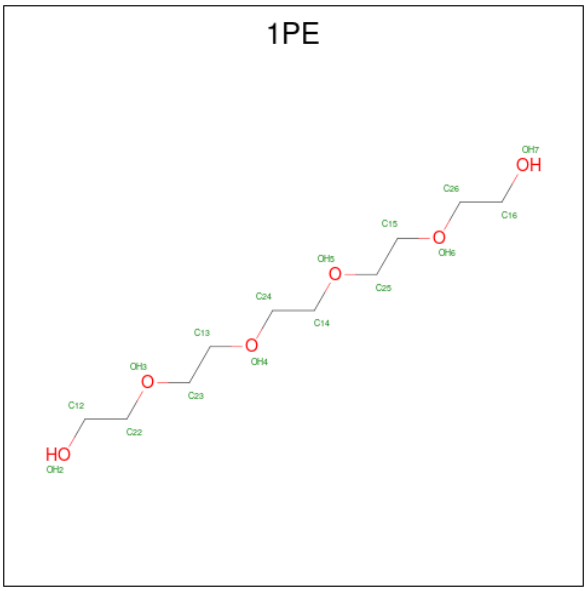
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 26 12 4 7 2 1	0	0
4	B	1	Total C N O P S 26 12 4 7 2 1	0	0
4	C	1	Total C N O P S 26 12 4 7 2 1	0	0
4	D	1	Total C N O P S 26 12 4 7 2 1	0	0
4	E	1	Total C N O P S 26 12 4 7 2 1	0	0
4	F	1	Total C N O P S 26 12 4 7 2 1	0	0

- Molecule 5 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O S 8 4 2 2	0	0
5	B	1	Total C O S 8 4 2 2	0	0
5	C	1	Total C O S 8 4 2 2	0	0
5	D	1	Total C O S 8 4 2 2	0	0
5	E	1	Total C O S 8 4 2 2	0	0
5	F	1	Total C O S 8 4 2 2	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 32 20 12	0	1

- Molecule 7 is water.

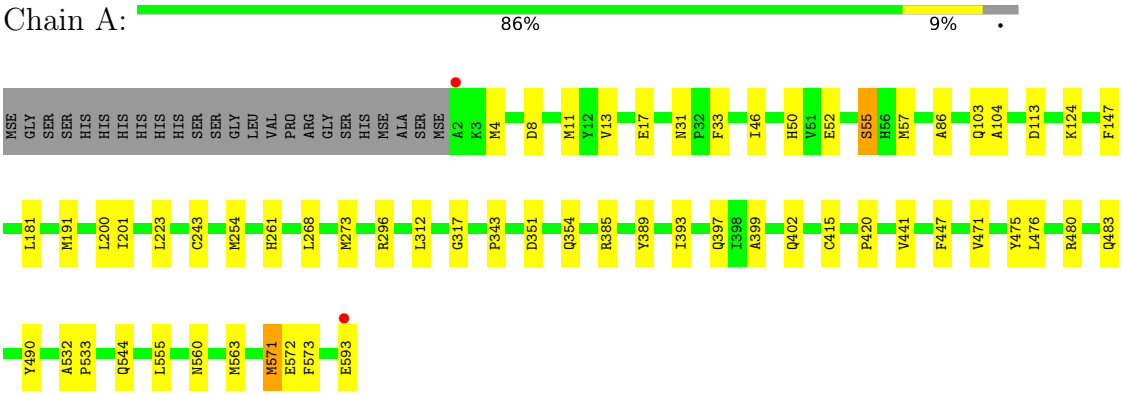
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	85	Total O 85 85	0	0
7	B	84	Total O 84 84	0	0
7	C	50	Total O 50 50	0	0
7	D	61	Total O 61 61	0	0
7	E	40	Total O 40 40	0	0
7	F	43	Total O 43 43	0	0

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.

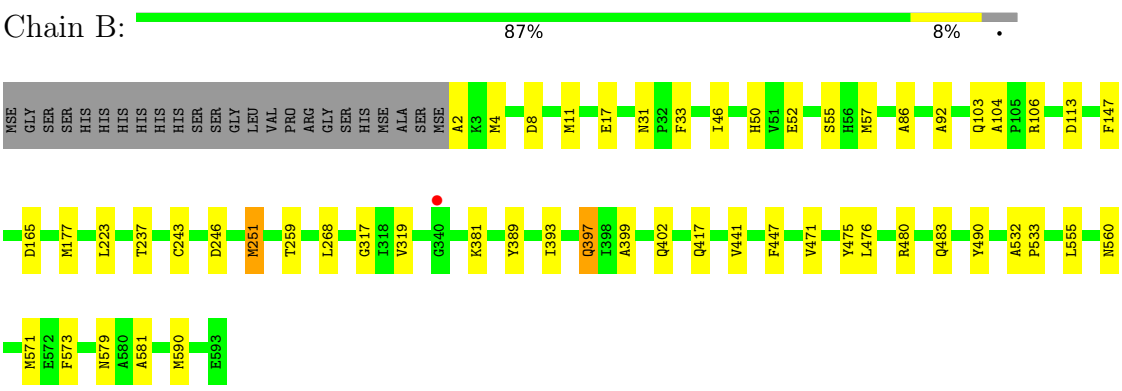
• Molecule 1: Glyoxylate carboligase

Chain A:



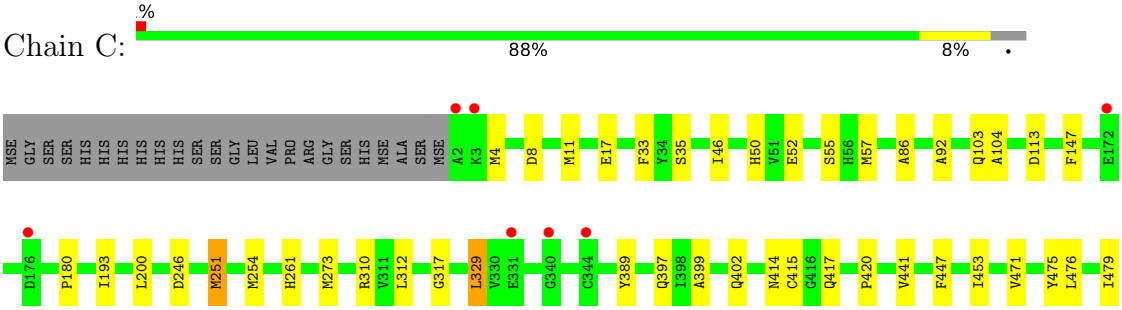
• Molecule 1: Glyoxylate carboligase

Chain B:

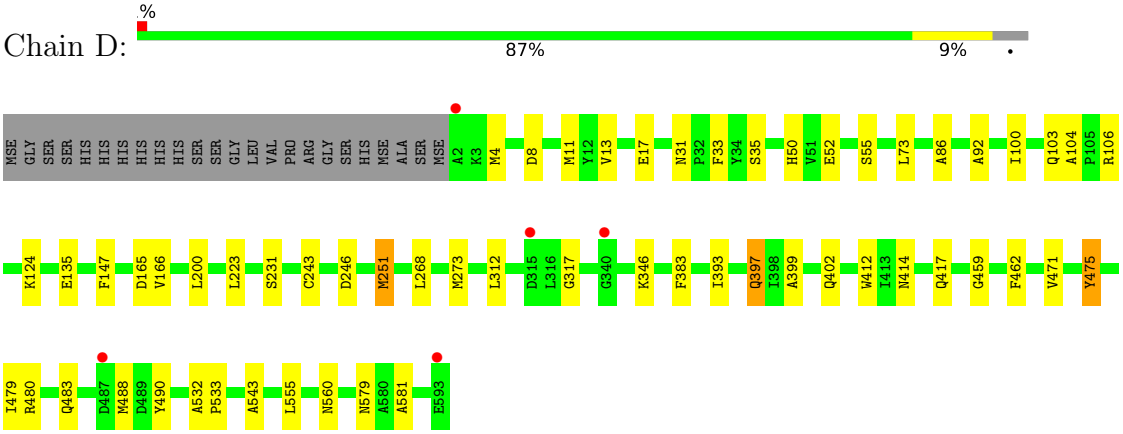


• Molecule 1: Glyoxylate carboligase

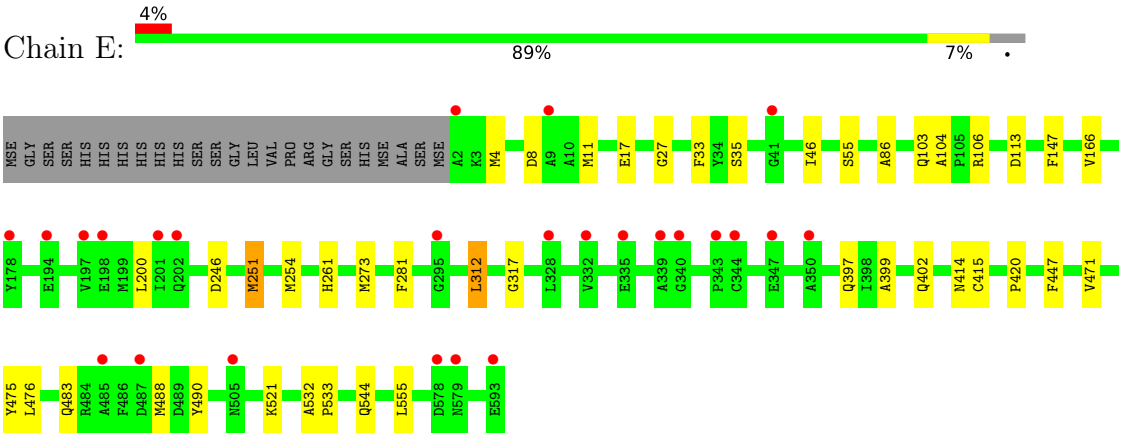
Chain C:



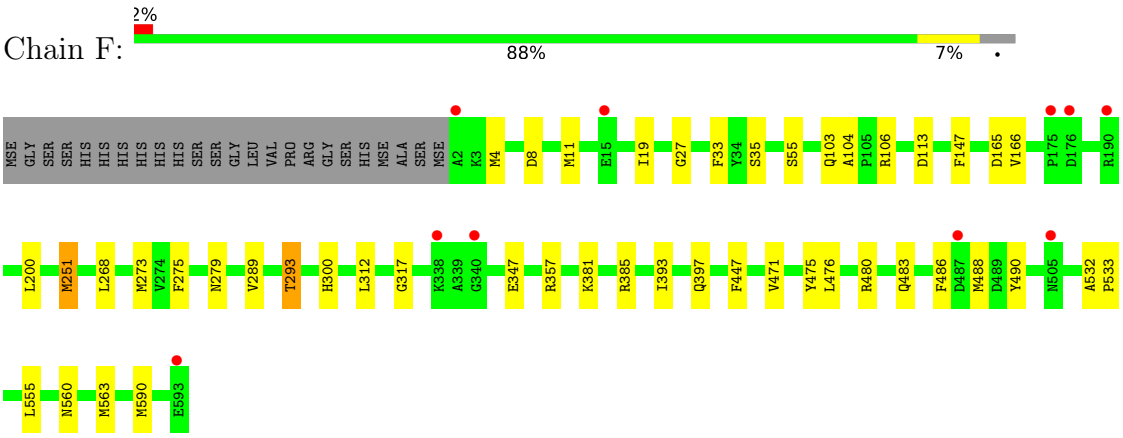
• Molecule 1: Glyoxylate carboligase



• Molecule 1: Glyoxylate carboligase



• Molecule 1: Glyoxylate carboligase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	188.18Å 188.18Å 249.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 48.14 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.70) 99.9 (48.14-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.219 , 0.253 0.223 , 0.255	Depositor DCC
R_{free} test set	2461 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	28107	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.0032e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: DTT, FAD, TPP, MG, 1PE

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	0.45	0/4600	0.63	1/6208 (0.0%)
1	B	0.43	0/4600	0.62	0/6208
1	C	0.41	0/4600	0.59	0/6208
1	D	0.40	0/4600	0.57	0/6208
1	E	0.40	0/4600	0.57	0/6208
1	F	0.40	0/4600	0.57	0/6208
All	All	0.42	0/27600	0.59	1/37248 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	296	ARG	NE-CZ-NH1	5.39	123.00	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4530	0	4534	43	0
1	B	4530	0	4534	36	0
1	C	4530	0	4534	34	0
1	D	4530	0	4534	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4530	0	4534	26	0
1	F	4530	0	4534	26	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	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	1	0
3	E	53	0	31	0	0
3	F	53	0	31	0	0
4	A	26	0	16	0	0
4	B	26	0	16	1	0
4	C	26	0	16	1	0
4	D	26	0	16	1	0
4	E	26	0	16	2	0
4	F	26	0	16	0	0
5	A	8	0	10	1	0
5	B	8	0	10	0	0
5	C	8	0	10	1	0
5	D	8	0	10	0	0
5	E	8	0	10	0	0
5	F	8	0	10	1	0
6	A	32	0	42	8	0
7	A	85	0	0	0	0
7	B	84	0	0	3	0
7	C	50	0	0	1	0
7	D	61	0	0	2	0
7	E	40	0	0	0	0
7	F	43	0	0	0	0
All	All	28107	0	27588	196	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (196) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:MSE:SE	1:A:571:MSE:CE	2.14	1.44
1:A:572:GLU:H	6:A:951[A]:1PE:H122	1.34	0.91
1:C:397:GLN:HE21	1:C:414:ASN:HD21	1.33	0.76
1:C:103:GLN:HE21	1:C:104:ALA:H	1.37	0.71
1:B:17:GLU:HG2	1:B:147:PHE:CD2	2.28	0.68
1:B:103:GLN:HE21	1:B:104:ALA:H	1.41	0.67
1:C:483:GLN:HE22	1:C:490:TYR:H	1.41	0.66
1:A:572:GLU:H	6:A:951[A]:1PE:C12	2.09	0.65
1:A:483:GLN:HE22	1:A:490:TYR:H	1.43	0.65
1:D:17:GLU:HG2	1:D:147:PHE:CD2	2.32	0.64
1:F:393:ILE:HA	1:F:397:GLN:HG2	1.80	0.63
1:A:103:GLN:HE21	1:A:104:ALA:H	1.47	0.63
1:D:483:GLN:HE22	1:D:490:TYR:H	1.46	0.63
1:A:11:MSE:HE1	1:A:33:PHE:CZ	2.35	0.62
1:C:200:LEU:HD13	1:C:273:MSE:HE1	1.82	0.62
1:A:393:ILE:HA	1:A:397:GLN:HG2	1.81	0.62
1:D:393:ILE:HA	1:D:397:GLN:HG2	1.81	0.62
1:C:251:MSE:HE1	7:C:1100:HOH:O	2.01	0.61
1:E:471:VAL:HB	1:E:555:LEU:HD11	1.83	0.61
1:C:17:GLU:HG2	1:C:147:PHE:CD2	2.37	0.60
1:A:471:VAL:HB	1:A:555:LEU:HD11	1.84	0.59
1:A:573:PHE:HA	6:A:951[A]:1PE:H141	1.84	0.59
1:D:471:VAL:HB	1:D:555:LEU:HD11	1.84	0.59
1:F:483:GLN:HE22	1:F:490:TYR:H	1.50	0.59
1:C:471:VAL:HB	1:C:555:LEU:HD11	1.85	0.58
1:C:17:GLU:HG2	1:C:147:PHE:CG	2.38	0.58
1:F:200:LEU:HD13	1:F:273:MSE:HE1	1.86	0.57
1:D:200:LEU:HD13	1:D:273:MSE:HE1	1.86	0.57
1:B:17:GLU:HG2	1:B:147:PHE:CG	2.40	0.57
1:D:393:ILE:CA	1:D:397:GLN:HG2	2.34	0.57
1:A:480:ARG:HH12	1:A:560:ASN:HD21	1.52	0.57
1:A:393:ILE:CA	1:A:397:GLN:HG2	2.35	0.57
1:F:103:GLN:HE21	1:F:104:ALA:H	1.51	0.57
1:E:11:MSE:HE1	1:E:33:PHE:CZ	2.41	0.56
1:A:4:MSE:HG2	1:A:8:ASP:HB2	1.87	0.56
1:B:483:GLN:HE22	1:B:490:TYR:H	1.53	0.56
1:B:55:SER:HB3	1:B:86:ALA:CB	2.36	0.56
1:B:237:THR:HG21	3:B:701:FAD:P	2.46	0.56
1:A:201:ILE:HG23	1:A:343:PRO:HD3	1.87	0.56
1:C:55:SER:HB3	1:C:86:ALA:CB	2.36	0.56
1:A:572:GLU:N	6:A:951[A]:1PE:H122	2.15	0.55
1:E:483:GLN:HE22	1:E:490:TYR:H	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:HIS:HD2	1:A:52:GLU:H	1.54	0.55
1:A:254:MSE:H	1:A:261:HIS:HD2	1.54	0.55
1:D:11:MSE:HE1	1:D:33:PHE:CZ	2.41	0.55
1:E:17:GLU:HG2	1:E:147:PHE:CG	2.42	0.55
1:F:106:ARG:HD2	1:F:166:VAL:HG23	1.88	0.54
1:A:571:MSE:CE	6:A:951[B]:1PE:H122	2.38	0.54
1:F:11:MSE:HE1	1:F:33:PHE:CZ	2.43	0.54
1:B:11:MSE:HE1	1:B:33:PHE:CZ	2.43	0.54
1:D:4:MSE:HG2	1:D:8:ASP:HB2	1.89	0.54
1:A:46:ILE:HG21	1:A:57:MSE:HE1	1.90	0.53
1:B:471:VAL:HB	1:B:555:LEU:HD11	1.89	0.53
1:E:11:MSE:HE1	1:E:33:PHE:CE1	2.44	0.53
1:F:563:MSE:HE3	5:F:901:DTT:H3	1.90	0.53
1:A:11:MSE:HE1	1:A:33:PHE:CE1	2.44	0.52
1:F:393:ILE:CA	1:F:397:GLN:HG2	2.39	0.52
1:B:251:MSE:HE1	7:B:2003:HOH:O	2.09	0.52
1:B:393:ILE:HA	1:B:397:GLN:HG2	1.92	0.52
1:B:381:LYS:HG2	1:B:590:MSE:HE1	1.93	0.51
1:D:103:GLN:HE21	1:D:104:ALA:H	1.58	0.51
1:F:106:ARG:HD3	1:F:165:ASP:OD2	2.10	0.51
1:B:476:LEU:HD13	4:B:801:TPP:HM41	1.93	0.51
1:A:17:GLU:HG2	1:A:147:PHE:CD2	2.46	0.51
1:A:532:ALA:HB3	1:A:533:PRO:HD3	1.93	0.50
1:D:532:ALA:HB3	1:D:533:PRO:HD3	1.94	0.50
1:E:476:LEU:HD13	4:E:801:TPP:HM41	1.93	0.50
1:F:279:ASN:O	1:F:300:HIS:HE1	1.93	0.50
1:E:17:GLU:HG2	1:E:147:PHE:CD2	2.46	0.49
1:A:17:GLU:HG2	1:A:147:PHE:CG	2.47	0.49
1:C:35:SER:HA	1:E:488:MSE:HE1	1.93	0.49
1:D:17:GLU:HG2	1:D:147:PHE:CG	2.47	0.49
1:E:246:ASP:HA	1:E:251:MSE:HG2	1.95	0.49
1:B:532:ALA:HB3	1:B:533:PRO:HD3	1.95	0.49
1:C:532:ALA:HB3	1:C:533:PRO:HD3	1.94	0.49
1:A:571:MSE:SE	6:A:951[B]:1PE:H122	2.62	0.49
1:D:488:MSE:HE1	1:F:35:SER:HA	1.94	0.49
1:B:4:MSE:HG2	1:B:8:ASP:HB2	1.96	0.48
1:F:532:ALA:HB3	1:F:533:PRO:HD3	1.96	0.48
1:C:447:PHE:CD2	1:C:476:LEU:HD22	2.48	0.48
1:C:4:MSE:HG2	1:C:8:ASP:HB2	1.94	0.48
1:E:106:ARG:HD2	1:E:166:VAL:HG23	1.95	0.48
1:F:447:PHE:CD2	1:F:476:LEU:HD22	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ILE:HG23	1:C:329:LEU:HD13	1.95	0.48
1:C:488:MSE:HE1	1:E:35:SER:HA	1.94	0.48
1:A:55:SER:HB2	1:A:86:ALA:HB2	1.95	0.48
1:B:480:ARG:HH12	1:B:560:ASN:HD21	1.60	0.48
1:B:393:ILE:CA	1:B:397:GLN:HG2	2.44	0.48
1:B:393:ILE:HA	1:B:397:GLN:CG	2.44	0.47
1:D:73:LEU:HD23	1:D:100:ILE:HB	1.96	0.47
1:E:532:ALA:HB3	1:E:533:PRO:HD3	1.97	0.47
1:E:397:GLN:HE21	1:E:414:ASN:HD21	1.63	0.47
1:A:447:PHE:CD2	1:A:476:LEU:HD22	2.50	0.47
1:A:571:MSE:HB3	1:A:571:MSE:HE2	1.97	0.47
1:E:447:PHE:CD2	1:E:476:LEU:HD22	2.50	0.47
1:C:479:ILE:HD12	1:E:27:GLY:HA2	1.98	0.46
1:A:385:ARG:H	1:A:593:GLU:HG3	1.80	0.46
1:C:563:MSE:HE3	5:C:901:DTT:H3	1.98	0.46
1:F:471:VAL:HB	1:F:555:LEU:HD11	1.97	0.46
1:B:2:ALA:N	7:B:3063:HOH:O	2.49	0.46
1:C:11:MSE:HE1	1:C:33:PHE:CZ	2.49	0.46
1:D:106:ARG:HD3	1:D:165:ASP:OD2	2.16	0.46
1:D:383:PHE:O	7:D:3011:HOH:O	2.20	0.46
1:E:415:CYS:SG	1:E:420:PRO:HD2	2.56	0.46
1:B:571:MSE:HG2	1:B:573:PHE:CZ	2.51	0.46
1:C:500:ASN:HD21	1:E:521:LYS:NZ	2.13	0.46
1:F:486:PHE:HB3	1:F:488:MSE:HE3	1.98	0.46
1:A:393:ILE:HA	1:A:397:GLN:CG	2.46	0.45
1:B:46:ILE:HG21	1:B:57:MSE:HE1	1.98	0.45
1:B:246:ASP:HA	1:B:251:MSE:HG2	1.98	0.45
1:F:480:ARG:HH12	1:F:560:ASN:HD21	1.64	0.45
1:A:571:MSE:CE	1:A:571:MSE:HB3	2.46	0.45
1:B:251:MSE:HE3	7:B:2145:HOH:O	2.16	0.45
1:C:92:ALA:HB1	1:C:417:GLN:CG	2.47	0.45
1:A:223:LEU:HD22	1:A:243:CYS:SG	2.57	0.45
1:B:106:ARG:HD3	1:B:165:ASP:OD2	2.16	0.45
1:D:246:ASP:HA	1:D:251:MSE:HG2	1.98	0.45
1:C:50:HIS:HD2	1:C:52:GLU:H	1.64	0.45
1:C:246:ASP:HA	1:C:251:MSE:HG2	1.98	0.45
1:D:480:ARG:HH12	1:D:560:ASN:HD21	1.65	0.45
1:D:92:ALA:HB1	1:D:417:GLN:CG	2.47	0.44
1:E:55:SER:HB2	1:E:86:ALA:CB	2.47	0.44
1:F:4:MSE:HG2	1:F:8:ASP:HB2	1.99	0.44
1:D:479:ILE:HD12	1:F:27:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HD13	1:A:273:MSE:HE1	1.98	0.44
1:C:415:CYS:SG	1:C:420:PRO:HD2	2.58	0.44
1:A:563:MSE:HE3	5:A:901:DTT:C4	2.47	0.44
1:A:571:MSE:CE	6:A:951[B]:1PE:C12	2.96	0.44
1:B:50:HIS:HD2	1:B:52:GLU:H	1.66	0.44
1:B:11:MSE:HE1	1:B:33:PHE:CE1	2.53	0.44
1:E:399:ALA:HA	1:E:402:GLN:HG2	1.99	0.44
1:B:399:ALA:HA	1:B:402:GLN:HG2	2.00	0.44
1:C:254:MSE:H	1:C:261:HIS:HD2	1.65	0.44
1:D:543:ALA:HB3	7:D:3092:HOH:O	2.16	0.44
1:D:13:VAL:O	1:D:17:GLU:HB2	2.18	0.43
1:E:200:LEU:HD13	1:E:273:MSE:HE1	1.99	0.43
1:C:453:ILE:HD13	1:C:514:VAL:HG11	2.00	0.43
1:F:393:ILE:HA	1:F:397:GLN:CG	2.48	0.43
1:F:289:VAL:O	1:F:293:THR:OG1	2.32	0.43
1:F:381:LYS:HG2	1:F:590:MSE:HE1	2.01	0.43
1:B:237:THR:HG21	3:B:701:FAD:O5'	2.18	0.43
1:C:17:GLU:OE2	1:C:180:PRO:HB3	2.19	0.43
1:D:459:GLY:O	1:D:462:PHE:O	2.36	0.43
1:F:11:MSE:HE1	1:F:33:PHE:CE2	2.53	0.43
1:A:399:ALA:HA	1:A:402:GLN:HG2	2.01	0.43
1:D:393:ILE:HA	1:D:397:GLN:CG	2.49	0.43
1:D:475:TYR:CE2	1:D:480:ARG:HD3	2.53	0.43
4:C:801:TPP:H61	4:C:801:TPP:HM41	1.85	0.43
1:C:399:ALA:HA	1:C:402:GLN:HG2	2.01	0.42
1:E:103:GLN:HE21	1:E:104:ALA:H	1.67	0.42
1:D:106:ARG:HD2	1:D:166:VAL:HG23	2.00	0.42
1:E:4:MSE:HG2	1:E:8:ASP:HB2	2.01	0.42
1:D:50:HIS:HD2	1:D:52:GLU:H	1.68	0.42
1:A:13:VAL:O	1:A:17:GLU:HB2	2.20	0.42
1:B:579:ASN:HD21	1:B:581:ALA:HB3	1.84	0.42
1:B:259:THR:OG1	3:B:701:FAD:C4X	2.67	0.42
1:B:393:ILE:N	1:B:397:GLN:HG2	2.35	0.42
1:C:46:ILE:HG21	1:C:57:MSE:HE1	2.02	0.42
1:D:399:ALA:HA	1:D:402:GLN:HG2	2.02	0.42
1:D:579:ASN:HD21	1:D:581:ALA:HB3	1.85	0.42
1:F:273:MSE:HE3	1:F:275:PHE:HB2	2.02	0.42
1:A:415:CYS:SG	1:A:420:PRO:HD2	2.60	0.41
3:A:701:FAD:H9	3:A:701:FAD:H1'1	1.86	0.41
1:D:55:SER:HB3	1:D:86:ALA:CB	2.50	0.41
1:D:223:LEU:HD22	1:D:243:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:ILE:CD1	1:F:147:PHE:HZ	2.34	0.41
1:A:389:TYR:HA	1:A:441:VAL:O	2.21	0.41
1:F:251:MSE:O	1:F:251:MSE:HG3	2.19	0.41
1:A:571:MSE:HA	6:A:951[A]:1PE:OH2	2.20	0.41
3:C:701:FAD:H9	3:C:701:FAD:H1'1	1.89	0.41
3:D:701:FAD:H9	3:D:701:FAD:H1'1	1.92	0.41
4:E:801:TPP:HM41	4:E:801:TPP:H61	1.84	0.41
1:C:389:TYR:HA	1:C:441:VAL:O	2.21	0.41
1:E:447:PHE:CG	1:E:476:LEU:HD22	2.56	0.41
1:E:281:PHE:CD1	1:E:312:LEU:HD11	2.55	0.41
1:A:351:ASP:HA	1:A:354:GLN:HB2	2.02	0.41
1:A:385:ARG:H	1:A:593:GLU:CG	2.33	0.41
1:B:92:ALA:HB1	1:B:417:GLN:CG	2.51	0.41
1:B:223:LEU:HD22	1:B:243:CYS:SG	2.61	0.41
1:C:200:LEU:CD1	1:C:273:MSE:HE1	2.49	0.41
1:D:11:MSE:HE1	1:D:33:PHE:CE1	2.56	0.41
1:A:181:LEU:HD21	1:B:319:VAL:HG11	2.03	0.41
4:D:801:TPP:H61	4:D:801:TPP:HM41	1.88	0.41
1:A:31:ASN:HD22	1:A:31:ASN:HA	1.70	0.40
1:A:191:MSE:HG2	1:B:177:MSE:HE1	2.02	0.40
1:B:389:TYR:HA	1:B:441:VAL:O	2.22	0.40
1:E:254:MSE:H	1:E:261:HIS:HD2	1.69	0.40
1:C:310:ARG:O	1:D:135:GLU:HG3	2.21	0.40
1:D:92:ALA:HB1	1:D:417:GLN:HG2	2.02	0.40
1:D:251:MSE:O	1:D:251:MSE:HG3	2.21	0.40
1:D:35:SER:HA	1:F:488:MSE:HE1	2.03	0.40
1:D:412:TRP:HE1	1:D:414:ASN:HD22	1.70	0.40
1:B:447:PHE:CG	1:B:476:LEU:HD22	2.57	0.40
1:C:397:GLN:NE2	1:C:414:ASN:HD21	2.09	0.40
1:C:447:PHE:CG	1:C:476:LEU:HD22	2.57	0.40
1:C:500:ASN:ND2	1:E:521:LYS:NZ	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	590/616 (96%)	578 (98%)	11 (2%)	1 (0%)	47	73
1	B	590/616 (96%)	578 (98%)	11 (2%)	1 (0%)	47	73
1	C	590/616 (96%)	578 (98%)	11 (2%)	1 (0%)	47	73
1	D	590/616 (96%)	578 (98%)	11 (2%)	1 (0%)	47	73
1	E	590/616 (96%)	578 (98%)	11 (2%)	1 (0%)	47	73
1	F	590/616 (96%)	578 (98%)	11 (2%)	1 (0%)	47	73
All	All	3540/3696 (96%)	3468 (98%)	66 (2%)	6 (0%)	47	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	GLY
1	C	317	GLY
1	E	317	GLY
1	D	317	GLY
1	F	317	GLY
1	B	317	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	474/469 (101%)	466 (98%)	8 (2%)	60	84
1	B	474/469 (101%)	468 (99%)	6 (1%)	69	87
1	C	474/469 (101%)	469 (99%)	5 (1%)	73	90
1	D	474/469 (101%)	465 (98%)	9 (2%)	57	82
1	E	474/469 (101%)	468 (99%)	6 (1%)	69	87
1	F	474/469 (101%)	464 (98%)	10 (2%)	53	80
All	All	2844/2814 (101%)	2800 (98%)	44 (2%)	65	86

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	SER
1	A	113	ASP
1	A	124	LYS
1	A	268	LEU
1	A	312	LEU
1	A	475	TYR
1	A	544	GLN
1	A	571	MSE
1	B	31	ASN
1	B	113	ASP
1	B	251	MSE
1	B	268	LEU
1	B	397	GLN
1	B	475	TYR
1	C	113	ASP
1	C	251	MSE
1	C	312	LEU
1	C	329	LEU
1	C	475	TYR
1	D	31	ASN
1	D	124	LYS
1	D	231	SER
1	D	251	MSE
1	D	268	LEU
1	D	312	LEU
1	D	346	LYS
1	D	397	GLN
1	D	475	TYR
1	E	46	ILE
1	E	113	ASP
1	E	251	MSE
1	E	312	LEU
1	E	475	TYR
1	E	544	GLN
1	F	55	SER
1	F	113	ASP
1	F	251	MSE
1	F	268	LEU
1	F	293	THR
1	F	312	LEU
1	F	347	GLU
1	F	357	ARG

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Mol	Chain	Res	Type
1	F	385	ARG
1	F	475	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	50	HIS
1	A	103	GLN
1	A	261	HIS
1	A	397	GLN
1	A	402	GLN
1	A	414	ASN
1	A	483	GLN
1	A	560	ASN
1	B	31	ASN
1	B	50	HIS
1	B	103	GLN
1	B	261	HIS
1	B	402	GLN
1	B	414	ASN
1	B	483	GLN
1	B	560	ASN
1	B	579	ASN
1	C	31	ASN
1	C	50	HIS
1	C	103	GLN
1	C	261	HIS
1	C	414	ASN
1	C	483	GLN
1	C	500	ASN
1	C	560	ASN
1	D	31	ASN
1	D	50	HIS
1	D	103	GLN
1	D	261	HIS
1	D	397	GLN
1	D	402	GLN
1	D	414	ASN
1	D	483	GLN
1	D	500	ASN
1	D	560	ASN

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Mol	Chain	Res	Type
1	D	579	ASN
1	E	31	ASN
1	E	103	GLN
1	E	261	HIS
1	E	402	GLN
1	E	414	ASN
1	E	483	GLN
1	E	500	ASN
1	E	560	ASN
1	F	50	HIS
1	F	103	GLN
1	F	261	HIS
1	F	300	HIS
1	F	337	GLN
1	F	397	GLN
1	F	414	ASN
1	F	483	GLN
1	F	500	ASN
1	F	537	GLN
1	F	560	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 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	701	-	51,58,58	1.41	7 (13%)	60,89,89	1.78	8 (13%)
5	DTT	F	901	-	7,7,7	0.64	0	4,8,8	0.86	0
4	TPP	A	801	2	22,27,27	1.40	3 (13%)	29,40,40	2.19	8 (27%)
3	FAD	C	701	-	51,58,58	1.36	6 (11%)	60,89,89	1.82	9 (15%)
4	TPP	C	801	2	22,27,27	1.47	3 (13%)	29,40,40	2.20	9 (31%)
5	DTT	A	901	-	7,7,7	0.62	0	4,8,8	1.20	0
3	FAD	E	701	-	51,58,58	1.40	6 (11%)	60,89,89	1.71	8 (13%)
6	1PE	A	951[A]	-	15,15,15	1.06	1 (6%)	14,14,14	0.65	0
5	DTT	D	901	-	7,7,7	0.66	0	4,8,8	0.66	0
6	1PE	A	951[B]	-	15,15,15	1.07	1 (6%)	14,14,14	0.55	0
3	FAD	B	701	-	51,58,58	1.46	7 (13%)	60,89,89	1.93	10 (16%)
5	DTT	B	901	-	7,7,7	0.56	0	4,8,8	1.52	1 (25%)
4	TPP	F	801	2	22,27,27	1.58	4 (18%)	29,40,40	2.06	6 (20%)
5	DTT	C	901	-	7,7,7	0.68	0	4,8,8	0.73	0
4	TPP	E	801	2	22,27,27	1.47	3 (13%)	29,40,40	2.31	7 (24%)
5	DTT	E	901	-	7,7,7	0.66	0	4,8,8	0.77	0
4	TPP	B	801	2	22,27,27	1.46	3 (13%)	29,40,40	2.09	7 (24%)
3	FAD	A	701	-	51,58,58	1.34	6 (11%)	60,89,89	1.74	8 (13%)
3	FAD	D	701	-	51,58,58	1.48	7 (13%)	60,89,89	1.81	7 (11%)
4	TPP	D	801	2	22,27,27	1.41	3 (13%)	29,40,40	2.22	7 (24%)

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	701	-	-	5/30/50/50	0/6/6/6
5	DTT	F	901	-	-	3/8/8/8	-
4	TPP	A	801	2	-	5/16/17/17	0/2/2/2
3	FAD	C	701	-	-	6/30/50/50	0/6/6/6
4	TPP	C	801	2	-	3/16/17/17	0/2/2/2
5	DTT	A	901	-	-	1/8/8/8	-
3	FAD	E	701	-	-	5/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	A	951[A]	-	-	7/13/13/13	-
5	DTT	D	901	-	-	2/8/8/8	-
6	1PE	A	951[B]	-	-	5/13/13/13	-
3	FAD	B	701	-	-	4/30/50/50	0/6/6/6
5	DTT	B	901	-	-	3/8/8/8	-
4	TPP	F	801	2	-	4/16/17/17	0/2/2/2
5	DTT	C	901	-	-	2/8/8/8	-
4	TPP	E	801	2	-	5/16/17/17	0/2/2/2
5	DTT	E	901	-	-	2/8/8/8	-
4	TPP	B	801	2	-	5/16/17/17	0/2/2/2
3	FAD	A	701	-	-	7/30/50/50	0/6/6/6
3	FAD	D	701	-	-	6/30/50/50	0/6/6/6
4	TPP	D	801	2	-	3/16/17/17	0/2/2/2

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	FAD	C1'-N10	4.54	1.52	1.48
4	C	801	TPP	C5'-C4'	4.43	1.50	1.42
3	E	701	FAD	C10-N1	4.42	1.38	1.33
4	F	801	TPP	C5'-C4'	4.26	1.50	1.42
3	D	701	FAD	C10-N1	4.19	1.38	1.33
3	D	701	FAD	C2A-N3A	4.17	1.38	1.32
3	D	701	FAD	C4X-N5	4.16	1.39	1.33
3	B	701	FAD	C4X-N5	4.08	1.39	1.33
3	C	701	FAD	C2A-N3A	4.07	1.38	1.32
3	B	701	FAD	C2A-N3A	4.02	1.38	1.32
4	B	801	TPP	C5'-C4'	3.98	1.49	1.42
4	E	801	TPP	C5'-C4'	3.94	1.49	1.42
3	F	701	FAD	C2A-N3A	3.93	1.38	1.32
3	F	701	FAD	C4X-N5	3.90	1.38	1.33
3	E	701	FAD	C4X-N5	3.82	1.38	1.33
4	D	801	TPP	C5'-C4'	3.81	1.49	1.42
6	A	951[B]	1PE	OH7-C16	-3.76	1.22	1.42
3	F	701	FAD	C1'-N10	3.76	1.52	1.48
3	E	701	FAD	C2A-N3A	3.76	1.38	1.32
3	F	701	FAD	C10-N1	3.74	1.38	1.33
4	A	801	TPP	C5'-C4'	3.67	1.49	1.42
3	C	701	FAD	C4X-N5	3.64	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	951[A]	1PE	OH7-C16	-3.62	1.23	1.42
3	D	701	FAD	C1'-N10	3.52	1.51	1.48
3	A	701	FAD	C4X-N5	3.52	1.38	1.33
3	A	701	FAD	C2A-N3A	3.50	1.37	1.32
3	D	701	FAD	C4-N3	3.47	1.39	1.33
3	C	701	FAD	C10-N1	3.45	1.37	1.33
3	A	701	FAD	C10-N1	3.43	1.37	1.33
3	C	701	FAD	C4-N3	3.41	1.39	1.33
3	B	701	FAD	C10-N1	3.40	1.37	1.33
3	A	701	FAD	C1'-N10	3.38	1.51	1.48
3	F	701	FAD	C4-N3	3.31	1.38	1.33
4	F	801	TPP	C4-N3	3.26	1.42	1.39
3	B	701	FAD	C4-N3	3.22	1.38	1.33
4	A	801	TPP	C2-N3	3.21	1.42	1.36
4	B	801	TPP	C4-N3	3.16	1.42	1.39
3	E	701	FAD	C1'-N10	3.15	1.51	1.48
4	E	801	TPP	C4-N3	3.12	1.42	1.39
4	C	801	TPP	C2-N3	3.10	1.42	1.36
3	A	701	FAD	C4-N3	3.08	1.38	1.33
3	E	701	FAD	C4-N3	3.07	1.38	1.33
4	E	801	TPP	C2-N3	3.06	1.42	1.36
4	F	801	TPP	C2-N3	2.99	1.42	1.36
4	B	801	TPP	C2-N3	2.95	1.42	1.36
4	D	801	TPP	C2-N3	2.95	1.42	1.36
4	A	801	TPP	C4-N3	2.93	1.42	1.39
3	C	701	FAD	C1'-N10	2.91	1.51	1.48
4	D	801	TPP	C4-N3	2.83	1.42	1.39
4	C	801	TPP	C4-N3	2.76	1.42	1.39
4	F	801	TPP	C6-C5	2.75	1.52	1.50
3	E	701	FAD	C2A-N1A	2.69	1.38	1.33
3	C	701	FAD	C2A-N1A	2.53	1.38	1.33
3	D	701	FAD	C2A-N1A	2.46	1.38	1.33
3	B	701	FAD	C2A-N1A	2.34	1.38	1.33
3	F	701	FAD	C2A-N1A	2.29	1.38	1.33
3	D	701	FAD	C5X-N5	2.22	1.39	1.35
3	A	701	FAD	C2A-N1A	2.20	1.38	1.33
3	F	701	FAD	C5X-N5	2.14	1.38	1.35
3	B	701	FAD	C5X-N5	2.12	1.38	1.35

All (95) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	701	FAD	C4-N3-C2	7.58	121.54	115.14
3	D	701	FAD	C4-N3-C2	7.44	121.42	115.14
3	A	701	FAD	C4-N3-C2	7.42	121.41	115.14
3	E	701	FAD	C4-N3-C2	7.18	121.21	115.14
3	B	701	FAD	C1'-N10-C9A	7.12	123.90	118.29
3	F	701	FAD	C4-N3-C2	6.98	121.04	115.14
3	B	701	FAD	C4-N3-C2	6.96	121.02	115.14
3	D	701	FAD	C1'-N10-C9A	6.05	123.06	118.29
4	D	801	TPP	C5'-C7'-N3	-5.88	103.49	113.28
4	B	801	TPP	C5'-C7'-N3	-5.73	103.75	113.28
3	C	701	FAD	N3A-C2A-N1A	-5.65	119.85	128.68
3	A	701	FAD	N3A-C2A-N1A	-5.63	119.88	128.68
4	E	801	TPP	C6-C5-C4	-5.63	122.92	127.43
3	F	701	FAD	N3A-C2A-N1A	-5.63	119.88	128.68
4	E	801	TPP	C5'-C7'-N3	-5.57	104.00	113.28
3	E	701	FAD	N3A-C2A-N1A	-5.41	120.22	128.68
4	E	801	TPP	C7'-N3-C2	-5.39	115.61	125.35
4	C	801	TPP	C7'-N3-C2	-5.37	115.64	125.35
3	D	701	FAD	N3A-C2A-N1A	-5.35	120.31	128.68
3	B	701	FAD	N3A-C2A-N1A	-5.23	120.51	128.68
3	C	701	FAD	C1'-N10-C9A	5.19	122.38	118.29
4	C	801	TPP	C6-C5-C4	-5.17	123.28	127.43
4	A	801	TPP	C6-C5-C4	-5.14	123.31	127.43
4	D	801	TPP	C7'-N3-C2	-5.09	116.15	125.35
4	A	801	TPP	C5'-C7'-N3	-5.05	104.88	113.28
4	D	801	TPP	C6-C5-C4	-4.92	123.49	127.43
4	F	801	TPP	C7'-N3-C2	-4.91	116.48	125.35
3	F	701	FAD	C1'-N10-C9A	4.78	122.05	118.29
4	C	801	TPP	C5'-C7'-N3	-4.74	105.39	113.28
4	F	801	TPP	C6-C5-C4	-4.71	123.65	127.43
3	E	701	FAD	C1'-N10-C9A	4.57	121.89	118.29
4	A	801	TPP	C7'-N3-C2	-4.50	117.22	125.35
4	B	801	TPP	C6-C5-C4	-4.29	123.99	127.43
4	B	801	TPP	C7'-N3-C2	-4.23	117.70	125.35
3	A	701	FAD	C1'-N10-C9A	4.15	121.56	118.29
4	A	801	TPP	CM2-C2'-N1'	3.99	121.53	117.14
4	F	801	TPP	C5'-C7'-N3	-3.87	106.83	113.28
3	B	701	FAD	C5X-C9A-N10	3.87	120.52	117.72
4	C	801	TPP	C6'-N1'-C2'	3.72	122.30	115.96
4	E	801	TPP	C6'-N1'-C2'	3.67	122.20	115.96
3	C	701	FAD	C4X-C4-N3	-3.66	118.43	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	801	TPP	C6'-N1'-C2'	3.54	121.98	115.96
4	B	801	TPP	C6'-N1'-C2'	3.51	121.94	115.96
4	F	801	TPP	C6'-N1'-C2'	3.50	121.92	115.96
4	F	801	TPP	CM2-C2'-N1'	3.48	120.97	117.14
3	A	701	FAD	C4X-C4-N3	-3.46	118.70	123.43
3	D	701	FAD	C4X-C4-N3	-3.39	118.79	123.43
4	A	801	TPP	C6'-N1'-C2'	3.38	121.71	115.96
3	F	701	FAD	C4X-C4-N3	-3.27	118.96	123.43
3	B	701	FAD	C4X-C4-N3	-3.16	119.11	123.43
3	F	701	FAD	C4X-N5-C5X	3.15	119.92	116.77
3	E	701	FAD	C4X-N5-C5X	3.11	119.88	116.77
4	E	801	TPP	CM2-C2'-N1'	3.05	120.49	117.14
4	C	801	TPP	CM2-C2'-N1'	3.00	120.44	117.14
3	D	701	FAD	C5X-C9A-N10	2.95	119.85	117.72
3	B	701	FAD	C9A-N10-C10	-2.91	118.09	121.91
3	D	701	FAD	C4X-N5-C5X	2.86	119.62	116.77
4	B	801	TPP	CM2-C2'-N1'	2.85	120.27	117.14
3	C	701	FAD	C4X-N5-C5X	2.83	119.60	116.77
4	A	801	TPP	N1'-C2'-N3'	-2.80	120.72	125.54
3	E	701	FAD	C4X-C4-N3	-2.77	119.64	123.43
5	B	901	DTT	C2-C1-S1	-2.76	106.45	114.47
3	A	701	FAD	C5X-C9A-N10	2.72	119.69	117.72
3	A	701	FAD	C4X-N5-C5X	2.65	119.42	116.77
3	A	701	FAD	O4B-C1B-C2B	-2.53	103.22	106.93
4	C	801	TPP	N1'-C2'-N3'	-2.51	121.22	125.54
4	F	801	TPP	N1'-C2'-N3'	-2.48	121.27	125.54
4	A	801	TPP	CM4-C4-N3	2.47	125.68	122.53
4	D	801	TPP	N1'-C2'-N3'	-2.45	121.33	125.54
4	D	801	TPP	CM2-C2'-N1'	2.44	119.82	117.14
4	E	801	TPP	N1'-C2'-N3'	-2.43	121.35	125.54
3	C	701	FAD	C5X-C9A-N10	2.43	119.47	117.72
4	B	801	TPP	N1'-C2'-N3'	-2.41	121.40	125.54
3	B	701	FAD	C4A-C5A-N7A	-2.38	106.92	109.40
3	F	701	FAD	C5X-C9A-N10	2.38	119.44	117.72
3	F	701	FAD	C10-C4X-N5	-2.37	119.62	121.26
4	E	801	TPP	C5'-C6'-N1'	-2.37	119.87	123.82
3	C	701	FAD	O4B-C1B-C2B	-2.36	103.48	106.93
3	B	701	FAD	O4B-C1B-C2B	-2.33	103.53	106.93
4	C	801	TPP	CM4-C4-N3	2.31	125.47	122.53
3	B	701	FAD	C4X-N5-C5X	2.26	119.03	116.77
3	E	701	FAD	C5X-C9A-N10	2.26	119.36	117.72
4	C	801	TPP	C5'-C6'-N1'	-2.24	120.09	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	801	TPP	C5'-C6'-N1'	-2.20	120.16	123.82
3	A	701	FAD	C4A-C5A-N7A	-2.19	107.12	109.40
4	C	801	TPP	O3B-PB-O2B	2.16	115.87	107.64
3	C	701	FAD	C10-C4X-N5	-2.15	119.77	121.26
4	A	801	TPP	C2'-N3'-C4'	2.13	121.40	118.08
3	F	701	FAD	C9A-N10-C10	-2.12	119.13	121.91
3	C	701	FAD	C8M-C8-C9	-2.10	115.31	120.34
3	B	701	FAD	O4'-C4'-C3'	2.10	114.20	109.10
4	B	801	TPP	C5'-C6'-N1'	-2.08	120.35	123.82
3	E	701	FAD	C1B-N9A-C4A	-2.04	123.05	126.64
3	D	701	FAD	C9A-N10-C10	-2.02	119.26	121.91
3	E	701	FAD	C4A-C5A-N7A	-2.01	107.31	109.40

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	FAD	C5B-O5B-PA-O3P
3	A	701	FAD	C5'-O5'-P-O1P
3	A	701	FAD	C5'-O5'-P-O3P
3	B	701	FAD	C5B-O5B-PA-O3P
3	C	701	FAD	C5B-O5B-PA-O3P
3	D	701	FAD	C5B-O5B-PA-O3P
3	D	701	FAD	C5'-O5'-P-O1P
3	D	701	FAD	C5'-O5'-P-O3P
3	E	701	FAD	C5B-O5B-PA-O3P
3	F	701	FAD	C5B-O5B-PA-O3P
4	A	801	TPP	C5'-C7'-N3-C2
4	B	801	TPP	C5'-C7'-N3-C2
4	B	801	TPP	C7-O7-PA-O2A
4	B	801	TPP	PB-O3A-PA-O7
4	C	801	TPP	C5'-C7'-N3-C2
4	D	801	TPP	C5'-C7'-N3-C2
4	D	801	TPP	PB-O3A-PA-O7
4	E	801	TPP	C5'-C7'-N3-C2
4	E	801	TPP	C7-O7-PA-O2A
4	F	801	TPP	C4'-C5'-C7'-N3
4	F	801	TPP	C5'-C7'-N3-C2
4	F	801	TPP	PB-O3A-PA-O7
5	B	901	DTT	S1-C1-C2-O2
5	C	901	DTT	S1-C1-C2-O2
5	C	901	DTT	S1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	D	901	DTT	C2-C3-C4-S4
5	E	901	DTT	S1-C1-C2-C3
5	F	901	DTT	S1-C1-C2-O2
5	F	901	DTT	C2-C3-C4-S4
5	F	901	DTT	O3-C3-C4-S4
6	A	951[B]	1PE	C13-C23-OH3-C22
6	A	951[A]	1PE	OH4-C13-C23-OH3
6	A	951[B]	1PE	OH7-C16-C26-OH6
6	A	951[B]	1PE	OH6-C15-C25-OH5
6	A	951[A]	1PE	C23-C13-OH4-C24
3	E	701	FAD	C3'-C4'-C5'-O5'
6	A	951[A]	1PE	OH5-C14-C24-OH4
4	C	801	TPP	PB-O3A-PA-O7
4	E	801	TPP	PB-O3A-PA-O7
6	A	951[A]	1PE	C13-C23-OH3-C22
3	A	701	FAD	O2'-C2'-C3'-C4'
4	E	801	TPP	C7-O7-PA-O3A
3	A	701	FAD	P-O3P-PA-O1A
3	D	701	FAD	P-O3P-PA-O1A
6	A	951[A]	1PE	C24-C14-OH5-C25
3	A	701	FAD	C5B-O5B-PA-O1A
3	A	701	FAD	C5B-O5B-PA-O2A
3	B	701	FAD	C5B-O5B-PA-O1A
3	B	701	FAD	C5B-O5B-PA-O2A
3	C	701	FAD	C5B-O5B-PA-O1A
3	C	701	FAD	C5B-O5B-PA-O2A
3	D	701	FAD	C5B-O5B-PA-O1A
3	D	701	FAD	C5B-O5B-PA-O2A
3	E	701	FAD	C5B-O5B-PA-O1A
3	E	701	FAD	C5B-O5B-PA-O2A
3	F	701	FAD	C5B-O5B-PA-O1A
3	F	701	FAD	C5B-O5B-PA-O2A
4	A	801	TPP	C7-O7-PA-O2A
5	A	901	DTT	S1-C1-C2-O2
5	B	901	DTT	O3-C3-C4-S4
5	D	901	DTT	O3-C3-C4-S4
5	E	901	DTT	S1-C1-C2-O2
3	E	701	FAD	O4'-C4'-C5'-O5'
6	A	951[A]	1PE	C14-C24-OH4-C13
6	A	951[B]	1PE	C23-C13-OH4-C24
6	A	951[B]	1PE	OH4-C13-C23-OH3
5	B	901	DTT	C2-C3-C4-S4

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Mol	Chain	Res	Type	Atoms
4	A	801	TPP	C4'-C5'-C7'-N3
4	C	801	TPP	C4'-C5'-C7'-N3
4	A	801	TPP	C7-O7-PA-O3A
4	B	801	TPP	C7-O7-PA-O3A
3	C	701	FAD	P-O3P-PA-O1A
3	C	701	FAD	P-O3P-PA-O2A
3	F	701	FAD	P-O3P-PA-O1A
6	A	951[A]	1PE	C15-C25-OH5-C14
3	B	701	FAD	C3'-C4'-C5'-O5'
3	C	701	FAD	C5'-O5'-P-O1P
3	F	701	FAD	C5'-O5'-P-O1P
4	A	801	TPP	C7-O7-PA-O1A
4	B	801	TPP	C7-O7-PA-O1A
4	D	801	TPP	C7-O7-PA-O1A
4	E	801	TPP	C7-O7-PA-O1A
4	F	801	TPP	C7-O7-PA-O1A

There are no ring outliers.

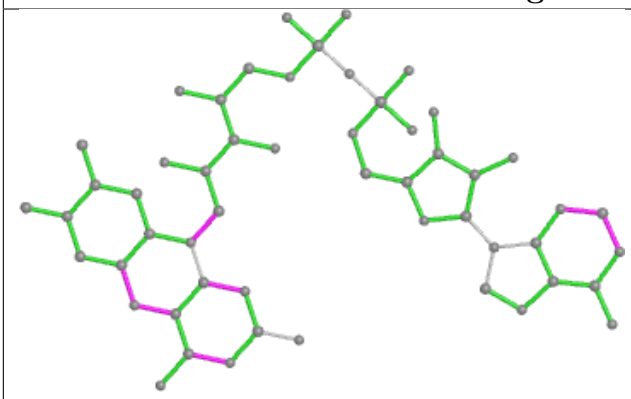
13 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	901	DTT	1	0
3	C	701	FAD	1	0
4	C	801	TPP	1	0
5	A	901	DTT	1	0
6	A	951[A]	1PE	5	0
6	A	951[B]	1PE	3	0
3	B	701	FAD	3	0
5	C	901	DTT	1	0
4	E	801	TPP	2	0
4	B	801	TPP	1	0
3	A	701	FAD	1	0
3	D	701	FAD	1	0
4	D	801	TPP	1	0

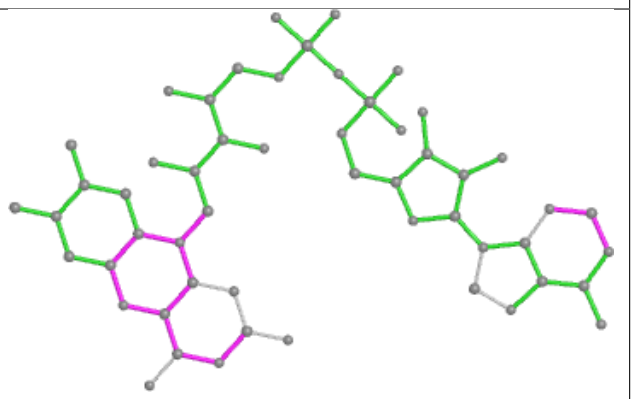
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

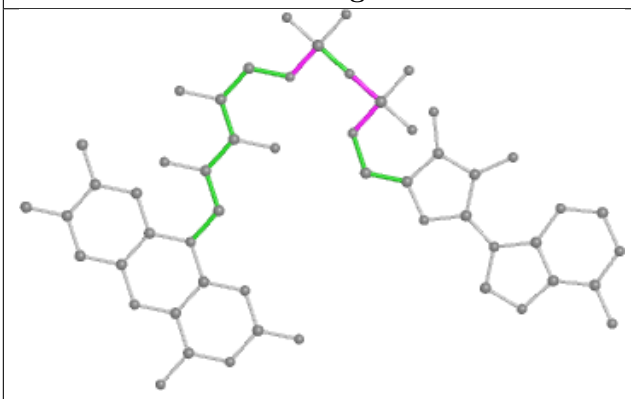
Ligand FAD F 701



Bond lengths



Bond angles



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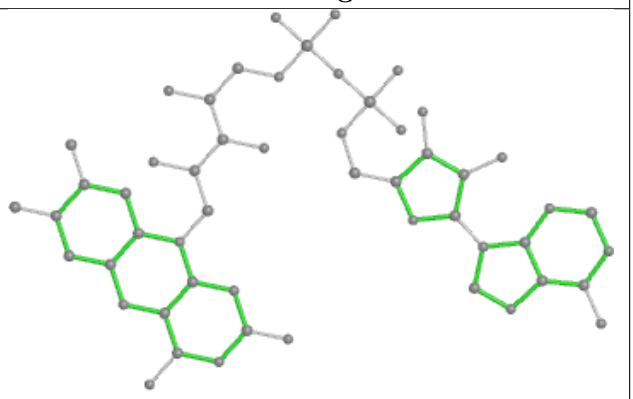
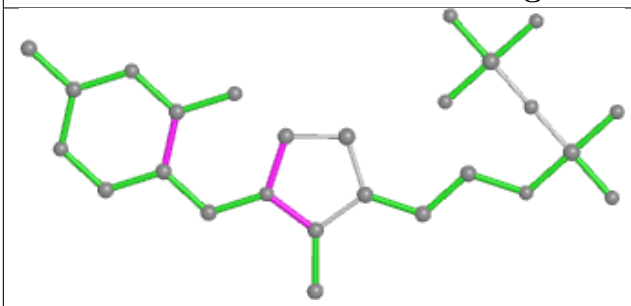


Rings

Ligand TPP A 801



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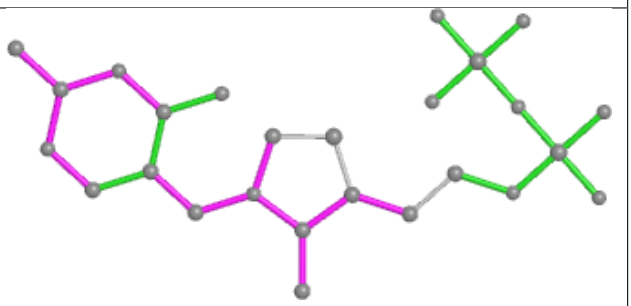

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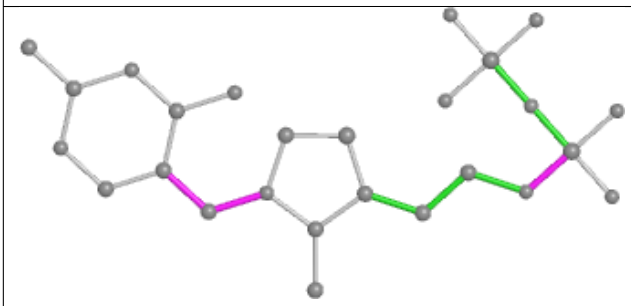

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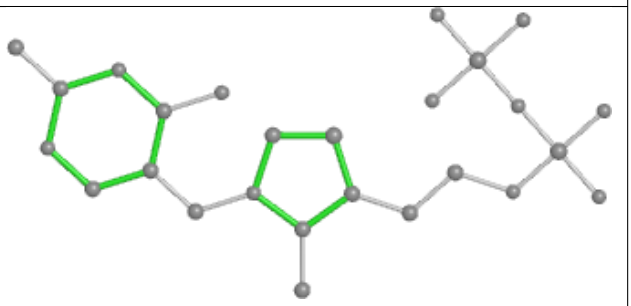
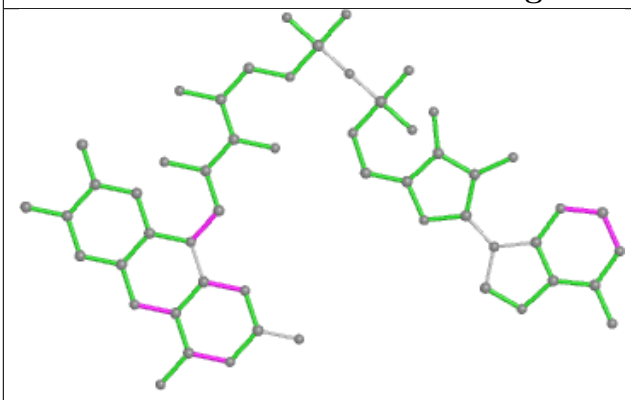


Rings

Ligand FAD C 701



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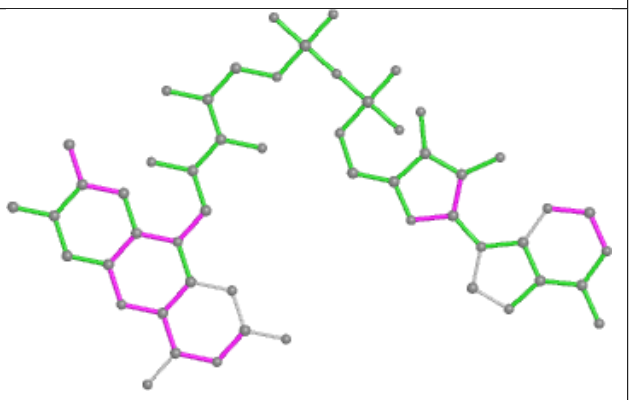

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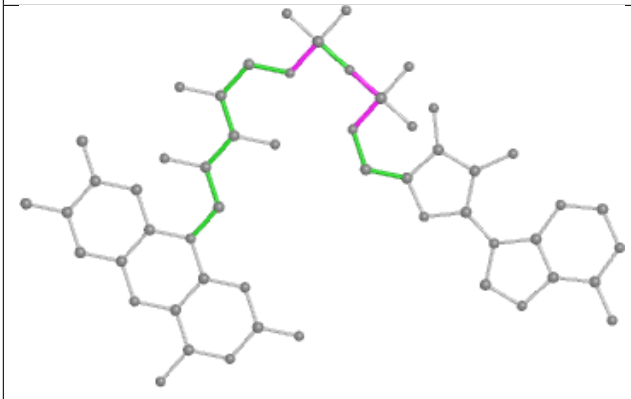

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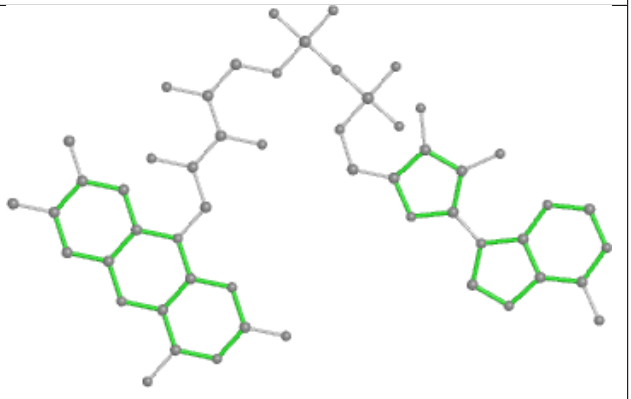
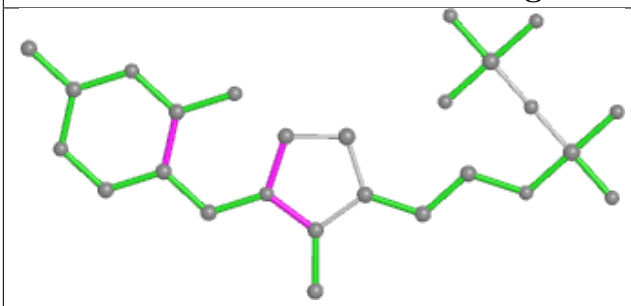


Rings

Ligand TPP C 801



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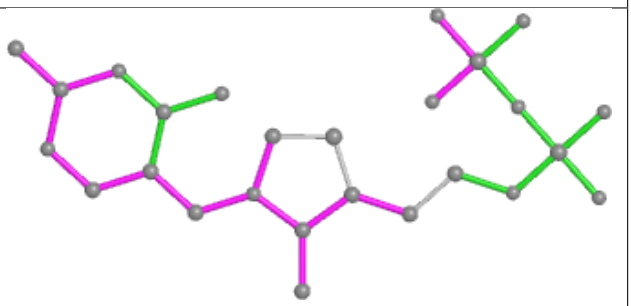

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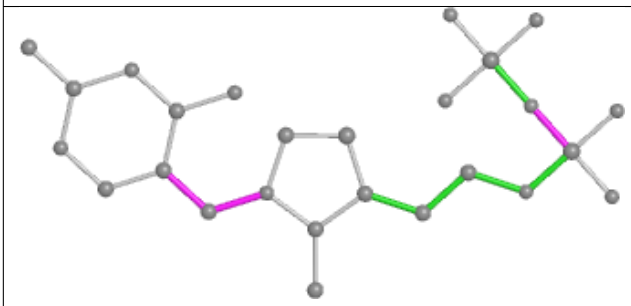

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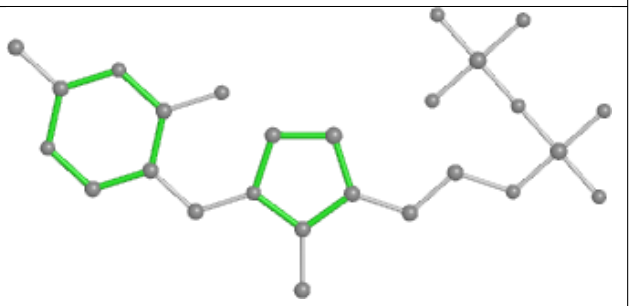
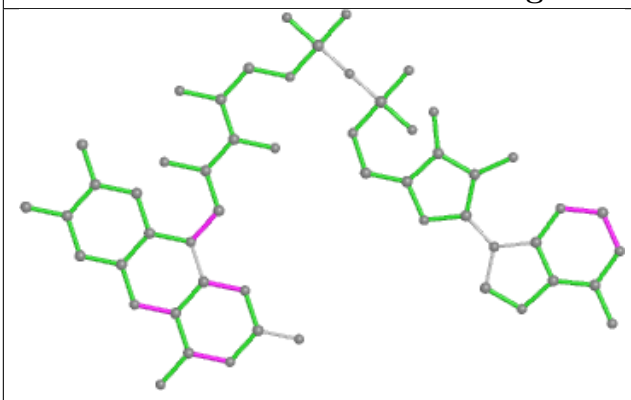


Rings

Ligand FAD E 701



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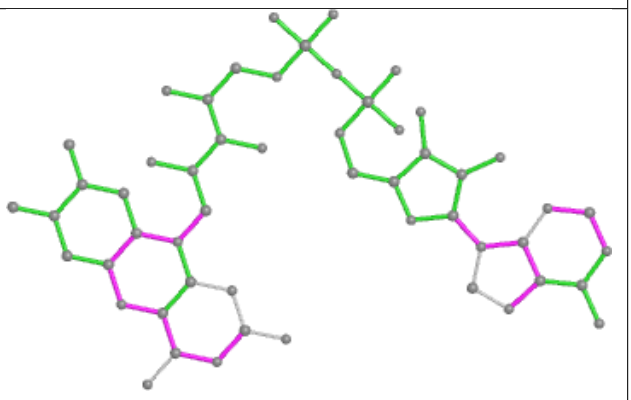

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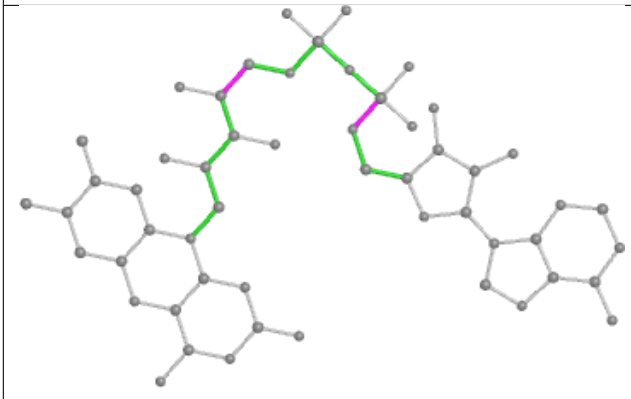

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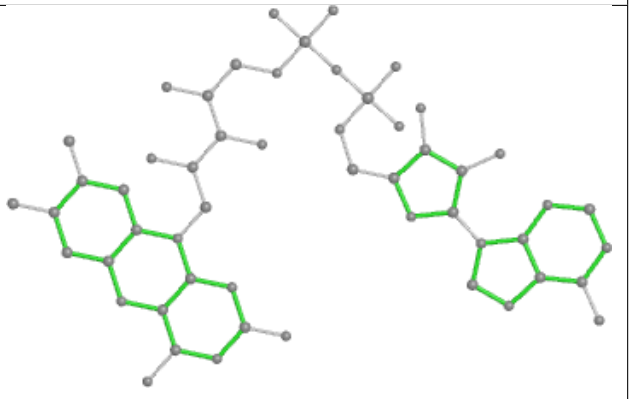
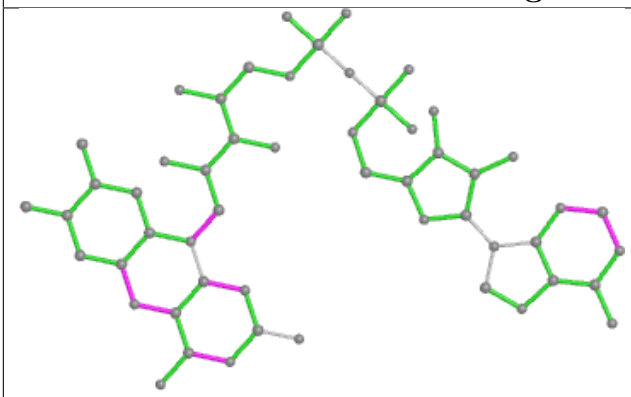


Rings

Ligand FAD B 701



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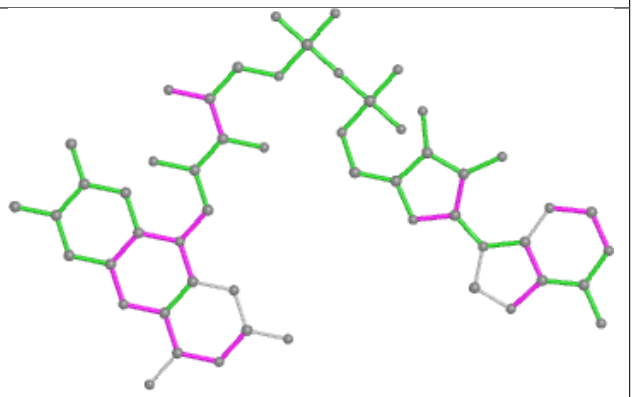

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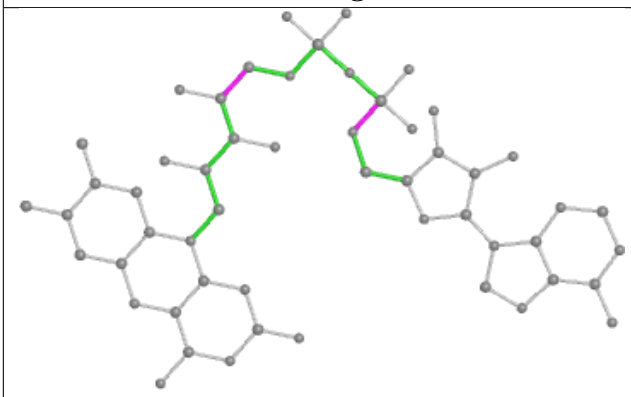

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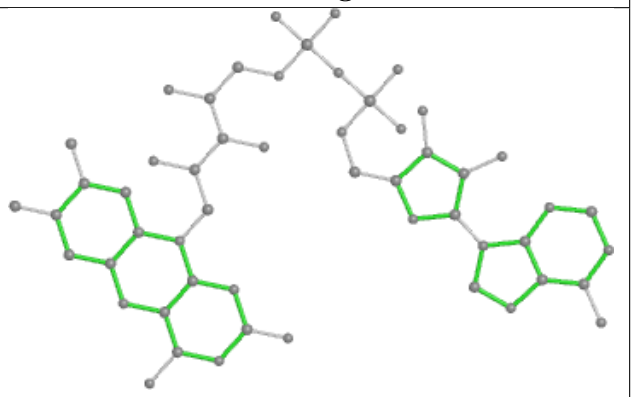
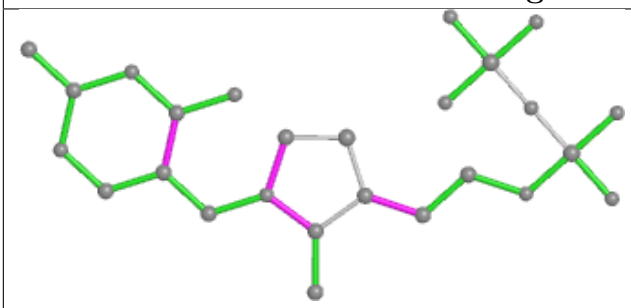


Rings

Ligand TPP F 801



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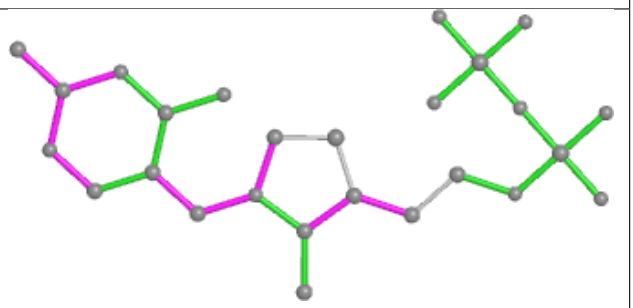

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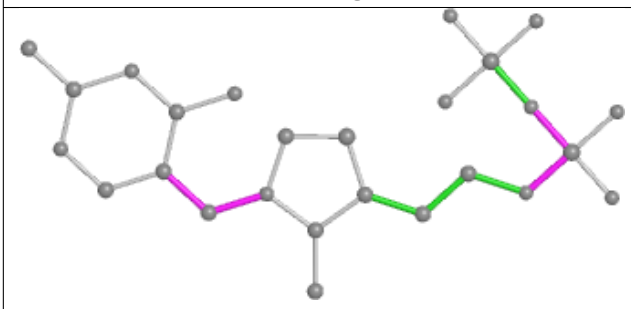

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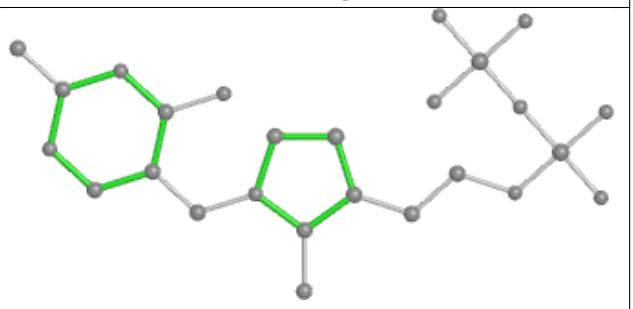
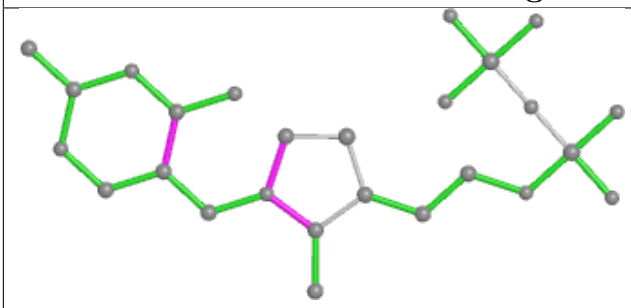


Rings

Ligand TPP E 801



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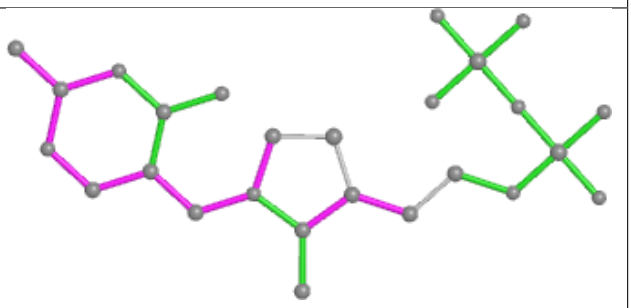

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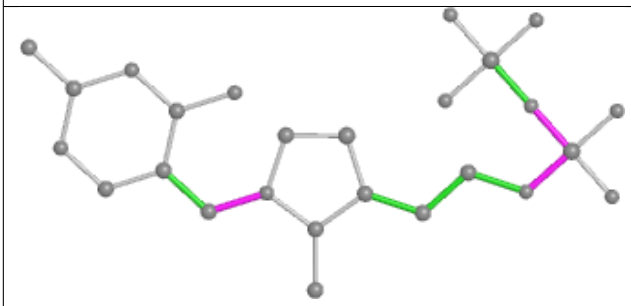

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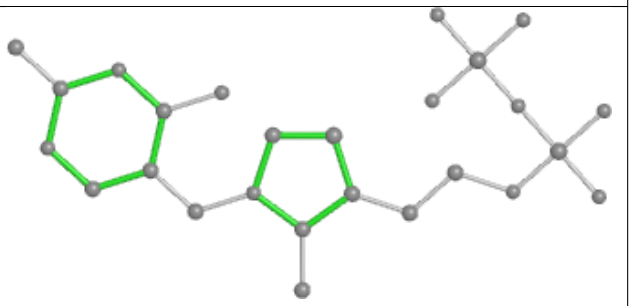
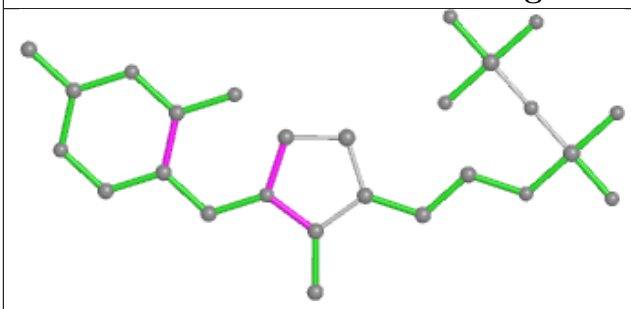


Rings

Ligand TPP B 801



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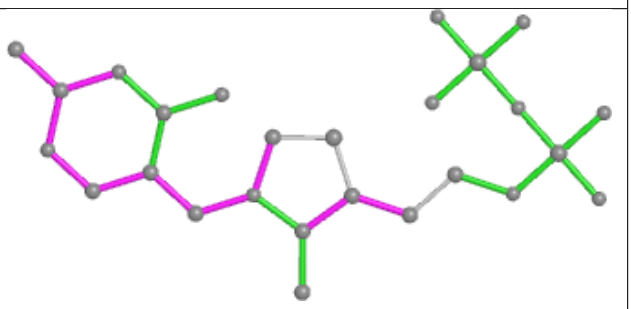

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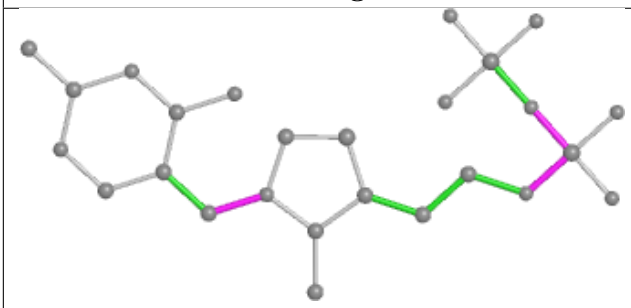

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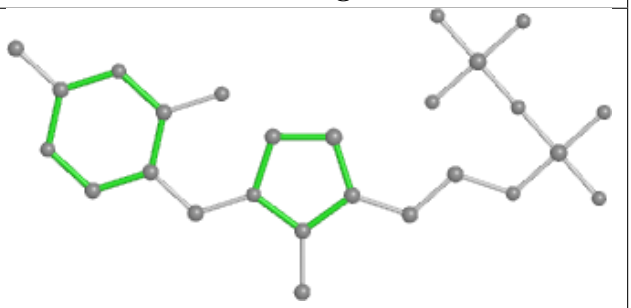
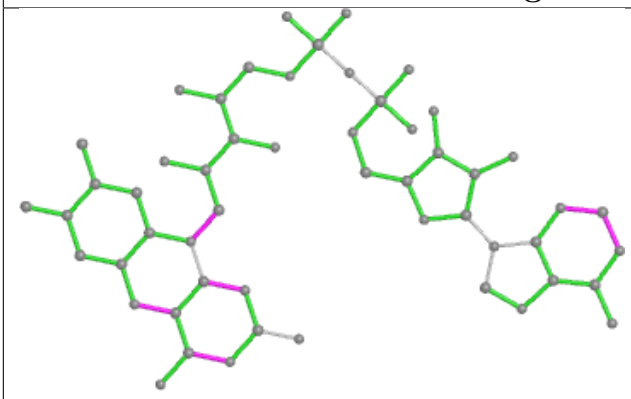


Rings

Ligand FAD A 701



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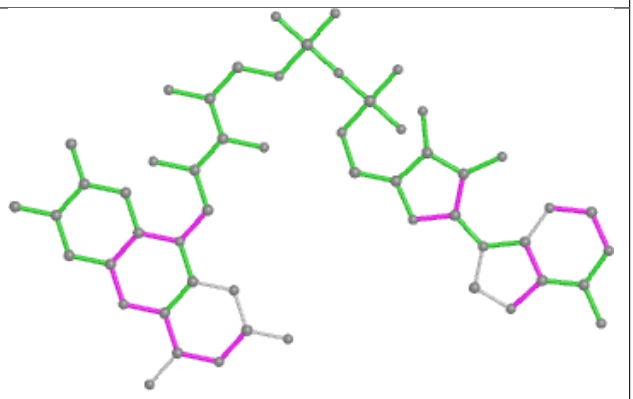

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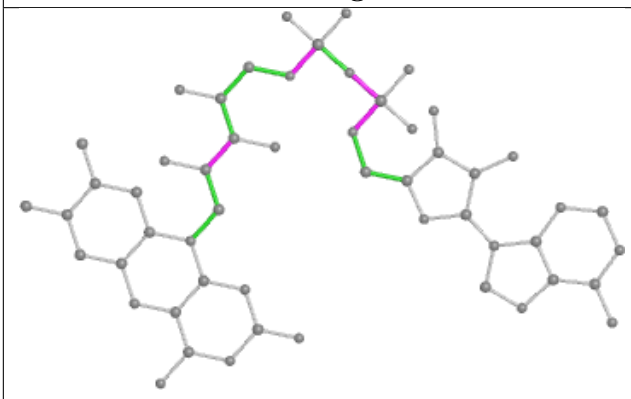

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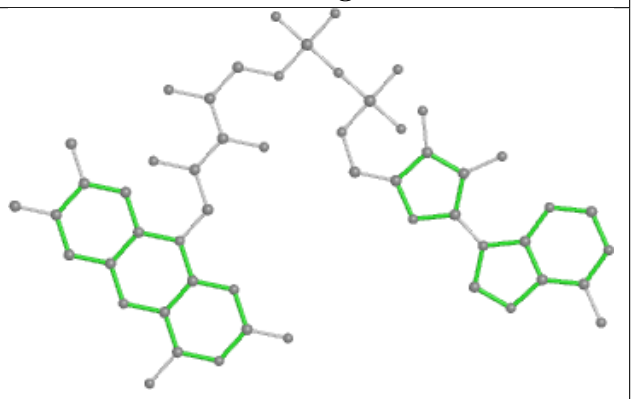
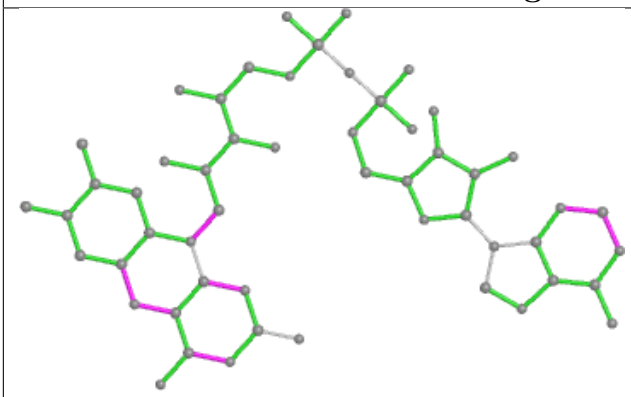
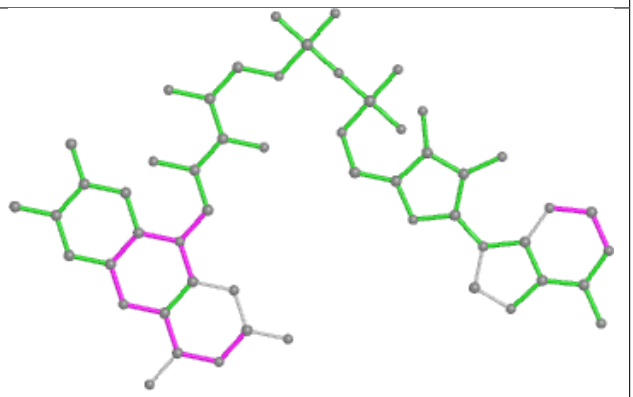


Rings

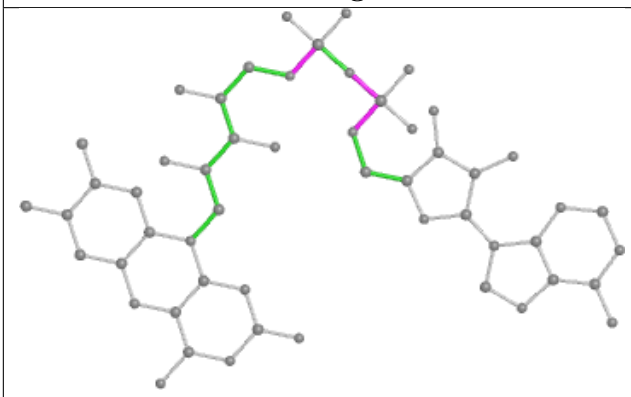
Ligand FAD D 701



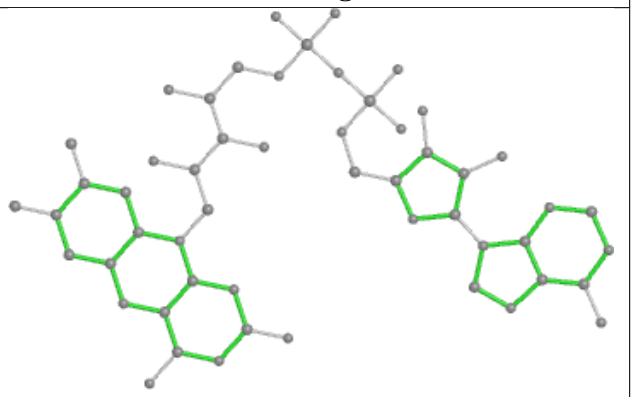
Bond lengths



Bond angles

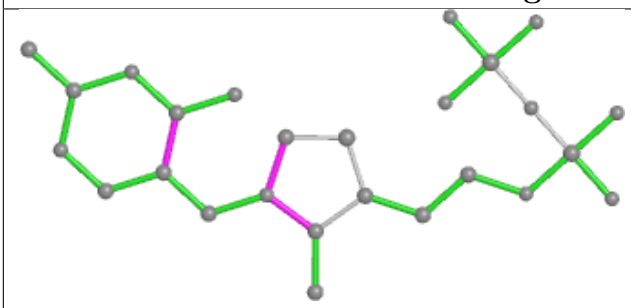


Torsions

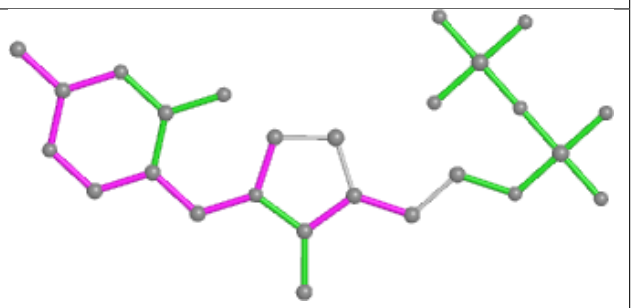


Rings

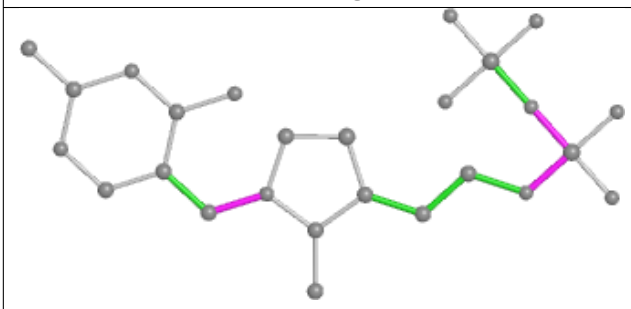
Ligand TPP D 801



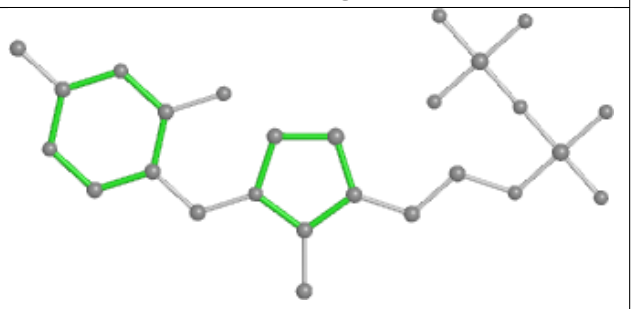
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	570/616 (92%)	-0.42	2 (0%)	92	93	20, 26, 37, 48	0
1	B	570/616 (92%)	-0.32	1 (0%)	95	96	21, 27, 39, 53	0
1	C	570/616 (92%)	-0.12	9 (1%)	72	74	33, 39, 51, 68	0
1	D	570/616 (92%)	-0.18	5 (0%)	84	85	35, 41, 53, 68	0
1	E	570/616 (92%)	0.01	25 (4%)	34	33	34, 45, 61, 79	0
1	F	570/616 (92%)	-0.06	10 (1%)	68	70	36, 45, 60, 73	0
All	All	3420/3696 (92%)	-0.18	52 (1%)	73	76	20, 39, 55, 79	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	4.4
1	E	201	ILE	3.9
1	E	593	GLU	3.8
1	A	2	ALA	3.8
1	F	175	PRO	3.7
1	F	2	ALA	3.4
1	F	176	ASP	3.2
1	E	2	ALA	3.2
1	B	340	GLY	3.1
1	E	9	ALA	3.1
1	E	578	ASP	3.0
1	F	593	GLU	3.0
1	E	295	GLY	3.0
1	C	3	LYS	2.9
1	E	487	ASP	2.8
1	D	487	ASP	2.8
1	E	344	CYS	2.7
1	E	340	GLY	2.7
1	D	2	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	197	VAL	2.7
1	C	344	CYS	2.6
1	D	340	GLY	2.6
1	C	172	GLU	2.6
1	C	340	GLY	2.6
1	F	190	ARG	2.6
1	E	41	GLY	2.5
1	E	198	GLU	2.5
1	E	347	GLU	2.5
1	C	540	ALA	2.5
1	D	593	GLU	2.5
1	E	339	ALA	2.4
1	C	176	ASP	2.4
1	F	505	ASN	2.4
1	E	328	LEU	2.4
1	E	579	ASN	2.3
1	E	343	PRO	2.3
1	E	335	GLU	2.3
1	A	593	GLU	2.3
1	C	331	GLU	2.2
1	E	332	VAL	2.2
1	E	202	GLN	2.2
1	F	340	GLY	2.2
1	E	178	TYR	2.1
1	F	15	GLU	2.1
1	F	487	ASP	2.1
1	E	194	GLU	2.1
1	E	350	ALA	2.1
1	E	505	ASN	2.1
1	C	588	CYS	2.1
1	E	485	ALA	2.1
1	F	338	LYS	2.1
1	D	315	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)

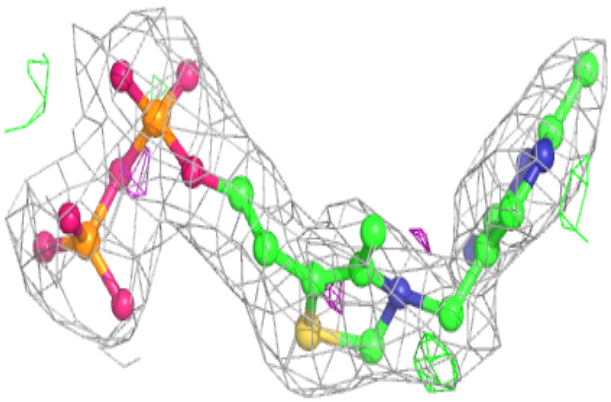
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

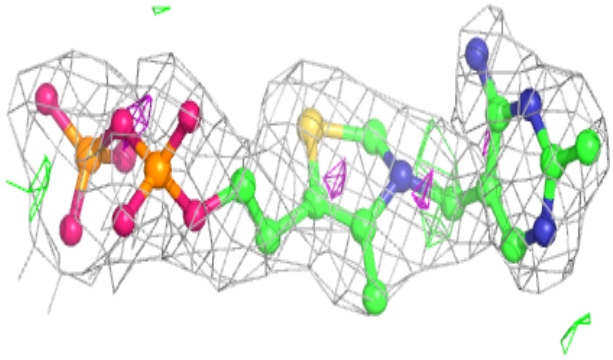
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DTT	C	901	8/8	0.74	0.45	45,46,47,47	8
5	DTT	B	901	8/8	0.80	0.34	25,26,27,29	8
2	MG	C	851	1/1	0.80	0.09	25,25,25,25	0
6	1PE	A	951[A]	16/16	0.81	0.31	59,60,61,62	16
6	1PE	A	951[B]	16/16	0.81	0.31	57,59,59,59	16
5	DTT	F	901	8/8	0.83	0.38	39,39,40,40	8
5	DTT	E	901	8/8	0.84	0.34	38,38,39,39	8
2	MG	B	851	1/1	0.86	0.12	16,16,16,16	0
5	DTT	A	901	8/8	0.86	0.28	24,24,25,27	8
2	MG	F	851	1/1	0.87	0.11	37,37,37,37	0
2	MG	A	851	1/1	0.87	0.16	30,30,30,30	0
5	DTT	D	901	8/8	0.88	0.39	40,41,41,42	8
2	MG	E	851	1/1	0.90	0.17	41,41,41,41	0
2	MG	D	851	1/1	0.91	0.08	33,33,33,33	0
4	TPP	F	801	26/26	0.95	0.14	36,45,46,46	0
3	FAD	E	701	53/53	0.96	0.14	33,36,37,37	0
3	FAD	F	701	53/53	0.96	0.13	32,36,38,38	0
4	TPP	D	801	26/26	0.96	0.13	38,42,43,43	0
2	MG	E	1501	1/1	0.96	0.29	31,31,31,31	0
4	TPP	E	801	26/26	0.97	0.14	36,40,42,42	0
2	MG	F	1501	1/1	0.97	0.20	35,35,35,35	0
3	FAD	C	701	53/53	0.97	0.12	28,31,33,34	0
4	TPP	C	801	26/26	0.97	0.14	32,41,43,43	0
3	FAD	D	701	53/53	0.97	0.11	30,32,38,38	0
2	MG	A	1501	1/1	0.98	0.20	14,14,14,14	1
4	TPP	A	801	26/26	0.98	0.13	20,24,25,26	0
4	TPP	B	801	26/26	0.98	0.12	19,28,29,29	0
3	FAD	A	701	53/53	0.98	0.11	14,17,20,20	0
3	FAD	B	701	53/53	0.98	0.12	14,16,19,20	0
2	MG	B	1501	1/1	0.99	0.21	21,21,21,21	1

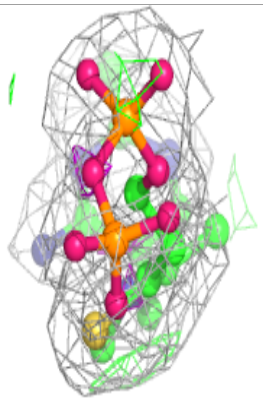
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP F 801:

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

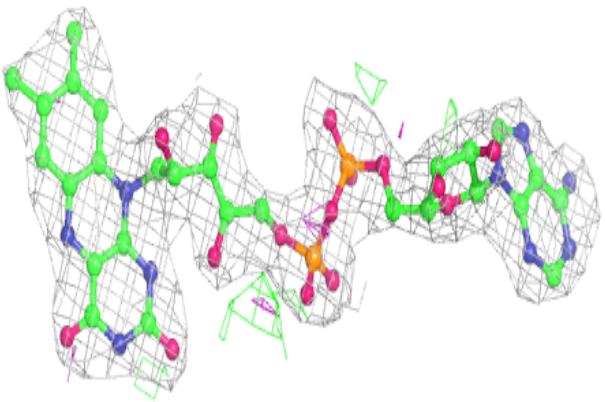


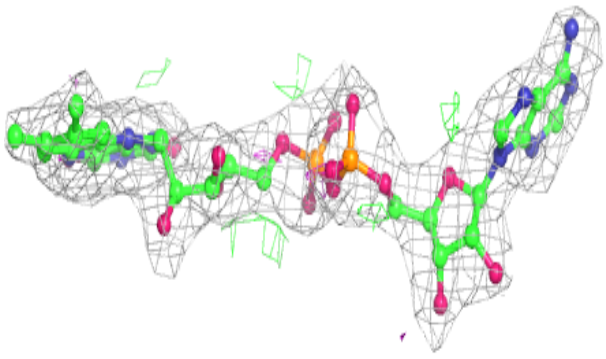


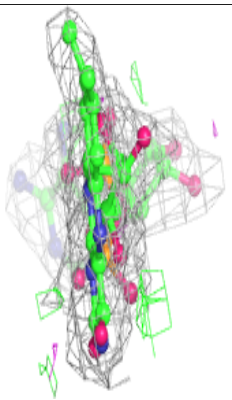


Electron density around FAD E 701:

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

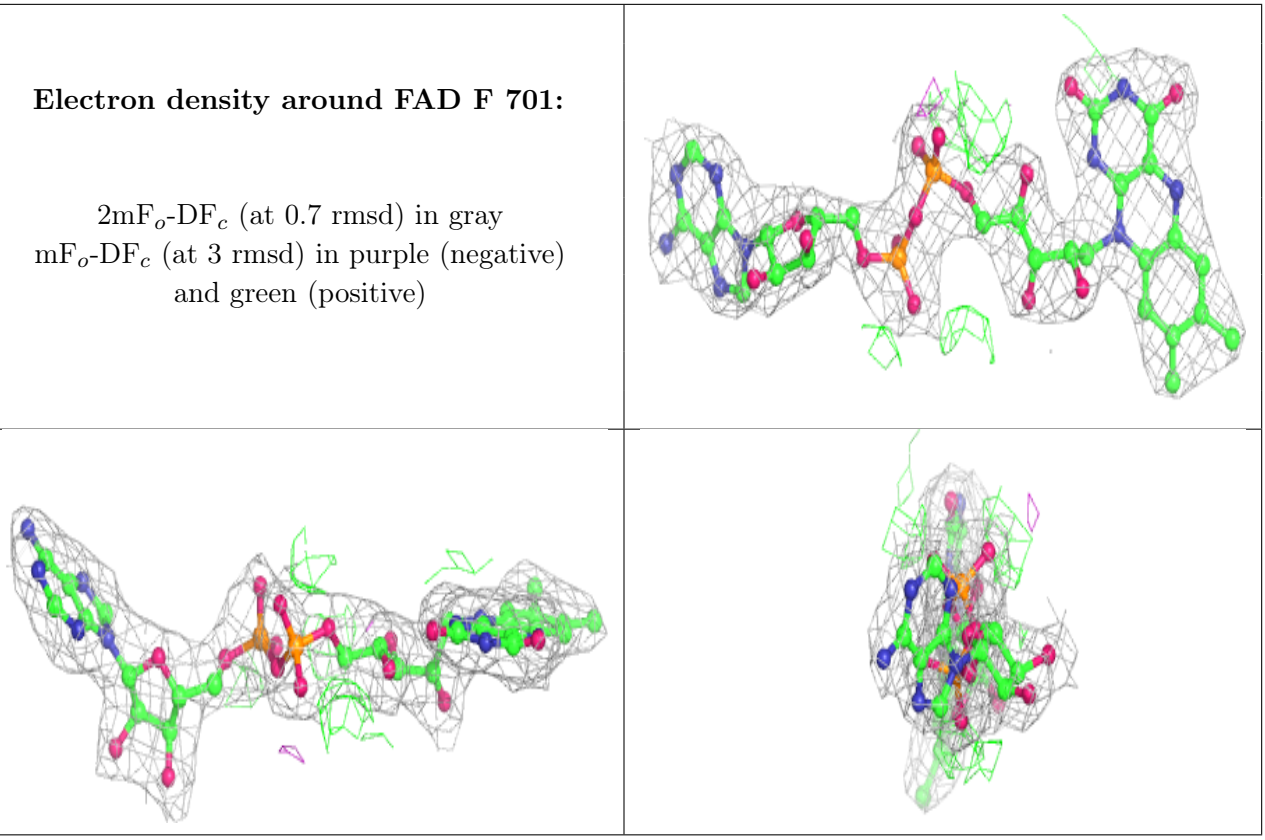






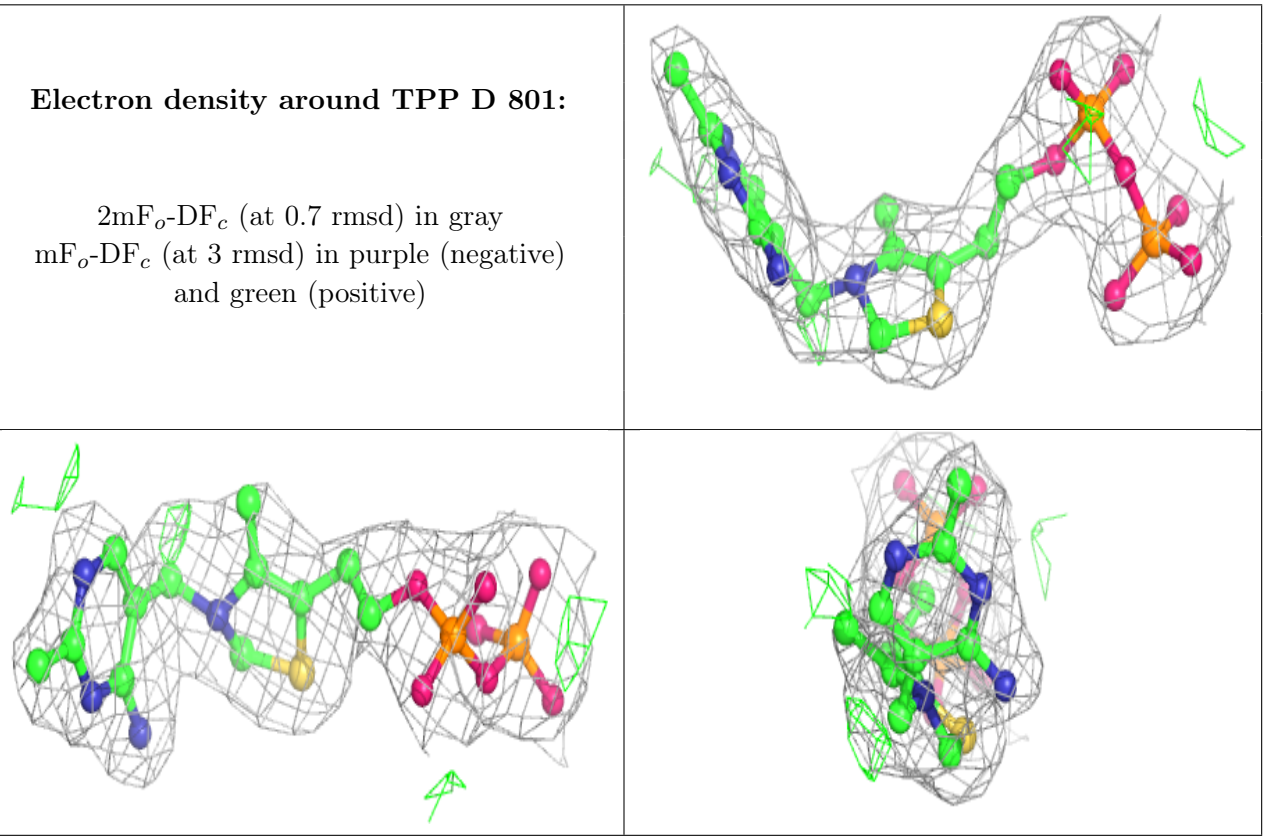
Electron density around FAD F 701:

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



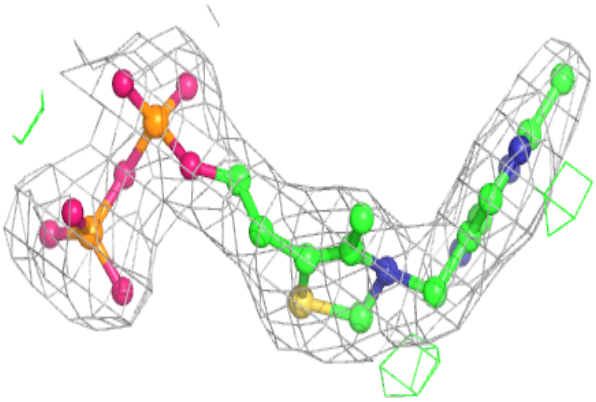
Electron density around TPP D 801:

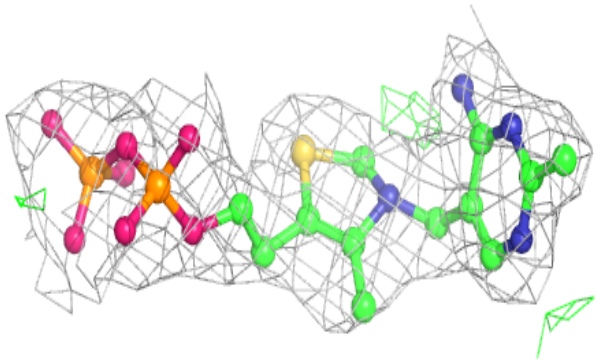
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

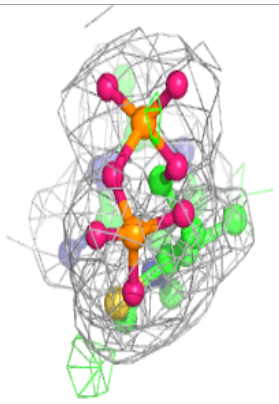


Electron density around TPP E 801:

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

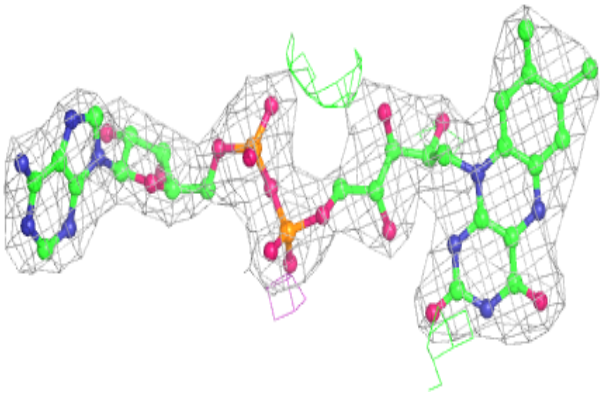


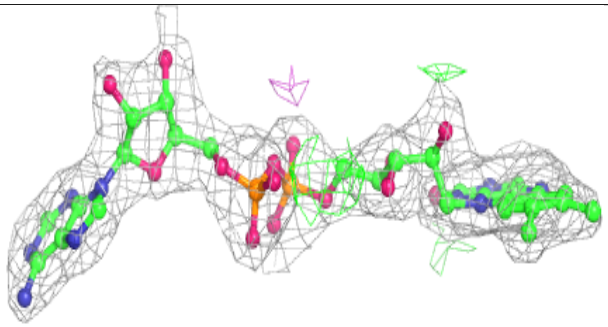


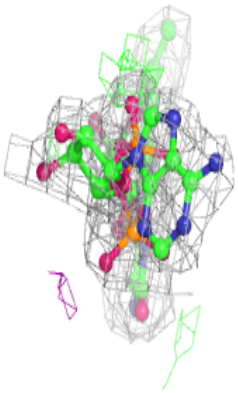


Electron density around FAD C 701:

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

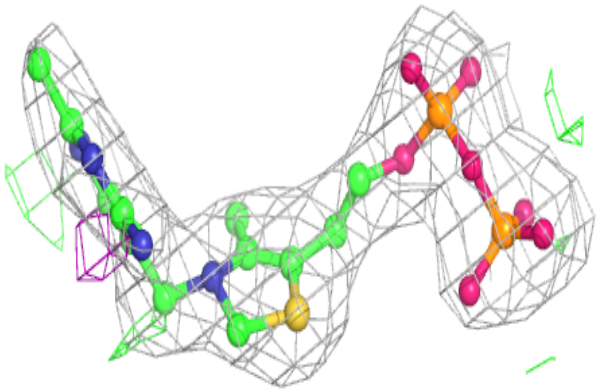


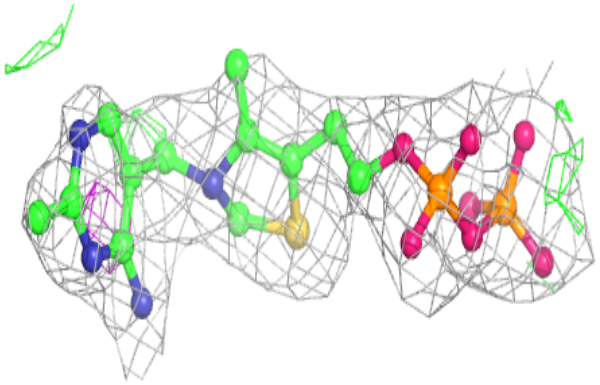


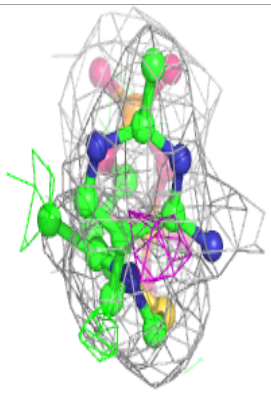


Electron density around TPP C 801:

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

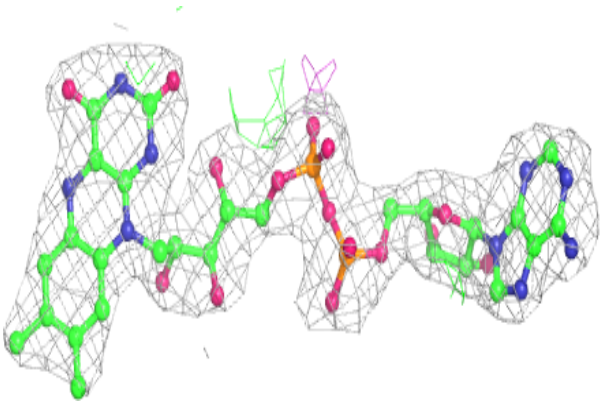


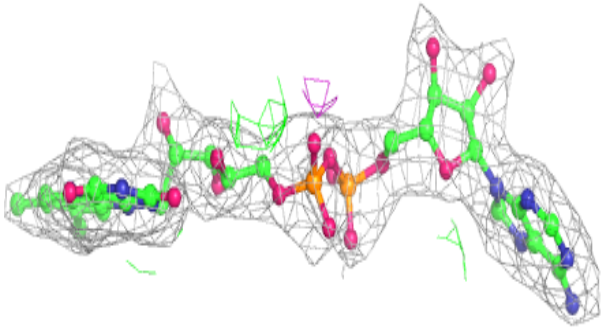


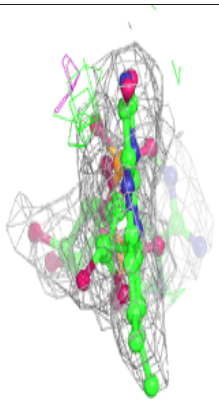


Electron density around FAD D 701:

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

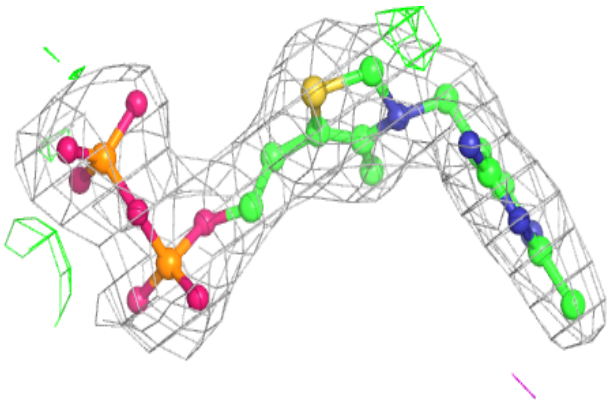


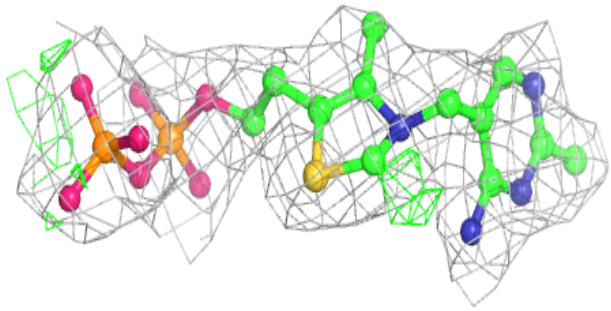


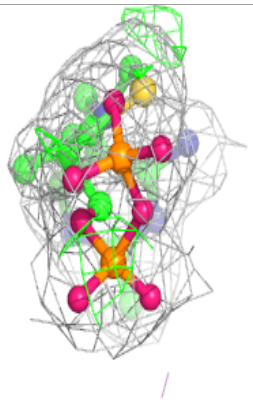


Electron density around TPP A 801:

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

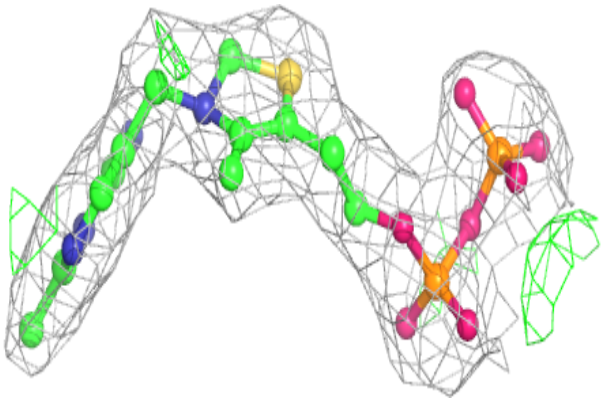


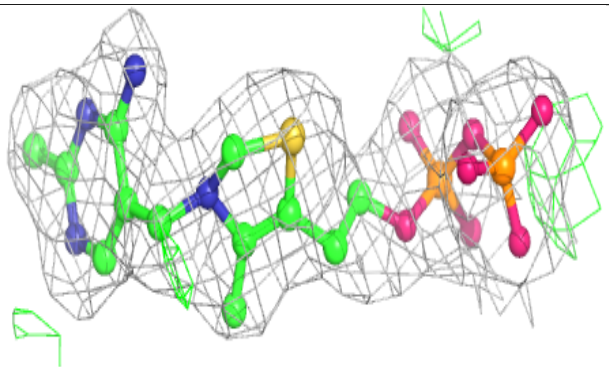


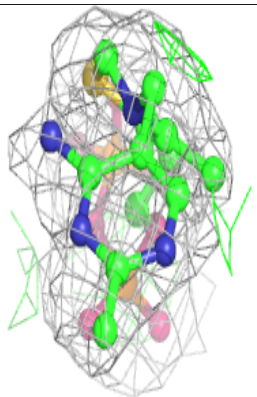


Electron density around TPP B 801:

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

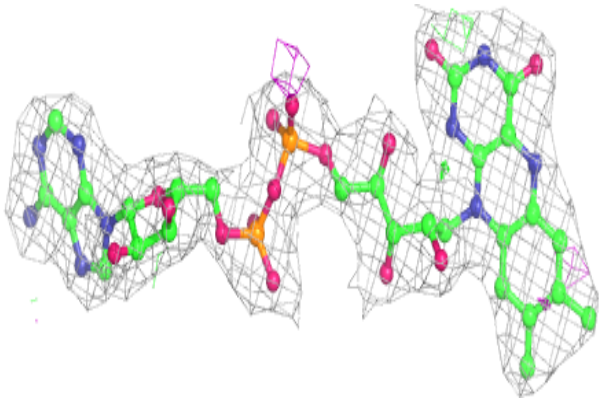


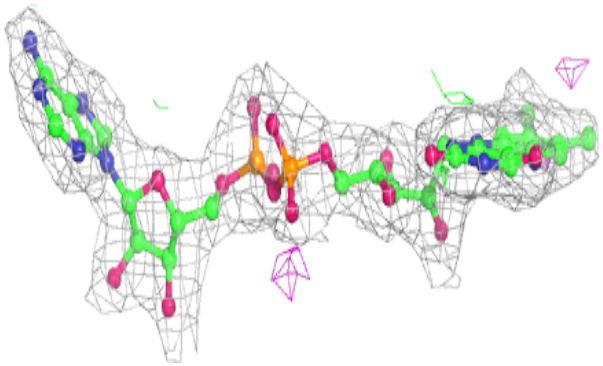


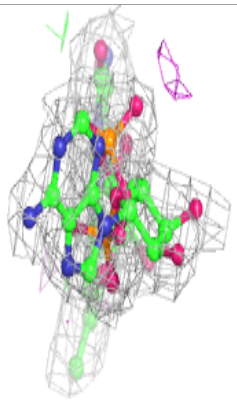


Electron density around FAD A 701:

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

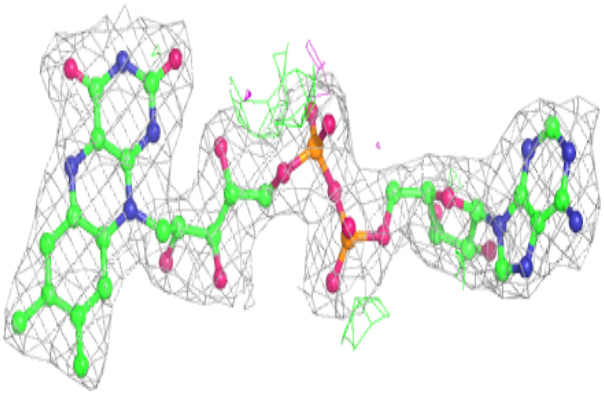


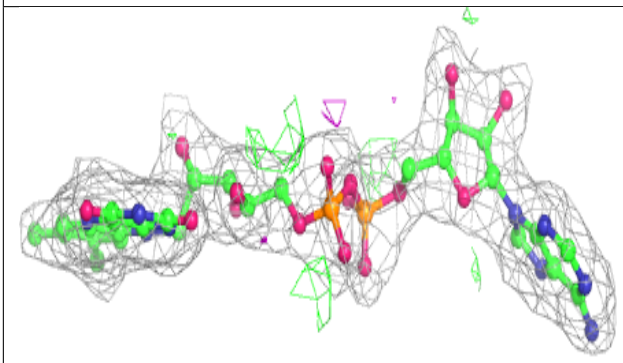


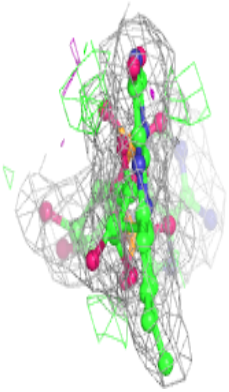


Electron density around FAD B 701:

$2mF_o$-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.