Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 11:27 PM EDT

PDB ID	:	4F07
Title	:	Structure of the Styrene Monooxygenase Flavin Reductase (SMOB) from Pseudomonas putida S12
Authors	:	Sazinsky, M.H.; Morrison, E.; Kantz, A.; Gassner, G.
Deposited on	:	2012-05-03
Resolution	:	2.30 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

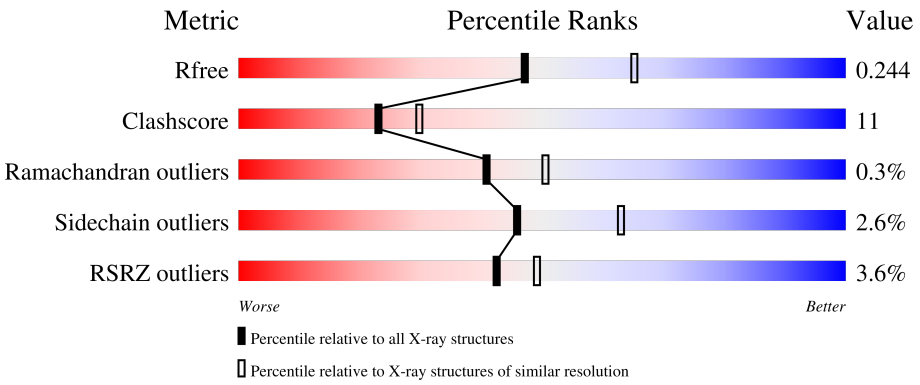
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	190	3%, 56%, 23%, •, 20%
1	B	190	2%, 68%, 12%, •, 19%
1	C	190	2%, 59%, 20%, •, 20%
1	D	190	4%, 63%, 16%, •, 19%
1	E	190	3%, 63%, 15%, •, 22%

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Mol	Chain	Length	Quality of chain
1	F	190	4% 64% 16% 18%
1	G	190	% 63% 17% 19%
1	H	190	5% 64% 16% 19%
1	I	190	2% 62% 18% 18%
1	J	190	6% 63% 17% 18%
1	K	190	2% 63% 18% 18%
1	L	190	2% 59% 19% 21%

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
3	NO3	H	202	-	-	X	-
3	NO3	J	202	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15130 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 Styrene monooxygenase component 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	152	1149	735	194	213	7	0	0	0
1	B	154	1168	746	198	217	7	0	1	0
1	C	152	1144	732	194	211	7	0	0	0
1	D	153	1152	737	195	213	7	0	0	0
1	E	149	1124	721	191	205	7	0	0	0
1	F	155	1167	745	198	217	7	0	0	0
1	G	153	1159	741	196	215	7	0	1	0
1	H	154	1158	740	196	215	7	0	0	0
1	I	155	1166	744	198	217	7	0	0	0
1	J	155	1167	745	198	217	7	0	0	0
1	K	155	1163	746	198	212	7	0	1	0
1	L	151	1138	729	193	209	7	0	0	0

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O33495
A	-18	GLY	-	expression tag	UNP O33495
A	-17	SER	-	expression tag	UNP O33495
A	-16	SER	-	expression tag	UNP O33495
A	-15	HIS	-	expression tag	UNP O33495

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP O33495
A	-13	HIS	-	expression tag	UNP O33495
A	-12	HIS	-	expression tag	UNP O33495
A	-11	HIS	-	expression tag	UNP O33495
A	-10	HIS	-	expression tag	UNP O33495
A	-9	SER	-	expression tag	UNP O33495
A	-8	SER	-	expression tag	UNP O33495
A	-7	GLY	-	expression tag	UNP O33495
A	-6	LEU	-	expression tag	UNP O33495
A	-5	VAL	-	expression tag	UNP O33495
A	-4	PRO	-	expression tag	UNP O33495
A	-3	ARG	-	expression tag	UNP O33495
A	-2	GLY	-	expression tag	UNP O33495
A	-1	SER	-	expression tag	UNP O33495
A	0	HIS	-	expression tag	UNP O33495
A	151	THR	ALA	engineered mutation	UNP O33495
A	164	GLY	SER	engineered mutation	UNP O33495
B	-19	MET	-	expression tag	UNP O33495
B	-18	GLY	-	expression tag	UNP O33495
B	-17	SER	-	expression tag	UNP O33495
B	-16	SER	-	expression tag	UNP O33495
B	-15	HIS	-	expression tag	UNP O33495
B	-14	HIS	-	expression tag	UNP O33495
B	-13	HIS	-	expression tag	UNP O33495
B	-12	HIS	-	expression tag	UNP O33495
B	-11	HIS	-	expression tag	UNP O33495
B	-10	HIS	-	expression tag	UNP O33495
B	-9	SER	-	expression tag	UNP O33495
B	-8	SER	-	expression tag	UNP O33495
B	-7	GLY	-	expression tag	UNP O33495
B	-6	LEU	-	expression tag	UNP O33495
B	-5	VAL	-	expression tag	UNP O33495
B	-4	PRO	-	expression tag	UNP O33495
B	-3	ARG	-	expression tag	UNP O33495
B	-2	GLY	-	expression tag	UNP O33495
B	-1	SER	-	expression tag	UNP O33495
B	0	HIS	-	expression tag	UNP O33495
B	151	THR	ALA	engineered mutation	UNP O33495
B	164	GLY	SER	engineered mutation	UNP O33495
C	-19	MET	-	expression tag	UNP O33495
C	-18	GLY	-	expression tag	UNP O33495
C	-17	SER	-	expression tag	UNP O33495

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	SER	-	expression tag	UNP O33495
C	-15	HIS	-	expression tag	UNP O33495
C	-14	HIS	-	expression tag	UNP O33495
C	-13	HIS	-	expression tag	UNP O33495
C	-12	HIS	-	expression tag	UNP O33495
C	-11	HIS	-	expression tag	UNP O33495
C	-10	HIS	-	expression tag	UNP O33495
C	-9	SER	-	expression tag	UNP O33495
C	-8	SER	-	expression tag	UNP O33495
C	-7	GLY	-	expression tag	UNP O33495
C	-6	LEU	-	expression tag	UNP O33495
C	-5	VAL	-	expression tag	UNP O33495
C	-4	PRO	-	expression tag	UNP O33495
C	-3	ARG	-	expression tag	UNP O33495
C	-2	GLY	-	expression tag	UNP O33495
C	-1	SER	-	expression tag	UNP O33495
C	0	HIS	-	expression tag	UNP O33495
C	151	THR	ALA	engineered mutation	UNP O33495
C	164	GLY	SER	engineered mutation	UNP O33495
D	-19	MET	-	expression tag	UNP O33495
D	-18	GLY	-	expression tag	UNP O33495
D	-17	SER	-	expression tag	UNP O33495
D	-16	SER	-	expression tag	UNP O33495
D	-15	HIS	-	expression tag	UNP O33495
D	-14	HIS	-	expression tag	UNP O33495
D	-13	HIS	-	expression tag	UNP O33495
D	-12	HIS	-	expression tag	UNP O33495
D	-11	HIS	-	expression tag	UNP O33495
D	-10	HIS	-	expression tag	UNP O33495
D	-9	SER	-	expression tag	UNP O33495
D	-8	SER	-	expression tag	UNP O33495
D	-7	GLY	-	expression tag	UNP O33495
D	-6	LEU	-	expression tag	UNP O33495
D	-5	VAL	-	expression tag	UNP O33495
D	-4	PRO	-	expression tag	UNP O33495
D	-3	ARG	-	expression tag	UNP O33495
D	-2	GLY	-	expression tag	UNP O33495
D	-1	SER	-	expression tag	UNP O33495
D	0	HIS	-	expression tag	UNP O33495
D	151	THR	ALA	engineered mutation	UNP O33495
D	164	GLY	SER	engineered mutation	UNP O33495
E	-19	MET	-	expression tag	UNP O33495

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-18	GLY	-	expression tag	UNP O33495
E	-17	SER	-	expression tag	UNP O33495
E	-16	SER	-	expression tag	UNP O33495
E	-15	HIS	-	expression tag	UNP O33495
E	-14	HIS	-	expression tag	UNP O33495
E	-13	HIS	-	expression tag	UNP O33495
E	-12	HIS	-	expression tag	UNP O33495
E	-11	HIS	-	expression tag	UNP O33495
E	-10	HIS	-	expression tag	UNP O33495
E	-9	SER	-	expression tag	UNP O33495
E	-8	SER	-	expression tag	UNP O33495
E	-7	GLY	-	expression tag	UNP O33495
E	-6	LEU	-	expression tag	UNP O33495
E	-5	VAL	-	expression tag	UNP O33495
E	-4	PRO	-	expression tag	UNP O33495
E	-3	ARG	-	expression tag	UNP O33495
E	-2	GLY	-	expression tag	UNP O33495
E	-1	SER	-	expression tag	UNP O33495
E	0	HIS	-	expression tag	UNP O33495
E	151	THR	ALA	engineered mutation	UNP O33495
E	164	GLY	SER	engineered mutation	UNP O33495
F	-19	MET	-	expression tag	UNP O33495
F	-18	GLY	-	expression tag	UNP O33495
F	-17	SER	-	expression tag	UNP O33495
F	-16	SER	-	expression tag	UNP O33495
F	-15	HIS	-	expression tag	UNP O33495
F	-14	HIS	-	expression tag	UNP O33495
F	-13	HIS	-	expression tag	UNP O33495
F	-12	HIS	-	expression tag	UNP O33495
F	-11	HIS	-	expression tag	UNP O33495
F	-10	HIS	-	expression tag	UNP O33495
F	-9	SER	-	expression tag	UNP O33495
F	-8	SER	-	expression tag	UNP O33495
F	-7	GLY	-	expression tag	UNP O33495
F	-6	LEU	-	expression tag	UNP O33495
F	-5	VAL	-	expression tag	UNP O33495
F	-4	PRO	-	expression tag	UNP O33495
F	-3	ARG	-	expression tag	UNP O33495
F	-2	GLY	-	expression tag	UNP O33495
F	-1	SER	-	expression tag	UNP O33495
F	0	HIS	-	expression tag	UNP O33495
F	151	THR	ALA	engineered mutation	UNP O33495

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Chain	Residue	Modelled	Actual	Comment	Reference
F	164	GLY	SER	engineered mutation	UNP O33495
G	-19	MET	-	expression tag	UNP O33495
G	-18	GLY	-	expression tag	UNP O33495
G	-17	SER	-	expression tag	UNP O33495
G	-16	SER	-	expression tag	UNP O33495
G	-15	HIS	-	expression tag	UNP O33495
G	-14	HIS	-	expression tag	UNP O33495
G	-13	HIS	-	expression tag	UNP O33495
G	-12	HIS	-	expression tag	UNP O33495
G	-11	HIS	-	expression tag	UNP O33495
G	-10	HIS	-	expression tag	UNP O33495
G	-9	SER	-	expression tag	UNP O33495
G	-8	SER	-	expression tag	UNP O33495
G	-7	GLY	-	expression tag	UNP O33495
G	-6	LEU	-	expression tag	UNP O33495
G	-5	VAL	-	expression tag	UNP O33495
G	-4	PRO	-	expression tag	UNP O33495
G	-3	ARG	-	expression tag	UNP O33495
G	-2	GLY	-	expression tag	UNP O33495
G	-1	SER	-	expression tag	UNP O33495
G	0	HIS	-	expression tag	UNP O33495
G	151	THR	ALA	engineered mutation	UNP O33495
G	164	GLY	SER	engineered mutation	UNP O33495
H	-19	MET	-	expression tag	UNP O33495
H	-18	GLY	-	expression tag	UNP O33495
H	-17	SER	-	expression tag	UNP O33495
H	-16	SER	-	expression tag	UNP O33495
H	-15	HIS	-	expression tag	UNP O33495
H	-14	HIS	-	expression tag	UNP O33495
H	-13	HIS	-	expression tag	UNP O33495
H	-12	HIS	-	expression tag	UNP O33495
H	-11	HIS	-	expression tag	UNP O33495
H	-10	HIS	-	expression tag	UNP O33495
H	-9	SER	-	expression tag	UNP O33495
H	-8	SER	-	expression tag	UNP O33495
H	-7	GLY	-	expression tag	UNP O33495
H	-6	LEU	-	expression tag	UNP O33495
H	-5	VAL	-	expression tag	UNP O33495
H	-4	PRO	-	expression tag	UNP O33495
H	-3	ARG	-	expression tag	UNP O33495
H	-2	GLY	-	expression tag	UNP O33495
H	-1	SER	-	expression tag	UNP O33495

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	HIS	-	expression tag	UNP O33495
H	151	THR	ALA	engineered mutation	UNP O33495
H	164	GLY	SER	engineered mutation	UNP O33495
I	-19	MET	-	expression tag	UNP O33495
I	-18	GLY	-	expression tag	UNP O33495
I	-17	SER	-	expression tag	UNP O33495
I	-16	SER	-	expression tag	UNP O33495
I	-15	HIS	-	expression tag	UNP O33495
I	-14	HIS	-	expression tag	UNP O33495
I	-13	HIS	-	expression tag	UNP O33495
I	-12	HIS	-	expression tag	UNP O33495
I	-11	HIS	-	expression tag	UNP O33495
I	-10	HIS	-	expression tag	UNP O33495
I	-9	SER	-	expression tag	UNP O33495
I	-8	SER	-	expression tag	UNP O33495
I	-7	GLY	-	expression tag	UNP O33495
I	-6	LEU	-	expression tag	UNP O33495
I	-5	VAL	-	expression tag	UNP O33495
I	-4	PRO	-	expression tag	UNP O33495
I	-3	ARG	-	expression tag	UNP O33495
I	-2	GLY	-	expression tag	UNP O33495
I	-1	SER	-	expression tag	UNP O33495
I	0	HIS	-	expression tag	UNP O33495
I	151	THR	ALA	engineered mutation	UNP O33495
I	164	GLY	SER	engineered mutation	UNP O33495
J	-19	MET	-	expression tag	UNP O33495
J	-18	GLY	-	expression tag	UNP O33495
J	-17	SER	-	expression tag	UNP O33495
J	-16	SER	-	expression tag	UNP O33495
J	-15	HIS	-	expression tag	UNP O33495
J	-14	HIS	-	expression tag	UNP O33495
J	-13	HIS	-	expression tag	UNP O33495
J	-12	HIS	-	expression tag	UNP O33495
J	-11	HIS	-	expression tag	UNP O33495
J	-10	HIS	-	expression tag	UNP O33495
J	-9	SER	-	expression tag	UNP O33495
J	-8	SER	-	expression tag	UNP O33495
J	-7	GLY	-	expression tag	UNP O33495
J	-6	LEU	-	expression tag	UNP O33495
J	-5	VAL	-	expression tag	UNP O33495
J	-4	PRO	-	expression tag	UNP O33495
J	-3	ARG	-	expression tag	UNP O33495

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-2	GLY	-	expression tag	UNP O33495
J	-1	SER	-	expression tag	UNP O33495
J	0	HIS	-	expression tag	UNP O33495
J	151	THR	ALA	engineered mutation	UNP O33495
J	164	GLY	SER	engineered mutation	UNP O33495
K	-19	MET	-	expression tag	UNP O33495
K	-18	GLY	-	expression tag	UNP O33495
K	-17	SER	-	expression tag	UNP O33495
K	-16	SER	-	expression tag	UNP O33495
K	-15	HIS	-	expression tag	UNP O33495
K	-14	HIS	-	expression tag	UNP O33495
K	-13	HIS	-	expression tag	UNP O33495
K	-12	HIS	-	expression tag	UNP O33495
K	-11	HIS	-	expression tag	UNP O33495
K	-10	HIS	-	expression tag	UNP O33495
K	-9	SER	-	expression tag	UNP O33495
K	-8	SER	-	expression tag	UNP O33495
K	-7	GLY	-	expression tag	UNP O33495
K	-6	LEU	-	expression tag	UNP O33495
K	-5	VAL	-	expression tag	UNP O33495
K	-4	PRO	-	expression tag	UNP O33495
K	-3	ARG	-	expression tag	UNP O33495
K	-2	GLY	-	expression tag	UNP O33495
K	-1	SER	-	expression tag	UNP O33495
K	0	HIS	-	expression tag	UNP O33495
K	151	THR	ALA	engineered mutation	UNP O33495
K	164	GLY	SER	engineered mutation	UNP O33495
L	-19	MET	-	expression tag	UNP O33495
L	-18	GLY	-	expression tag	UNP O33495
L	-17	SER	-	expression tag	UNP O33495
L	-16	SER	-	expression tag	UNP O33495
L	-15	HIS	-	expression tag	UNP O33495
L	-14	HIS	-	expression tag	UNP O33495
L	-13	HIS	-	expression tag	UNP O33495
L	-12	HIS	-	expression tag	UNP O33495
L	-11	HIS	-	expression tag	UNP O33495
L	-10	HIS	-	expression tag	UNP O33495
L	-9	SER	-	expression tag	UNP O33495
L	-8	SER	-	expression tag	UNP O33495
L	-7	GLY	-	expression tag	UNP O33495
L	-6	LEU	-	expression tag	UNP O33495
L	-5	VAL	-	expression tag	UNP O33495

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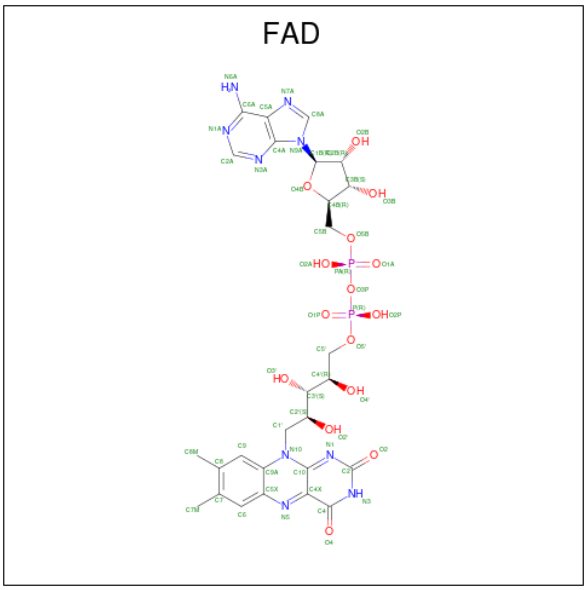
Chain	Residue	Modelled	Actual	Comment	Reference
L	-4	PRO	-	expression tag	UNP O33495
L	-3	ARG	-	expression tag	UNP O33495
L	-2	GLY	-	expression tag	UNP O33495
L	-1	SER	-	expression tag	UNP O33495
L	0	HIS	-	expression tag	UNP O33495
L	151	THR	ALA	engineered mutation	UNP O33495
L	164	GLY	SER	engineered mutation	UNP O33495

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

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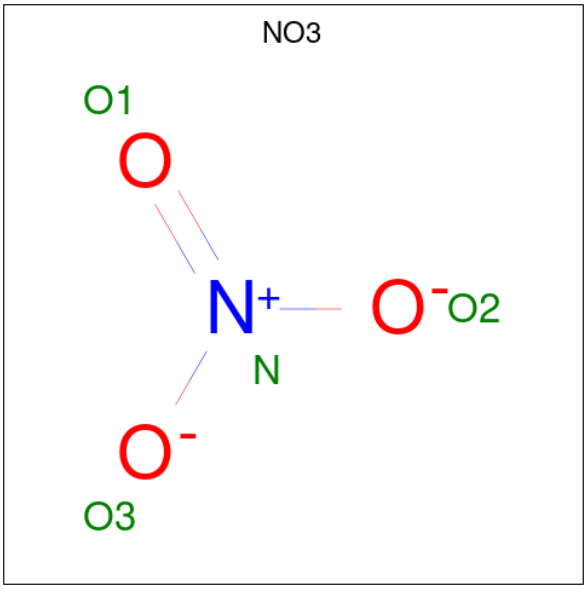
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	H	1	53	27	9	15	2	0	0
2	I	1	53	27	9	15	2	0	0
2	J	1	53	27	9	15	2	0	0
2	K	1	53	27	9	15	2	0	0
2	L	1	52	27	9	14	2	0	0

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
3	A	1	4	1	3	0	0
3	A	1	4	1	3	0	0
3	B	1	4	1	3	0	0
3	C	1	4	1	3	0	0
3	D	1	4	1	3	0	0
3	E	1	4	1	3	0	0

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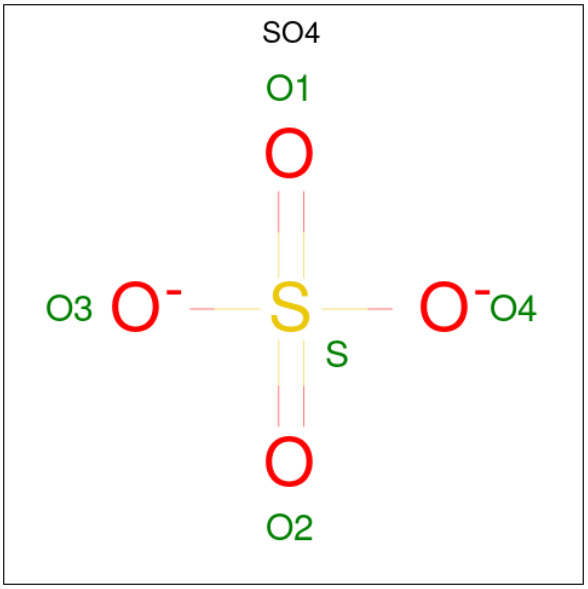
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
3	G	1	4	1	3	0	0
			Total	N	O		
3	H	1	4	1	3	0	0
			Total	N	O		
3	I	1	4	1	3	0	0
			Total	N	O		
3	J	1	4	1	3	0	0
			Total	N	O		
3	J	1	4	1	3	0	0
			Total	N	O		
3	L	1	4	1	3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

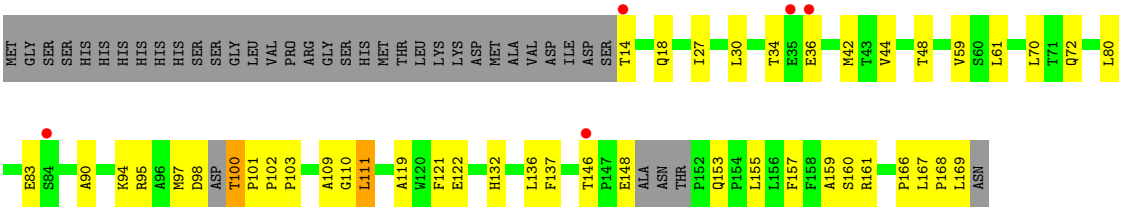
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	40	40	40	0	0
			Total	O		
5	B	61	61	61	0	0
			Total	O		
5	C	45	45	45	0	0
			Total	O		
5	D	33	33	33	0	0
			Total	O		
5	E	40	40	40	0	0
			Total	O		
5	F	45	45	45	0	0
			Total	O		
5	G	42	42	42	0	0
			Total	O		
5	H	35	35	35	0	0
			Total	O		
5	I	52	52	52	0	0
			Total	O		
5	J	66	66	66	0	0
			Total	O		
5	K	54	54	54	0	0
			Total	O		
5	L	64	64	64	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.

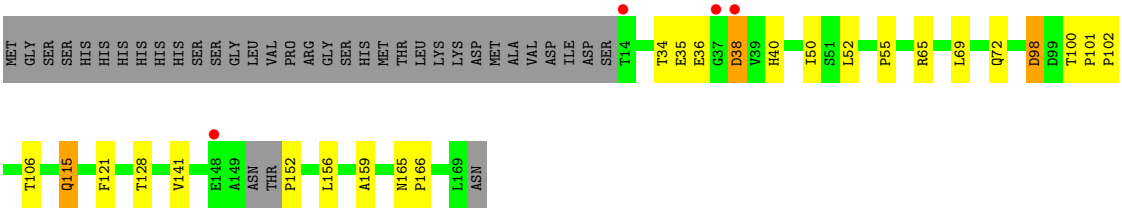
• Molecule 1: Styrene monooxygenase component 2

Chain A:



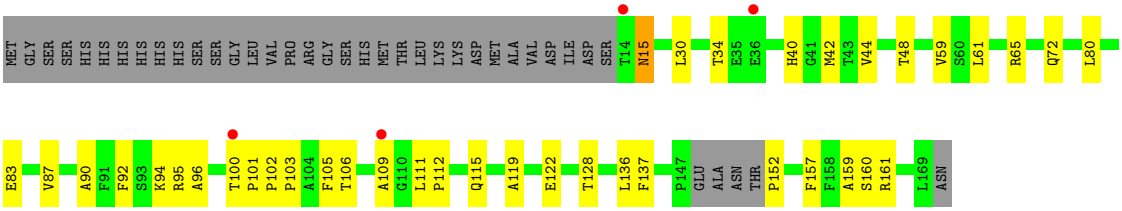
• Molecule 1: Styrene monooxygenase component 2

Chain B:



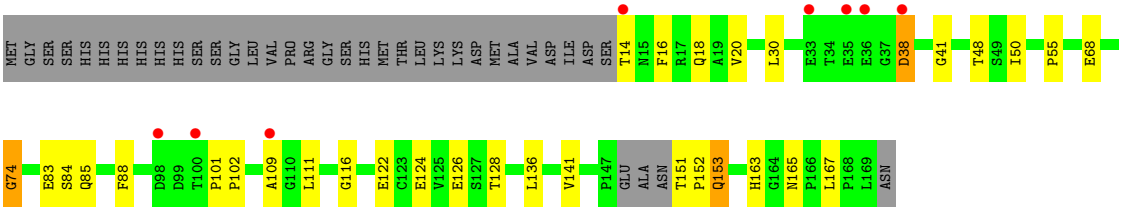
• Molecule 1: Styrene monooxygenase component 2

Chain C:



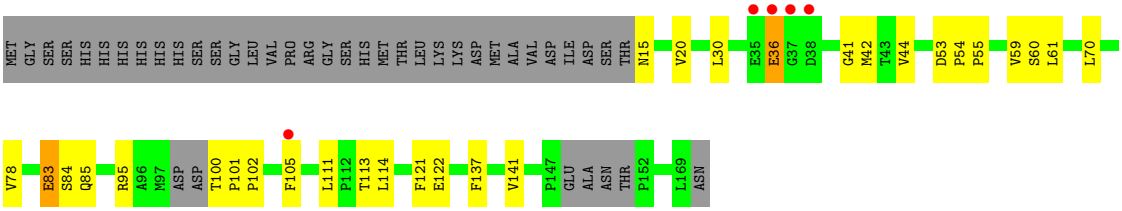
• Molecule 1: Styrene monooxygenase component 2

Chain D:



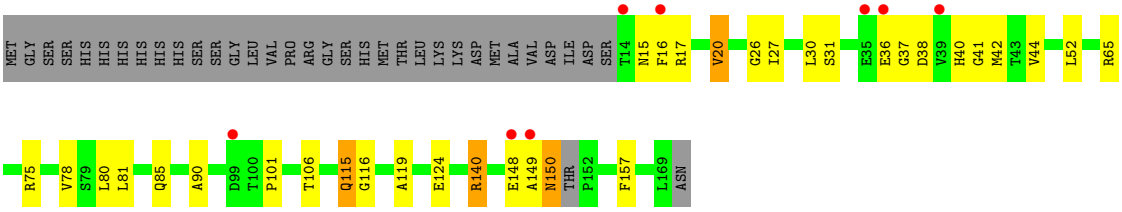
• Molecule 1: Styrene monooxygenase component 2

Chain E:



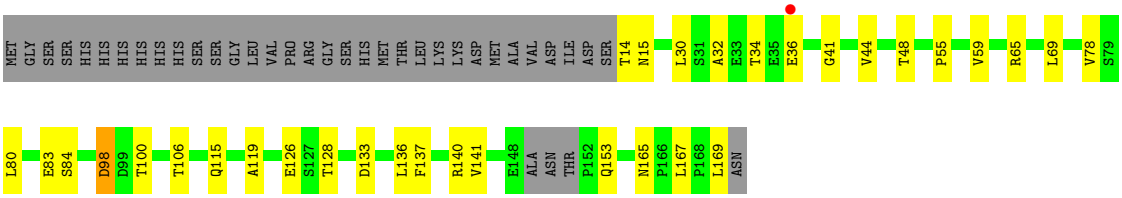
• Molecule 1: Styrene monooxygenase component 2

Chain F:



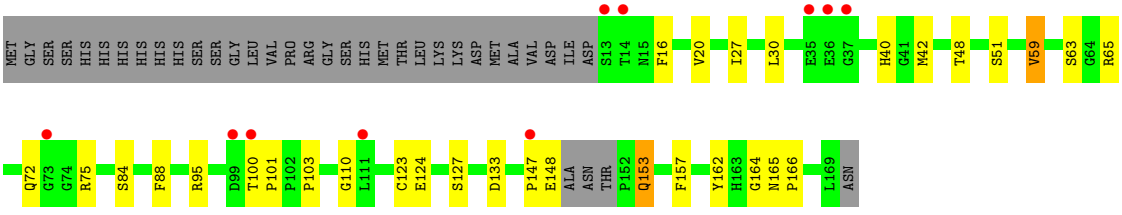
• Molecule 1: Styrene monooxygenase component 2

Chain G:



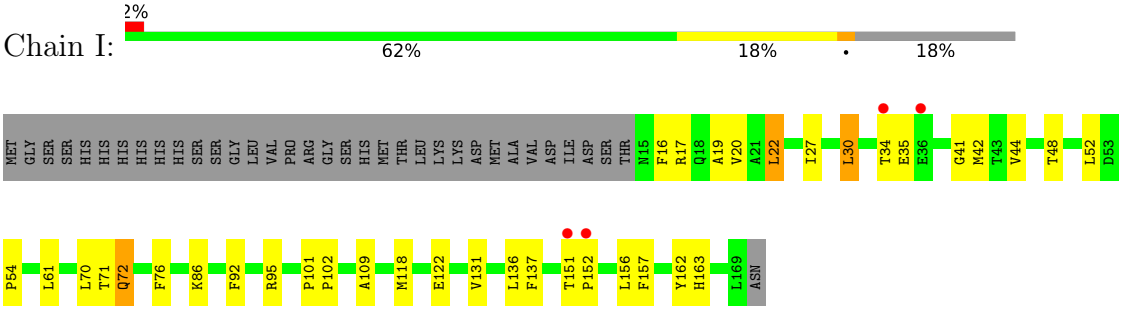
• Molecule 1: Styrene monooxygenase component 2

Chain H:



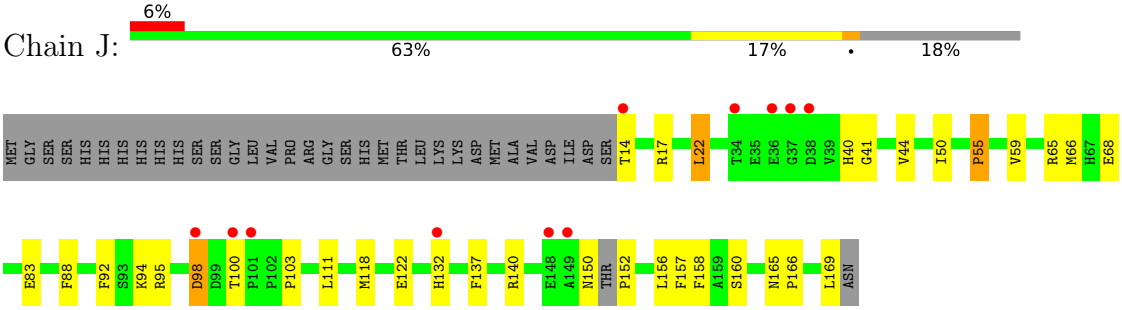
• Molecule 1: Styrene monooxygenase component 2

Chain I:



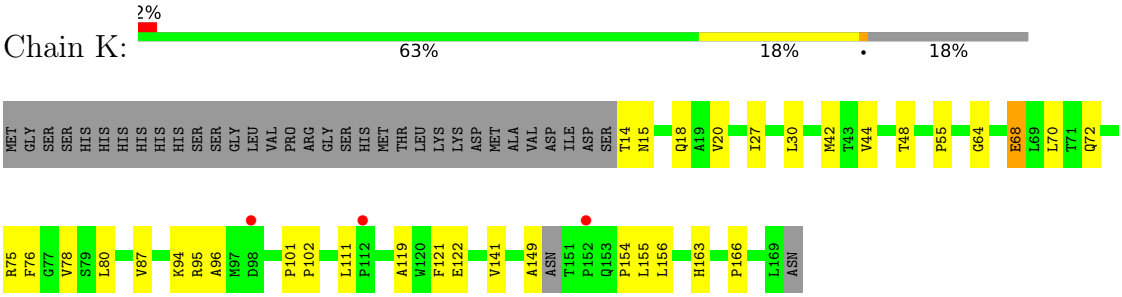
• Molecule 1: Styrene monooxygenase component 2

Chain J:



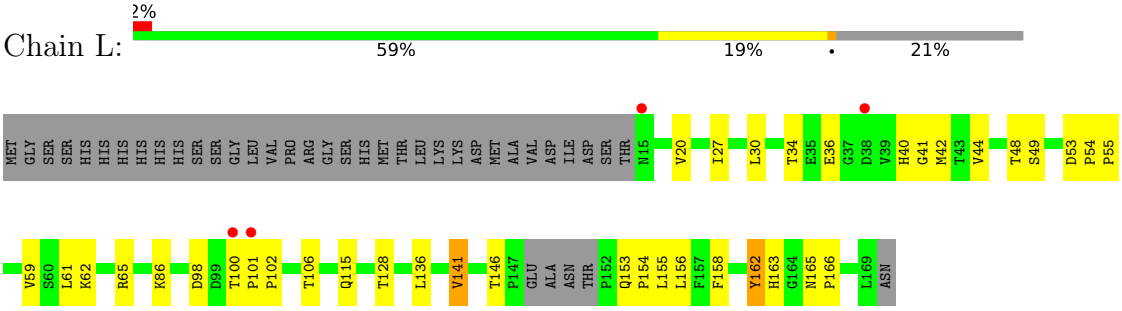
• Molecule 1: Styrene monooxygenase component 2

Chain K:



• Molecule 1: Styrene monooxygenase component 2

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	130.03Å 130.03Å 95.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.47 – 2.30 48.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.47-2.30) 100.0 (48.47-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$< I/\sigma(I) >$ [1]	5.04 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.185 , 0.248 0.199 , 0.244	Depositor DCC
R_{free} test set	3913 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	17.5	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	0.198 for -h,-k,l 0.008 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.884 for H, K, L 0.116 for -h,-k,l	Depositor
Outliers	0 of 79988 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15130	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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 28.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6803e-03. 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NO3, FAD, SO4

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	1.13	1/1177 (0.1%)	0.93	1/1598 (0.1%)
1	B	1.11	1/1197 (0.1%)	0.93	0/1627
1	C	0.97	0/1173	0.89	0/1594
1	D	1.08	1/1181 (0.1%)	0.87	1/1607 (0.1%)
1	E	1.12	1/1152 (0.1%)	0.90	0/1563
1	F	1.05	1/1196 (0.1%)	0.88	1/1626 (0.1%)
1	G	1.09	1/1191 (0.1%)	0.96	1/1619 (0.1%)
1	H	1.03	2/1187 (0.2%)	0.89	0/1614
1	I	1.25	3/1196 (0.3%)	0.96	1/1629 (0.1%)
1	J	1.14	0/1196	0.93	1/1626 (0.1%)
1	K	1.16	1/1195 (0.1%)	0.92	0/1625
1	L	1.24	3/1167 (0.3%)	0.98	0/1586
All	All	1.12	15/14208 (0.1%)	0.92	6/19314 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	68	GLU	CG-CD	5.55	1.60	1.51
1	L	162	TYR	CD1-CE1	5.46	1.47	1.39
1	E	83	GLU	CG-CD	5.43	1.60	1.51
1	A	121	PHE	CE2-CZ	5.42	1.47	1.37
1	L	141	VAL	CB-CG2	-5.37	1.41	1.52
1	L	162	TYR	CG-CD2	5.36	1.46	1.39
1	G	137	PHE	CE2-CZ	5.34	1.47	1.37
1	H	59	VAL	CB-CG2	5.34	1.64	1.52
1	I	131	VAL	CB-CG2	5.24	1.63	1.52
1	B	159	ALA	CA-CB	5.23	1.63	1.52
1	I	76	PHE	CE1-CZ	5.21	1.47	1.37
1	F	20	VAL	CB-CG1	-5.09	1.42	1.52
1	D	126	GLU	CG-CD	5.07	1.59	1.51
1	H	110	GLY	C-O	-5.07	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	137	PHE	CB-CG	5.01	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	81	LEU	CB-CG-CD1	-5.72	101.28	111.00
1	G	169	LEU	CA-CB-CG	5.47	127.89	115.30
1	D	167	LEU	CA-CB-CG	5.43	127.80	115.30
1	A	132	HIS	N-CA-C	-5.42	96.38	111.00
1	I	95	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	J	140	ARG	NE-CZ-NH2	-5.21	117.70	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1149	0	1128	39	0
1	B	1168	0	1143	17	0
1	C	1144	0	1121	32	0
1	D	1152	0	1131	25	0
1	E	1124	0	1107	24	0
1	F	1167	0	1142	30	0
1	G	1159	0	1137	20	0
1	H	1158	0	1131	30	0
1	I	1166	0	1140	31	0
1	J	1167	0	1142	38	0
1	K	1163	0	1144	30	0
1	L	1138	0	1118	34	0
2	A	53	0	31	2	0
2	B	53	0	31	0	0
2	C	53	0	31	3	0
2	D	53	0	31	2	0
2	E	53	0	31	3	0
2	F	53	0	31	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	53	0	31	1	0
2	H	53	0	31	6	0
2	I	53	0	31	3	0
2	J	53	0	31	2	0
2	K	53	0	31	4	0
2	L	52	0	31	4	0
3	A	8	0	0	1	0
3	B	4	0	0	0	0
3	C	4	0	0	1	0
3	D	4	0	0	1	0
3	E	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	2	0
3	I	4	0	0	0	0
3	J	8	0	0	3	0
3	L	4	0	0	1	0
4	D	10	0	0	0	0
4	J	5	0	0	1	0
5	A	40	0	0	0	0
5	B	61	0	0	2	0
5	C	45	0	0	3	0
5	D	33	0	0	0	0
5	E	40	0	0	0	0
5	F	45	0	0	2	0
5	G	42	0	0	0	0
5	H	35	0	0	0	0
5	I	52	0	0	2	0
5	J	66	0	0	2	0
5	K	54	0	0	4	0
5	L	64	0	0	1	0
All	All	15130	0	13956	326	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 11.

All (326) 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:D:83:GLU:OE1	1:H:84:SER:HB3	1.43	1.18
1:I:34:THR:CG2	1:I:35:GLU:H	1.65	1.10
1:A:110:GLY:C	1:A:111:LEU:HD13	1.76	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:34:THR:HG22	1:I:35:GLU:H	1.11	1.03
1:I:34:THR:HG22	1:I:35:GLU:N	1.65	1.01
1:A:110:GLY:O	1:A:111:LEU:HD13	1.64	0.97
1:G:106:THR:HG23	1:G:115[B]:GLN:HG2	1.43	0.96
1:J:40:HIS:HB2	1:J:65:ARG:HH21	1.30	0.95
1:F:42:MET:HE3	2:F:500:FAD:H5'2	1.50	0.94
1:E:36:GLU:HA	1:E:36:GLU:OE2	1.75	0.87
1:C:161:ARG:HD2	5:C:322:HOH:O	1.73	0.86
1:K:42:MET:HG3	2:K:500:FAD:H5'2	1.58	0.85
1:D:83:GLU:OE1	1:H:84:SER:CB	2.25	0.84
1:D:16:PHE:O	1:D:20:VAL:HG12	1.78	0.84
1:A:168:PRO:O	1:A:169:LEU:HD23	1.78	0.82
1:E:105:PHE:CE1	1:E:114:LEU:HG	2.17	0.79
1:A:136:LEU:HD21	1:D:50:ILE:HD12	1.67	0.77
1:A:30:LEU:HD11	1:A:59:VAL:HG21	1.65	0.77
1:A:100:THR:HB	1:A:101:PRO:HD3	1.67	0.77
1:I:136:LEU:HD21	1:J:50:ILE:HD12	1.67	0.76
1:A:98:ASP:O	1:A:100:THR:N	2.18	0.76
1:A:27:ILE:HD12	1:A:155:LEU:HG	1.66	0.76
1:G:32:ALA:HB3	1:G:69:LEU:HD13	1.67	0.75
1:L:153:GLN:HG3	1:L:166:PRO:HD2	1.69	0.74
1:C:92:PHE:HZ	1:C:103:PRO:HG3	1.52	0.73
1:F:90:ALA:HB2	5:F:644:HOH:O	1.87	0.73
1:H:95:ARG:HD3	3:H:202:NO3:O2	1.89	0.73
1:B:156:LEU:HD11	1:B:166:PRO:HG3	1.70	0.73
3:J:202:NO3:O3	1:K:95:ARG:HD2	1.89	0.73
1:F:15:ASN:HB3	5:F:616:HOH:O	1.87	0.72
1:F:150:ASN:HB2	1:J:150:ASN:HB2	1.70	0.72
1:G:106:THR:HG23	1:G:115[B]:GLN:CG	2.20	0.71
1:H:100:THR:HB	1:H:101:PRO:HD2	1.73	0.71
1:L:34:THR:OG1	1:L:36:GLU:HG2	1.89	0.71
1:E:111:LEU:HB2	1:E:122:GLU:HG2	1.73	0.71
1:D:38:ASP:OD1	1:D:38:ASP:N	2.22	0.70
1:J:14:THR:HG23	1:K:72:GLN:HE22	1.56	0.70
1:I:30:LEU:HD22	1:I:44:VAL:HG11	1.73	0.70
1:F:16:PHE:CE2	1:F:20:VAL:HG11	2.26	0.69
1:H:42:MET:HE3	2:H:201:FAD:H5'2	1.74	0.69
1:I:61:LEU:HD12	1:I:70:LEU:HD12	1.73	0.69
1:C:15:ASN:ND2	5:C:345:HOH:O	2.25	0.69
1:F:16:PHE:CZ	1:F:20:VAL:HG21	2.28	0.69
1:L:115:GLN:NE2	5:L:323:HOH:O	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ARG:HD2	3:C:202:NO3:O2	1.94	0.68
1:L:98:ASP:HB3	1:L:100:THR:HG23	1.76	0.67
1:H:40:HIS:CE1	1:H:65:ARG:HE	2.13	0.67
1:K:111:LEU:CD1	1:K:122:GLU:HG2	2.24	0.67
1:H:147:PRO:CA	1:H:148:GLU:HB2	2.25	0.67
1:F:16:PHE:CE1	1:F:20:VAL:HB	2.30	0.66
1:C:92:PHE:CZ	1:C:103:PRO:HG3	2.31	0.66
1:L:153:GLN:HG2	1:L:165:ASN:HA	1.77	0.66
1:C:100:THR:HG23	1:C:101:PRO:HD2	1.78	0.66
1:D:84:SER:HB2	1:H:165:ASN:HB2	1.78	0.66
1:L:40:HIS:CE1	1:L:65:ARG:HH11	2.13	0.65
1:A:110:GLY:O	1:A:111:LEU:CD1	2.42	0.65
1:H:42:MET:CE	2:H:201:FAD:H5'2	2.26	0.64
1:C:152:PRO:HG2	5:C:343:HOH:O	1.97	0.64
1:J:40:HIS:CD2	1:J:65:ARG:HG2	2.33	0.64
1:B:35:GLU:O	1:B:36:GLU:HB2	1.98	0.64
1:H:95:ARG:CD	3:H:202:NO3:O2	2.47	0.62
1:F:42:MET:CE	2:F:500:FAD:H5'2	2.25	0.62
1:L:62:LYS:NZ	3:L:202:NO3:O1	2.31	0.62
1:A:61:LEU:CD1	1:A:70:LEU:HD12	2.31	0.61
1:A:98:ASP:O	1:A:100:THR:HG23	2.01	0.60
1:I:61:LEU:CD1	1:I:70:LEU:HD12	2.31	0.60
1:L:30:LEU:CD1	1:L:61:LEU:HD21	2.32	0.60
1:J:68:GLU:CD	1:K:15:ASN:HD21	2.04	0.60
1:G:34:THR:HG21	1:G:65:ARG:HH21	1.67	0.60
1:A:30:LEU:CD1	1:A:61:LEU:HD21	2.32	0.59
1:J:65:ARG:NH1	4:J:204:SO4:O2	2.34	0.59
1:F:16:PHE:CZ	1:F:20:VAL:HG11	2.38	0.59
1:G:153:GLN:NE2	1:G:165:ASN:HA	2.17	0.59
1:A:153:GLN:OE1	1:A:166:PRO:HD2	2.03	0.58
1:C:103:PRO:HG2	1:C:105:PHE:CE2	2.38	0.58
1:I:34:THR:HG23	1:I:35:GLU:H	1.65	0.58
1:I:136:LEU:CD2	1:J:50:ILE:HD12	2.33	0.58
1:J:111:LEU:HD12	1:J:122:GLU:HB3	1.85	0.58
1:A:100:THR:CB	1:A:101:PRO:HD3	2.28	0.58
1:D:30:LEU:O	1:D:41:GLY:HA2	2.04	0.58
1:A:100:THR:CB	1:A:101:PRO:CD	2.82	0.58
1:F:26:GLY:O	1:F:27:ILE:HG13	2.03	0.57
1:I:54:PRO:HG2	1:J:132:HIS:NE2	2.19	0.57
1:J:40:HIS:HB2	1:J:65:ARG:NH2	2.12	0.57
1:K:55:PRO:HB2	1:K:141:VAL:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ARG:HD2	3:A:202:NO3:O3	2.05	0.57
1:B:166:PRO:HD3	5:B:306:HOH:O	2.04	0.57
1:E:59:VAL:HG22	1:E:60:SER:H	1.68	0.57
1:H:100:THR:CB	1:H:101:PRO:HD2	2.34	0.57
1:I:54:PRO:CG	1:J:132:HIS:CE1	2.88	0.56
1:H:147:PRO:HA	1:H:148:GLU:HB2	1.87	0.56
1:D:85:GLN:HG2	1:D:88:PHE:CE2	2.41	0.56
1:H:16:PHE:O	1:H:20:VAL:HG12	2.05	0.56
1:E:30:LEU:HD23	1:E:78:VAL:HG22	1.88	0.56
1:F:106:THR:HG21	1:F:115:GLN:OE1	2.05	0.56
1:F:40:HIS:CE1	1:F:65:ARG:HE	2.23	0.56
1:E:44:VAL:HA	2:E:201:FAD:N5	2.21	0.56
1:D:111:LEU:HB2	1:D:122:GLU:HG2	1.88	0.55
1:G:98:ASP:HB3	1:G:100:THR:H	1.70	0.55
1:I:54:PRO:CG	1:J:132:HIS:NE2	2.69	0.55
1:A:34:THR:C	1:A:36:GLU:H	2.10	0.55
1:B:34:THR:HG23	1:B:38:ASP:O	2.06	0.55
1:E:42:MET:HE3	2:E:201:FAD:H5'2	1.89	0.55
1:K:27:ILE:HD12	1:K:155:LEU:CD2	2.37	0.55
1:A:111:LEU:HD13	1:A:111:LEU:N	2.18	0.55
1:A:109:ALA:HB3	1:A:122:GLU:OE1	2.06	0.54
1:C:103:PRO:HG2	1:C:105:PHE:HE2	1.72	0.54
1:G:36:GLU:CD	1:G:36:GLU:O	2.45	0.54
1:K:156:LEU:HB2	1:K:163:HIS:HB2	1.89	0.54
1:B:55:PRO:HB2	1:B:141:VAL:HB	1.88	0.54
1:E:78:VAL:HB	1:E:121:PHE:HB2	1.88	0.54
1:H:75:ARG:NE	1:H:124:GLU:OE2	2.40	0.54
1:B:52:LEU:HD12	2:H:201:FAD:H2B	1.90	0.54
1:C:109:ALA:HB3	1:C:122:GLU:OE1	2.08	0.54
3:D:202:NO3:O3	1:E:95:ARG:HD2	2.07	0.54
1:D:85:GLN:NE2	1:D:116:GLY:O	2.39	0.54
1:B:50:ILE:HD12	1:C:136:LEU:HD21	1.90	0.53
1:L:42:MET:HE3	2:L:201:FAD:H5'2	1.90	0.53
1:C:159:ALA:O	1:C:161:ARG:HG3	2.07	0.53
1:E:59:VAL:HG22	1:E:60:SER:N	2.24	0.53
1:D:84:SER:CB	1:H:165:ASN:HB2	2.38	0.53
1:B:34:THR:O	1:B:35:GLU:C	2.47	0.53
1:B:72[B]:GLN:OE1	1:B:72[B]:GLN:HA	2.09	0.53
1:F:16:PHE:O	1:F:17:ARG:C	2.47	0.53
1:I:86:LYS:HB3	5:I:315:HOH:O	2.09	0.53
1:E:30:LEU:O	1:E:41:GLY:HA2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:40:HIS:CE1	1:L:65:ARG:NH1	2.76	0.52
1:A:14:THR:HG22	1:A:18:GLN:OE1	2.09	0.52
1:L:86:LYS:HD2	1:L:162:TYR:CD2	2.45	0.52
1:K:149:ALA:C	5:K:653:HOH:O	2.47	0.52
1:C:61:LEU:HD12	1:C:137:PHE:CE2	2.45	0.52
1:G:55:PRO:HB2	1:G:141:VAL:HB	1.91	0.52
1:F:30:LEU:O	1:F:41:GLY:HA2	2.10	0.52
1:I:54:PRO:HG3	1:J:132:HIS:CE1	2.45	0.52
1:H:147:PRO:CB	1:H:148:GLU:HB2	2.40	0.52
1:I:34:THR:CG2	1:I:35:GLU:N	2.30	0.52
1:J:150:ASN:O	1:J:152:PRO:HD3	2.10	0.52
1:A:48:THR:HG21	1:D:48:THR:OG1	2.10	0.51
1:E:42:MET:SD	1:E:61:LEU:HD22	2.50	0.51
2:I:201:FAD:H8A	2:I:201:FAD:H52A	1.92	0.51
1:K:78:VAL:HB	1:K:121:PHE:HB2	1.92	0.51
1:K:94[B]:LYS:NZ	1:K:96:ALA:O	2.43	0.51
1:I:30:LEU:HD22	1:I:44:VAL:CG1	2.40	0.50
1:F:75:ARG:HG2	1:F:124:GLU:HG3	1.93	0.50
1:D:74:GLY:O	1:D:124:GLU:HA	2.11	0.50
1:K:14:THR:HA	1:K:18:GLN:OE1	2.12	0.50
1:L:55:PRO:HB2	1:L:141:VAL:HB	1.93	0.50
1:J:98:ASP:HB3	1:J:100:THR:HG23	1.94	0.50
1:A:98:ASP:O	1:A:98:ASP:OD2	2.30	0.50
1:I:16:PHE:CD2	1:J:55:PRO:HB3	2.47	0.50
1:L:128:THR:HA	1:L:136:LEU:O	2.12	0.50
1:D:109:ALA:HB3	1:D:122:GLU:OE1	2.12	0.49
1:A:80:LEU:HD12	1:A:119:ALA:HB3	1.92	0.49
1:F:27:ILE:HD11	1:F:157:PHE:HB2	1.94	0.49
1:E:61:LEU:HD12	1:E:137:PHE:CD2	2.46	0.49
1:G:128:THR:HA	1:G:136:LEU:O	2.12	0.49
1:K:70:LEU:HD21	1:K:76:PHE:HB3	1.93	0.49
1:I:109:ALA:HB3	1:I:122:GLU:OE1	2.13	0.49
1:K:154:PRO:HD3	1:L:158:PHE:CZ	2.47	0.49
1:C:44:VAL:HA	2:C:201:FAD:N5	2.27	0.49
1:H:88:PHE:CE1	1:H:103:PRO:HB3	2.47	0.49
1:A:42:MET:HE3	2:A:201:FAD:H5'2	1.94	0.49
1:J:41:GLY:HA3	1:J:92:PHE:CD1	2.47	0.49
1:K:75:ARG:HD2	5:K:649:HOH:O	2.13	0.49
1:H:30:LEU:HD21	1:H:59:VAL:HG21	1.93	0.49
1:A:27:ILE:HD12	1:A:155:LEU:CG	2.38	0.48
1:K:44:VAL:HA	2:K:500:FAD:N5	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:MET:HE2	2:E:201:FAD:H2'	1.93	0.48
1:C:87:VAL:HG22	1:E:101:PRO:HB3	1.95	0.48
1:D:14:THR:HG22	1:D:18:GLN:HB3	1.95	0.48
1:G:80:LEU:HD12	1:G:119:ALA:HB3	1.94	0.48
1:J:59:VAL:HG23	1:J:137:PHE:HB2	1.94	0.48
1:F:42:MET:HE3	2:F:500:FAD:O2P	2.14	0.48
1:A:97:MET:O	1:A:98:ASP:HB3	2.12	0.48
1:F:149:ALA:O	1:F:150:ASN:C	2.52	0.48
1:I:27:ILE:HD11	1:I:157:PHE:HB2	1.95	0.48
1:G:30:LEU:O	1:G:41:GLY:HA2	2.13	0.48
1:J:95:ARG:NH1	3:J:203:NO3:O1	2.42	0.48
1:I:19:ALA:O	1:I:22:LEU:HB2	2.14	0.47
1:I:156:LEU:O	1:I:162:TYR:HA	2.14	0.47
1:J:44:VAL:HA	2:J:201:FAD:N5	2.29	0.47
1:A:100:THR:HB	1:A:101:PRO:CD	2.41	0.47
1:L:153:GLN:CG	1:L:166:PRO:HD2	2.41	0.47
1:A:90:ALA:O	1:A:94:LYS:HG3	2.14	0.47
1:J:83:GLU:OE2	1:J:165:ASN:N	2.46	0.47
1:L:40:HIS:CE1	1:L:65:ARG:HD2	2.49	0.47
1:C:111:LEU:HB3	1:C:112:PRO:HD2	1.96	0.47
2:C:201:FAD:H52A	2:C:201:FAD:H8A	1.96	0.47
1:D:165:ASN:HB2	1:H:84:SER:HB2	1.97	0.47
1:B:165:ASN:N	1:B:166:PRO:HD3	2.29	0.47
1:K:64:GLY:O	1:K:68:GLU:HG3	2.15	0.47
1:C:42:MET:SD	1:C:61:LEU:HD22	2.55	0.46
1:A:61:LEU:HD12	1:A:137:PHE:CE2	2.49	0.46
1:B:152:PRO:HG2	5:B:310:HOH:O	2.14	0.46
1:D:68:GLU:OE1	1:E:15:ASN:ND2	2.48	0.46
1:F:148:GLU:HA	1:F:149:ALA:HA	1.70	0.46
1:J:14:THR:HA	1:K:68:GLU:CD	2.36	0.46
1:E:55:PRO:HB2	1:E:141:VAL:HB	1.97	0.46
1:L:53:ASP:HA	1:L:54:PRO:HA	1.82	0.46
1:F:26:GLY:C	1:F:27:ILE:HG13	2.35	0.46
1:L:30:LEU:CD1	1:L:44:VAL:HG11	2.46	0.46
1:L:30:LEU:HD11	1:L:59:VAL:HG21	1.98	0.46
1:B:106:THR:HG23	1:B:115:GLN:HB2	1.96	0.46
1:G:14:THR:OG1	1:G:15:ASN:N	2.49	0.46
1:J:92:PHE:CE2	1:J:103:PRO:HG2	2.50	0.45
1:C:90:ALA:O	1:C:94:LYS:HG3	2.16	0.45
1:C:109:ALA:HB3	1:C:122:GLU:CD	2.37	0.45
2:D:201:FAD:C6A	1:F:52:LEU:HD21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:118:MET:HG3	1:I:152:PRO:HD2	1.98	0.45
1:J:22:LEU:HD12	1:J:158:PHE:CE1	2.52	0.45
1:J:111:LEU:O	5:J:301:HOH:O	2.20	0.45
1:C:80:LEU:HD12	1:C:119:ALA:HB3	1.98	0.45
1:D:128:THR:HA	1:D:136:LEU:O	2.17	0.45
1:H:27:ILE:HD11	1:H:157:PHE:HB2	1.99	0.45
1:K:14:THR:HG21	1:L:146:THR:OG1	2.17	0.45
1:C:40:HIS:CD2	1:C:65:ARG:HG2	2.52	0.45
1:L:30:LEU:O	1:L:41:GLY:HA2	2.17	0.45
1:L:101:PRO:HA	1:L:102:PRO:HD2	1.80	0.45
1:B:101:PRO:HA	1:B:102:PRO:HD3	1.79	0.45
1:F:44:VAL:HA	2:F:500:FAD:N5	2.32	0.45
1:E:83:GLU:O	1:E:85:GLN:N	2.51	0.44
1:B:40:HIS:ND1	1:B:65:ARG:HD3	2.33	0.44
2:C:201:FAD:H52A	2:C:201:FAD:C8A	2.47	0.44
1:L:30:LEU:HD11	1:L:61:LEU:HD21	1.97	0.44
1:F:30:LEU:HD12	1:F:78:VAL:HG22	1.99	0.44
1:K:48:THR:HG21	1:L:48:THR:OG1	2.17	0.44
1:C:96:ALA:CB	1:H:162:TYR:CE2	3.00	0.44
1:C:157:PHE:CZ	1:C:160:SER:HA	2.52	0.44
1:H:133:ASP:OD1	1:H:133:ASP:N	2.50	0.44
1:E:30:LEU:CD2	1:E:78:VAL:HG22	2.47	0.44
1:I:17:ARG:HD2	5:I:339:HOH:O	2.17	0.44
1:J:14:THR:HG22	1:K:68:GLU:OE1	2.17	0.44
2:L:201:FAD:H9	2:L:201:FAD:H1'1	1.79	0.44
1:B:98:ASP:HB3	1:B:100:THR:H	1.82	0.44
1:H:63:SER:O	2:H:201:FAD:H3B	2.18	0.44
1:I:41:GLY:HA3	1:I:92:PHE:CD1	2.53	0.44
1:J:94:LYS:HE3	5:K:632:HOH:O	2.18	0.44
1:I:71:THR:HG22	1:I:72:GLN:HE21	1.83	0.44
1:A:157:PHE:CZ	1:A:160:SER:HA	2.52	0.43
1:H:42:MET:HE3	2:H:201:FAD:C5'	2.46	0.43
1:F:80:LEU:HD12	1:F:119:ALA:HB3	2.00	0.43
1:G:44:VAL:HA	2:G:201:FAD:N5	2.33	0.43
1:G:153:GLN:HE22	1:G:165:ASN:HA	1.83	0.43
2:J:201:FAD:H5'1	2:J:201:FAD:H51A	1.99	0.43
1:K:80:LEU:HD12	1:K:119:ALA:HB3	2.00	0.43
1:C:100:THR:CG2	1:C:101:PRO:HD2	2.47	0.43
1:B:121:PHE:N	1:B:121:PHE:CD2	2.86	0.43
1:H:100:THR:CB	1:H:101:PRO:CD	2.97	0.43
1:L:42:MET:SD	1:L:61:LEU:HD22	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:THR:HA	1:C:136:LEU:O	2.18	0.43
1:J:66:MET:HB2	1:J:66:MET:HE2	1.74	0.43
1:J:157:PHE:CE2	1:J:160:SER:HA	2.54	0.43
1:K:166:PRO:HB2	1:L:163:HIS:CD2	2.53	0.43
1:L:27:ILE:HD12	1:L:155:LEU:HG	1.99	0.43
1:L:153:GLN:HG3	1:L:154:PRO:HD2	1.99	0.43
1:A:30:LEU:CD1	1:A:44:VAL:HG11	2.48	0.43
1:D:151:THR:HB	1:D:152:PRO:HD2	2.00	0.43
1:L:153:GLN:HE21	1:L:153:GLN:HB2	1.66	0.42
1:C:106:THR:OG1	1:C:115:GLN:HB2	2.19	0.42
1:I:42:MET:HE1	1:I:61:LEU:HD22	2.02	0.42
1:C:42:MET:HE1	1:C:61:LEU:HD22	2.00	0.42
1:J:169:LEU:N	1:J:169:LEU:HD23	2.35	0.42
1:E:83:GLU:C	1:E:85:GLN:H	2.23	0.42
1:G:167:LEU:N	1:H:164:GLY:O	2.43	0.42
1:A:61:LEU:HD12	1:A:70:LEU:HD12	2.02	0.42
1:C:30:LEU:HD21	1:C:59:VAL:HG21	2.02	0.42
1:I:52:LEU:HD12	2:K:500:FAD:H2B	2.02	0.42
1:K:20:VAL:HG21	1:L:49:SER:HB2	2.02	0.42
1:F:31:SER:HA	1:F:40:HIS:O	2.19	0.42
1:D:83:GLU:OE2	1:D:153:GLN:HB2	2.19	0.42
1:H:75:ARG:HA	1:H:123:CYS:O	2.20	0.42
1:I:54:PRO:HD2	1:J:132:HIS:CG	2.55	0.42
1:J:150:ASN:C	1:J:152:PRO:HD3	2.40	0.42
1:E:70:LEU:N	1:E:70:LEU:HD23	2.34	0.42
1:A:34:THR:C	1:A:36:GLU:N	2.74	0.42
1:E:53:ASP:HA	1:E:54:PRO:HA	1.94	0.42
1:G:126:GLU:OE2	1:G:140:ARG:NH2	2.53	0.42
1:H:153:GLN:OE1	1:H:166:PRO:HD2	2.20	0.42
1:C:61:LEU:HD12	1:C:137:PHE:CD2	2.55	0.42
1:C:83:GLU:O	1:C:83:GLU:HG2	2.20	0.42
1:G:30:LEU:HD21	1:G:59:VAL:HG11	2.02	0.42
2:I:201:FAD:H1'1	2:I:201:FAD:H9	1.76	0.42
3:J:202:NO3:O3	1:K:95:ARG:CD	2.64	0.42
1:B:69:LEU:HD23	1:B:69:LEU:HA	1.83	0.41
1:E:105:PHE:HE1	1:E:114:LEU:HG	1.78	0.41
1:F:16:PHE:CZ	1:F:20:VAL:CG2	3.01	0.41
1:L:34:THR:OG1	1:L:36:GLU:CG	2.64	0.41
1:E:105:PHE:HD1	1:E:113:THR:C	2.24	0.41
1:J:17:ARG:HD2	5:K:624:HOH:O	2.19	0.41
1:D:83:GLU:CD	1:D:153:GLN:HB2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:156:LEU:HB2	1:I:163:HIS:HB2	2.02	0.41
1:K:111:LEU:HD11	1:K:122:GLU:HG2	2.02	0.41
1:L:42:MET:CE	2:L:201:FAD:H5'2	2.50	0.41
1:A:30:LEU:HD12	1:A:44:VAL:HG11	2.01	0.41
1:A:167:LEU:O	1:D:163:HIS:HA	2.21	0.41
1:A:102:PRO:HA	1:A:103:PRO:HD3	1.94	0.41
1:A:159:ALA:O	1:A:161:ARG:HG3	2.21	0.41
1:D:55:PRO:HB2	1:D:141:VAL:HB	2.02	0.41
1:J:88:PHE:CE1	1:J:103:PRO:HB3	2.55	0.41
1:F:16:PHE:CE1	1:F:20:VAL:CB	3.01	0.41
2:I:201:FAD:H52A	2:I:201:FAD:C8A	2.51	0.41
1:K:101:PRO:HA	1:K:102:PRO:HD2	1.63	0.41
1:C:34:THR:HG21	1:C:65:ARG:NH1	2.36	0.41
1:D:85:GLN:HG2	1:D:88:PHE:CD2	2.56	0.41
1:G:133:ASP:OD1	1:H:51:SER:OG	2.25	0.41
2:H:201:FAD:H9	2:H:201:FAD:H1'1	1.81	0.41
1:A:42:MET:CE	2:A:201:FAD:H5'2	2.51	0.41
1:C:101:PRO:HA	1:C:102:PRO:HD3	1.94	0.41
1:D:101:PRO:HA	1:D:102:PRO:HD3	1.95	0.41
1:G:30:LEU:HD23	1:G:78:VAL:HG22	2.02	0.41
1:G:83:GLU:HG3	1:G:84:SER:N	2.36	0.41
1:K:27:ILE:HD12	1:K:155:LEU:HD23	2.03	0.41
1:K:42:MET:CG	2:K:500:FAD:H5'2	2.39	0.41
1:L:42:MET:HE2	2:L:201:FAD:H2'	2.03	0.41
1:L:156:LEU:HB2	1:L:163:HIS:HB2	2.02	0.41
2:D:201:FAD:H5'1	2:D:201:FAD:H52A	2.02	0.41
1:H:100:THR:HB	1:H:101:PRO:CD	2.46	0.41
1:I:22:LEU:O	1:J:118:MET:CE	2.69	0.40
1:K:111:LEU:HG	1:K:122:GLU:HG2	2.03	0.40
1:A:119:ALA:HB2	1:A:146:THR:HG22	2.03	0.40
1:J:156:LEU:HD11	1:J:166:PRO:HG3	2.03	0.40
1:F:36:GLU:C	1:F:38:ASP:H	2.24	0.40
1:I:101:PRO:HA	1:I:102:PRO:HD3	1.91	0.40
1:F:140:ARG:HE	1:F:140:ARG:HB2	1.80	0.40
1:F:85:GLN:HE22	1:F:116:GLY:C	2.25	0.40
1:J:68:GLU:OE2	5:J:359:HOH:O	2.21	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	146/190 (77%)	138 (94%)	8 (6%)	0	100	100
1	B	151/190 (80%)	142 (94%)	9 (6%)	0	100	100
1	C	148/190 (78%)	140 (95%)	8 (5%)	0	100	100
1	D	149/190 (78%)	140 (94%)	8 (5%)	1 (1%)	22	26
1	E	143/190 (75%)	134 (94%)	7 (5%)	2 (1%)	11	11
1	F	151/190 (80%)	142 (94%)	7 (5%)	2 (1%)	12	12
1	G	150/190 (79%)	144 (96%)	6 (4%)	0	100	100
1	H	150/190 (79%)	139 (93%)	11 (7%)	0	100	100
1	I	153/190 (80%)	145 (95%)	8 (5%)	0	100	100
1	J	151/190 (80%)	144 (95%)	7 (5%)	0	100	100
1	K	152/190 (80%)	143 (94%)	9 (6%)	0	100	100
1	L	147/190 (77%)	140 (95%)	7 (5%)	0	100	100
All	All	1791/2280 (79%)	1691 (94%)	95 (5%)	5 (0%)	41	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	37	GLY
1	E	84	SER
1	F	101	PRO
1	E	102	PRO
1	D	74	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	125/159 (79%)	120 (96%)	5 (4%)	31	44
1	B	126/159 (79%)	122 (97%)	4 (3%)	39	54
1	C	124/159 (78%)	121 (98%)	3 (2%)	49	66
1	D	125/159 (79%)	123 (98%)	2 (2%)	62	78
1	E	122/159 (77%)	119 (98%)	3 (2%)	47	65
1	F	126/159 (79%)	123 (98%)	3 (2%)	49	66
1	G	126/159 (79%)	124 (98%)	2 (2%)	62	78
1	H	125/159 (79%)	121 (97%)	4 (3%)	39	54
1	I	126/159 (79%)	120 (95%)	6 (5%)	25	36
1	J	126/159 (79%)	123 (98%)	3 (2%)	49	66
1	K	124/159 (78%)	122 (98%)	2 (2%)	62	78
1	L	123/159 (77%)	121 (98%)	2 (2%)	62	78
All	All	1498/1908 (78%)	1459 (97%)	39 (3%)	46	63

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	83	GLU
1	A	100	THR
1	A	111	LEU
1	A	148	GLU
1	B	38	ASP
1	B	98	ASP
1	B	115	GLN
1	B	128	THR
1	C	15	ASN
1	C	48	THR
1	C	72	GLN
1	D	38	ASP
1	D	153	GLN
1	E	20	VAL
1	E	36	GLU
1	E	100	THR
1	F	115	GLN
1	F	140	ARG

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Mol	Chain	Res	Type
1	F	150	ASN
1	G	48	THR
1	G	98	ASP
1	H	48	THR
1	H	72	GLN
1	H	127	SER
1	H	153	GLN
1	I	20	VAL
1	I	22	LEU
1	I	30	LEU
1	I	48	THR
1	I	72	GLN
1	I	151	THR
1	J	22	LEU
1	J	55	PRO
1	J	98	ASP
1	K	30	LEU
1	K	87	VAL
1	L	20	VAL
1	L	106	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	115	GLN
1	G	153	GLN
1	G	165	ASN
1	H	72	GLN
1	I	72	GLN
1	J	115	GLN
1	K	72	GLN
1	L	153	GLN
1	L	165	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)

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NO3	I	202	-	1,3,3	4.39	1 (100%)	0,3,3	-	-
2	FAD	I	201	-	53,58,58	1.26	4 (7%)	68,89,89	1.76	17 (25%)
2	FAD	J	201	-	53,58,58	1.50	5 (9%)	68,89,89	1.65	16 (23%)
2	FAD	H	201	-	53,58,58	1.25	5 (9%)	68,89,89	1.62	12 (17%)
4	SO4	D	203	-	4,4,4	0.06	0	6,6,6	0.58	0
2	FAD	L	201	-	52,57,58	1.17	6 (11%)	63,86,89	1.61	12 (19%)
3	NO3	G	202	-	1,3,3	3.53	1 (100%)	0,3,3	-	-
3	NO3	E	202	-	1,3,3	4.06	1 (100%)	0,3,3	-	-
3	NO3	B	202	-	1,3,3	3.75	1 (100%)	0,3,3	-	-
2	FAD	D	201	-	53,58,58	1.36	6 (11%)	68,89,89	1.56	13 (19%)
2	FAD	E	201	-	53,58,58	1.21	3 (5%)	68,89,89	1.56	11 (16%)
3	NO3	A	203	-	1,3,3	3.30	1 (100%)	0,3,3	-	-
4	SO4	J	204	-	4,4,4	0.21	0	6,6,6	0.49	0
2	FAD	K	500	-	53,58,58	1.35	7 (13%)	68,89,89	1.96	20 (29%)
3	NO3	D	202	-	1,3,3	3.84	1 (100%)	0,3,3	-	-
4	SO4	D	204	-	4,4,4	0.15	0	6,6,6	0.21	0
3	NO3	L	202	-	1,3,3	2.86	1 (100%)	0,3,3	-	-
3	NO3	A	202	-	1,3,3	3.32	1 (100%)	0,3,3	-	-
3	NO3	J	202	-	1,3,3	3.64	1 (100%)	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	F	500	-	53,58,58	1.22	7 (13%)	68,89,89	1.63	12 (17%)
3	NO3	J	203	-	1,3,3	3.22	1 (100%)	0,3,3	-	-
2	FAD	C	201	-	53,58,58	1.22	4 (7%)	68,89,89	1.69	14 (20%)
2	FAD	A	201	-	53,58,58	1.21	4 (7%)	68,89,89	1.62	17 (25%)
3	NO3	C	202	-	1,3,3	3.55	1 (100%)	0,3,3	-	-
2	FAD	G	201	-	53,58,58	1.18	4 (7%)	68,89,89	1.60	10 (14%)
2	FAD	B	201	-	53,58,58	1.62	5 (9%)	68,89,89	1.75	14 (20%)
3	NO3	H	202	-	1,3,3	4.11	1 (100%)	0,3,3	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	K	500	-	-	9/30/50/50	0/6/6/6
2	FAD	F	500	-	-	12/30/50/50	0/6/6/6
2	FAD	D	201	-	-	11/30/50/50	0/6/6/6
2	FAD	I	201	-	-	2/30/50/50	0/6/6/6
2	FAD	J	201	-	-	9/30/50/50	0/6/6/6
2	FAD	C	201	-	-	7/30/50/50	0/6/6/6
2	FAD	E	201	-	-	8/30/50/50	0/6/6/6
2	FAD	A	201	-	-	3/30/50/50	0/6/6/6
2	FAD	H	201	-	-	2/30/50/50	0/6/6/6
2	FAD	L	201	-	-	10/24/48/50	0/6/6/6
2	FAD	G	201	-	-	6/30/50/50	0/6/6/6
2	FAD	B	201	-	-	9/30/50/50	0/6/6/6

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	FAD	C4X-N5	6.23	1.42	1.30
2	J	201	FAD	C2A-N3A	6.13	1.42	1.32
2	K	500	FAD	C2A-N3A	4.66	1.39	1.32
2	A	201	FAD	C4X-N5	4.65	1.39	1.30
2	B	201	FAD	C2A-N3A	4.56	1.39	1.32
2	E	201	FAD	C4X-N5	4.53	1.39	1.30
2	G	201	FAD	C4X-N5	4.40	1.39	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	202	NO3	O1-N	4.39	1.44	1.24
2	D	201	FAD	C2A-N3A	4.24	1.38	1.32
3	H	202	NO3	O1-N	4.11	1.43	1.24
3	E	202	NO3	O1-N	4.06	1.42	1.24
2	F	500	FAD	C2A-N3A	4.05	1.38	1.32
2	I	201	FAD	C2A-N3A	4.04	1.38	1.32
2	G	201	FAD	C2A-N3A	4.03	1.38	1.32
2	J	201	FAD	C4X-N5	4.00	1.38	1.30
2	C	201	FAD	C4X-N5	3.97	1.38	1.30
2	B	201	FAD	C10-N1	3.93	1.41	1.33
2	E	201	FAD	C2A-N3A	3.91	1.38	1.32
2	I	201	FAD	C4X-N5	3.84	1.38	1.30
3	D	202	NO3	O1-N	3.84	1.41	1.24
2	D	201	FAD	C4X-N5	3.80	1.38	1.30
2	H	201	FAD	C2A-N1A	3.76	1.40	1.33
3	B	202	NO3	O1-N	3.75	1.41	1.24
3	J	202	NO3	O1-N	3.64	1.40	1.24
3	C	202	NO3	O1-N	3.55	1.40	1.24
3	G	202	NO3	O1-N	3.53	1.40	1.24
2	H	201	FAD	C2A-N3A	3.48	1.37	1.32
2	D	201	FAD	C2A-N1A	3.45	1.40	1.33
3	A	202	NO3	O1-N	3.32	1.39	1.24
3	A	203	NO3	O1-N	3.30	1.39	1.24
2	J	201	FAD	C9A-N10	-3.22	1.35	1.41
3	J	203	NO3	O1-N	3.22	1.38	1.24
2	K	500	FAD	C2A-N1A	3.16	1.39	1.33
2	J	201	FAD	C10-N1	3.12	1.39	1.33
2	I	201	FAD	C1'-C2'	2.97	1.56	1.52
2	C	201	FAD	C2A-N3A	2.90	1.36	1.32
2	B	201	FAD	C2A-N1A	2.87	1.39	1.33
3	L	202	NO3	O1-N	2.86	1.37	1.24
2	H	201	FAD	C4X-N5	2.80	1.36	1.30
2	E	201	FAD	C2A-N1A	2.77	1.39	1.33
2	C	201	FAD	C10-N1	2.77	1.38	1.33
2	D	201	FAD	C10-N1	2.76	1.38	1.33
2	G	201	FAD	C10-N1	2.74	1.38	1.33
2	L	201	FAD	C4X-N5	2.73	1.36	1.30
2	A	201	FAD	C7M-C7	2.72	1.56	1.51
2	A	201	FAD	C2A-N3A	2.71	1.36	1.32
2	A	201	FAD	C2A-N1A	2.67	1.38	1.33
2	J	201	FAD	C2A-N1A	2.62	1.38	1.33
2	B	201	FAD	C1'-C2'	2.59	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	FAD	C1'-C2'	2.55	1.56	1.52
2	L	201	FAD	C9-C8	2.54	1.43	1.39
2	L	201	FAD	C2A-N3A	2.53	1.36	1.32
2	F	500	FAD	O2-C2	-2.49	1.19	1.24
2	D	201	FAD	O2-C2	-2.46	1.19	1.24
2	H	201	FAD	O4-C4	-2.44	1.19	1.23
2	K	500	FAD	C6-C7	2.41	1.43	1.39
2	K	500	FAD	C4'-C3'	2.41	1.58	1.53
2	K	500	FAD	O4-C4	2.31	1.28	1.23
2	F	500	FAD	C10-N1	2.30	1.37	1.33
2	H	201	FAD	C10-N1	2.28	1.37	1.33
2	F	500	FAD	C2A-N1A	2.26	1.38	1.33
2	I	201	FAD	C10-N1	2.25	1.37	1.33
2	L	201	FAD	C2A-N1A	2.23	1.38	1.33
2	G	201	FAD	C2A-N1A	2.14	1.37	1.33
2	L	201	FAD	C5X-N5	-2.14	1.35	1.39
2	L	201	FAD	C8M-C8	2.14	1.55	1.51
2	F	500	FAD	C6-C7	2.13	1.42	1.39
2	D	201	FAD	C2B-C1B	-2.07	1.50	1.53
2	F	500	FAD	O3'-C3'	-2.04	1.38	1.43
2	K	500	FAD	C1'-C2'	2.04	1.55	1.52
2	F	500	FAD	C2'-C3'	-2.02	1.49	1.53
2	K	500	FAD	C10-N10	2.02	1.41	1.37

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	201	FAD	N3A-C2A-N1A	-7.57	116.85	128.68
2	H	201	FAD	N3A-C2A-N1A	-6.82	118.01	128.68
2	E	201	FAD	N3A-C2A-N1A	-6.49	118.54	128.68
2	G	201	FAD	N3A-C2A-N1A	-6.33	118.78	128.68
2	B	201	FAD	N3A-C2A-N1A	-5.95	119.37	128.68
2	J	201	FAD	N3A-C2A-N1A	-5.81	119.59	128.68
2	L	201	FAD	N3A-C2A-N1A	-5.63	119.88	128.68
2	D	201	FAD	N3A-C2A-N1A	-5.47	120.13	128.68
2	C	201	FAD	N3A-C2A-N1A	-5.43	120.19	128.68
2	K	500	FAD	C4-N3-C2	-5.38	115.70	125.64
2	K	500	FAD	C5B-C4B-C3B	-4.96	96.60	115.18
2	F	500	FAD	N3A-C2A-N1A	-4.91	121.00	128.68
2	A	201	FAD	N3A-C2A-N1A	-4.72	121.30	128.68
2	K	500	FAD	O2-C2-N1	-4.69	114.06	121.83
2	F	500	FAD	C4X-C10-N10	4.57	123.16	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	FAD	P-O3P-PA	-4.41	117.69	132.83
2	B	201	FAD	C3B-C2B-C1B	4.30	107.45	100.98
2	K	500	FAD	N3A-C2A-N1A	-4.13	122.22	128.68
2	G	201	FAD	C5B-C4B-C3B	-4.11	99.79	115.18
2	D	201	FAD	C3B-C2B-C1B	3.91	106.87	100.98
2	C	201	FAD	C5B-C4B-C3B	-3.85	100.76	115.18
2	H	201	FAD	C4-N3-C2	-3.80	118.61	125.64
2	F	500	FAD	C10-C4X-N5	-3.77	116.86	124.86
2	K	500	FAD	C9A-N10-C10	-3.77	114.90	120.77
2	L	201	FAD	C4-N3-C2	-3.76	118.69	125.64
2	K	500	FAD	C4X-C10-N10	3.71	121.90	116.48
2	I	201	FAD	C4-N3-C2	-3.64	118.92	125.64
2	E	201	FAD	C4-N3-C2	-3.63	118.94	125.64
2	B	201	FAD	C4-N3-C2	-3.59	119.00	125.64
2	B	201	FAD	C5B-C4B-C3B	-3.58	101.75	115.18
2	F	500	FAD	C3B-C2B-C1B	3.50	106.25	100.98
2	B	201	FAD	C4X-C4-N3	3.47	122.01	113.19
2	A	201	FAD	C5B-C4B-C3B	-3.46	102.21	115.18
2	F	500	FAD	C4-C4X-C10	3.44	122.57	116.79
2	B	201	FAD	O4-C4-C4X	-3.41	117.56	126.60
2	K	500	FAD	C4X-C10-N1	-3.39	116.87	124.73
2	C	201	FAD	C4X-C10-N10	3.38	121.42	116.48
2	G	201	FAD	C4X-C10-N10	3.23	121.20	116.48
2	H	201	FAD	C4X-C4-N3	3.18	121.26	113.19
2	C	201	FAD	C5X-C9A-N10	3.17	121.23	117.95
2	L	201	FAD	C4X-C10-N10	3.15	121.09	116.48
2	B	201	FAD	C5X-C9A-N10	3.13	121.18	117.95
2	E	201	FAD	C10-C4X-N5	-3.12	118.24	124.86
2	D	201	FAD	C4-N3-C2	-3.11	119.89	125.64
2	G	201	FAD	O2A-PA-O1A	3.07	127.44	112.24
2	K	500	FAD	C4-C4X-C10	3.02	121.86	116.79
2	J	201	FAD	C4X-C4-N3	3.01	120.84	113.19
2	L	201	FAD	C4'-C3'-C2'	-3.01	107.09	113.36
2	I	201	FAD	O2-C2-N1	-2.97	116.91	121.83
2	A	201	FAD	C4-N3-C2	-2.95	120.19	125.64
2	D	201	FAD	C4X-C10-N10	2.94	120.79	116.48
2	B	201	FAD	P-O3P-PA	-2.94	122.75	132.83
2	J	201	FAD	P-O3P-PA	-2.91	122.85	132.83
2	A	201	FAD	C8M-C8-C9	-2.88	114.16	119.49
2	D	201	FAD	P-O3P-PA	-2.88	122.95	132.83
2	I	201	FAD	C4X-C10-N10	2.87	120.68	116.48
2	J	201	FAD	O4'-C4'-C5'	-2.86	103.49	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	500	FAD	C5X-C9A-N10	2.85	120.90	117.95
2	F	500	FAD	C4-N3-C2	-2.84	120.40	125.64
2	E	201	FAD	C4X-C10-N10	2.80	120.58	116.48
2	K	500	FAD	C4X-C4-N3	2.77	120.23	113.19
2	A	201	FAD	C7M-C7-C8	2.77	126.41	120.74
2	K	500	FAD	C10-N1-C2	2.76	122.43	116.90
2	I	201	FAD	O4-C4-C4X	-2.75	119.30	126.60
2	A	201	FAD	C9A-C5X-N5	-2.74	119.46	122.43
2	G	201	FAD	C4-N3-C2	-2.72	120.61	125.64
2	J	201	FAD	C5B-C4B-C3B	-2.72	104.98	115.18
2	A	201	FAD	C6-C7-C8	-2.72	115.77	119.67
2	B	201	FAD	O2-C2-N1	-2.72	117.32	121.83
2	F	500	FAD	C5X-N5-C4X	2.67	122.51	118.07
2	H	201	FAD	PA-O5B-C5B	-2.66	106.11	121.68
2	J	201	FAD	C4X-C10-N10	2.65	120.35	116.48
2	J	201	FAD	C9-C9A-N10	-2.64	118.27	121.84
2	H	201	FAD	C4X-C10-N1	-2.62	118.66	124.73
2	H	201	FAD	C4X-C10-N10	2.61	120.30	116.48
2	I	201	FAD	C5B-C4B-C3B	-2.61	105.40	115.18
2	I	201	FAD	O2'-C2'-C3'	-2.61	102.76	109.10
2	L	201	FAD	C10-C4X-N5	-2.60	119.35	124.86
2	H	201	FAD	C5B-C4B-C3B	-2.57	105.53	115.18
2	J	201	FAD	C4-N3-C2	-2.56	120.91	125.64
2	F	500	FAD	C4X-C10-N1	-2.55	118.81	124.73
2	F	500	FAD	C4'-C3'-C2'	-2.54	108.08	113.36
2	B	201	FAD	O2B-C2B-C3B	-2.53	103.64	111.82
2	E	201	FAD	C5B-C4B-C3B	-2.53	105.71	115.18
2	D	201	FAD	O2A-PA-O5B	2.52	119.45	107.75
2	A	201	FAD	C4X-C10-N10	2.52	120.16	116.48
2	I	201	FAD	C9A-C5X-N5	-2.51	119.70	122.43
2	C	201	FAD	O2-C2-N1	-2.51	117.67	121.83
2	J	201	FAD	C10-C4X-N5	-2.47	119.61	124.86
2	G	201	FAD	O4'-C4'-C3'	2.47	115.09	109.10
2	D	201	FAD	C5A-C6A-N6A	-2.46	116.61	120.35
2	C	201	FAD	O2P-P-O5'	2.46	119.18	107.75
2	I	201	FAD	C4X-C4-N3	2.45	119.41	113.19
2	C	201	FAD	C4'-C3'-C2'	-2.43	108.31	113.36
2	D	201	FAD	O2-C2-N1	-2.43	117.80	121.83
2	B	201	FAD	C4X-C10-N10	2.43	120.03	116.48
2	F	500	FAD	O3B-C3B-C4B	-2.43	104.03	111.05
2	E	201	FAD	C5X-N5-C4X	2.42	122.10	118.07
2	I	201	FAD	C10-C4X-N5	-2.42	119.72	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201	FAD	C5X-C9A-N10	2.42	120.45	117.95
2	I	201	FAD	C5X-C9A-N10	2.41	120.45	117.95
2	J	201	FAD	C3B-C2B-C1B	2.40	104.60	100.98
2	D	201	FAD	C5'-C4'-C3'	-2.39	107.58	112.20
2	J	201	FAD	C4X-C10-N1	-2.38	119.20	124.73
2	H	201	FAD	P-O3P-PA	-2.38	124.66	132.83
2	B	201	FAD	C9A-C5X-N5	-2.38	119.85	122.43
2	K	500	FAD	O4'-C4'-C5'	-2.38	104.58	109.92
2	E	201	FAD	C4-C4X-C10	2.38	120.78	116.79
2	J	201	FAD	O4-C4-N3	-2.37	115.57	120.12
2	C	201	FAD	C9A-C5X-N5	-2.35	119.87	122.43
2	H	201	FAD	O4-C4-C4X	-2.35	120.36	126.60
2	J	201	FAD	C10-N1-C2	2.35	121.61	116.90
2	K	500	FAD	C9-C9A-N10	-2.34	118.67	121.84
2	D	201	FAD	C10-C4X-N5	-2.34	119.88	124.86
2	A	201	FAD	C10-N1-C2	2.34	121.58	116.90
2	C	201	FAD	C4-N3-C2	-2.34	121.32	125.64
2	K	500	FAD	P-O3P-PA	-2.33	124.83	132.83
2	L	201	FAD	C4X-C10-N1	-2.33	119.33	124.73
2	E	201	FAD	C4X-C10-N1	-2.33	119.33	124.73
2	D	201	FAD	C4X-C4-N3	2.32	119.07	113.19
2	A	201	FAD	O4-C4-C4X	-2.31	120.47	126.60
2	J	201	FAD	C4-C4X-N5	2.29	121.50	118.23
2	C	201	FAD	O5'-C5'-C4'	-2.29	103.25	109.36
2	K	500	FAD	O2-C2-N3	2.29	123.09	118.65
2	L	201	FAD	C4-C4X-C10	2.26	120.59	116.79
2	C	201	FAD	C10-C4X-N5	-2.25	120.08	124.86
2	G	201	FAD	C4X-C4-N3	2.25	118.89	113.19
2	E	201	FAD	C4X-C4-N3	2.24	118.88	113.19
2	G	201	FAD	C4'-C3'-C2'	-2.23	108.72	113.36
2	A	201	FAD	C4X-C4-N3	2.23	118.86	113.19
2	K	500	FAD	C5'-C4'-C3'	2.22	116.50	112.20
2	D	201	FAD	O4-C4-C4X	-2.21	120.73	126.60
2	L	201	FAD	C4X-C4-N3	2.21	118.80	113.19
2	A	201	FAD	O4B-C4B-C3B	2.21	109.48	105.11
2	F	500	FAD	O4-C4-C4X	-2.20	120.76	126.60
2	L	201	FAD	C2B-C3B-C4B	2.18	106.88	102.64
2	I	201	FAD	C3B-C2B-C1B	2.18	104.26	100.98
2	F	500	FAD	C9A-C5X-N5	-2.18	120.07	122.43
2	E	201	FAD	C9A-C5X-N5	-2.17	120.08	122.43
2	I	201	FAD	O4B-C1B-C2B	2.16	110.08	106.93
2	K	500	FAD	C4-C4X-N5	-2.15	115.17	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	FAD	C10-C4X-N5	-2.15	120.30	124.86
2	A	201	FAD	O5'-P-O1P	2.15	117.45	109.07
2	J	201	FAD	O4B-C1B-C2B	2.14	110.06	106.93
2	K	500	FAD	O4-C4-C4X	-2.14	120.93	126.60
2	B	201	FAD	PA-O5B-C5B	-2.13	109.20	121.68
2	H	201	FAD	C1B-N9A-C4A	-2.12	122.91	126.64
2	C	201	FAD	C8M-C8-C9	-2.12	115.57	119.49
2	H	201	FAD	C10-C4X-N5	-2.12	120.36	124.86
2	J	201	FAD	O5B-PA-O1A	2.12	117.34	109.07
2	C	201	FAD	C4X-C4-N3	2.10	118.52	113.19
2	A	201	FAD	O3'-C3'-C4'	2.10	113.88	108.81
2	I	201	FAD	O4B-C4B-C3B	2.10	109.26	105.11
2	K	500	FAD	O4B-C4B-C3B	2.09	109.26	105.11
2	G	201	FAD	C4X-C10-N1	-2.09	119.88	124.73
2	D	201	FAD	O2'-C2'-C1'	2.07	114.81	109.80
2	B	201	FAD	O2-C2-N3	2.07	122.67	118.65
2	L	201	FAD	C6-C5X-C9A	2.07	121.86	118.94
2	A	201	FAD	O2'-C2'-C1'	2.06	114.79	109.80
2	E	201	FAD	C6-C5X-C9A	2.06	121.85	118.94
2	I	201	FAD	O2A-PA-O5B	2.05	117.27	107.75
2	H	201	FAD	C5X-C9A-N10	2.05	120.07	117.95
2	K	500	FAD	C1'-N10-C9A	2.04	123.91	120.51
2	A	201	FAD	C3B-C2B-C1B	2.03	104.04	100.98
2	L	201	FAD	O3B-C3B-C4B	-2.03	105.18	111.05
2	L	201	FAD	O2A-PA-O5B	2.01	117.08	107.75
2	I	201	FAD	C4X-C10-N1	-2.01	120.08	124.73
2	I	201	FAD	C2A-N1A-C6A	2.00	122.18	118.75

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	FAD	C5B-O5B-PA-O1A
2	B	201	FAD	C5B-O5B-PA-O2A
2	B	201	FAD	C5B-O5B-PA-O3P
2	B	201	FAD	C5'-O5'-P-O2P
2	B	201	FAD	C5'-O5'-P-O3P
2	D	201	FAD	C5B-O5B-PA-O1A
2	D	201	FAD	C5B-O5B-PA-O3P
2	D	201	FAD	O4B-C4B-C5B-O5B
2	D	201	FAD	C5'-O5'-P-O3P
2	E	201	FAD	C5B-O5B-PA-O3P

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Mol	Chain	Res	Type	Atoms
2	F	500	FAD	C5B-O5B-PA-O1A
2	F	500	FAD	C5B-O5B-PA-O3P
2	F	500	FAD	C5'-O5'-P-O2P
2	G	201	FAD	C5B-O5B-PA-O3P
2	H	201	FAD	C5B-O5B-PA-O3P
2	J	201	FAD	C5B-O5B-PA-O2A
2	J	201	FAD	C5B-O5B-PA-O3P
2	J	201	FAD	O4B-C4B-C5B-O5B
2	J	201	FAD	C3B-C4B-C5B-O5B
2	K	500	FAD	C5B-O5B-PA-O3P
2	K	500	FAD	O4'-C4'-C5'-O5'
2	K	500	FAD	C5'-O5'-P-O1P
2	K	500	FAD	C5'-O5'-P-O2P
2	L	201	FAD	C5B-O5B-PA-O3P
2	D	201	FAD	C3B-C4B-C5B-O5B
2	F	500	FAD	O4B-C4B-C5B-O5B
2	F	500	FAD	C3B-C4B-C5B-O5B
2	L	201	FAD	O4B-C4B-C5B-O5B
2	L	201	FAD	C3B-C4B-C5B-O5B
2	F	500	FAD	O3'-C3'-C4'-O4'
2	L	201	FAD	C2'-C3'-C4'-O4'
2	F	500	FAD	O3'-C3'-C4'-C5'
2	B	201	FAD	C3B-C4B-C5B-O5B
2	E	201	FAD	C3B-C4B-C5B-O5B
2	I	201	FAD	C3B-C4B-C5B-O5B
2	A	201	FAD	C2'-C3'-C4'-O4'
2	C	201	FAD	C2'-C3'-C4'-O4'
2	F	500	FAD	C2'-C3'-C4'-O4'
2	J	201	FAD	C2'-C3'-C4'-O4'
2	J	201	FAD	O3'-C3'-C4'-O4'
2	L	201	FAD	O3'-C3'-C4'-O4'
2	J	201	FAD	O3'-C3'-C4'-C5'
2	C	201	FAD	O4B-C4B-C5B-O5B
2	K	500	FAD	C3'-C4'-C5'-O5'
2	C	201	FAD	C2'-C3'-C4'-C5'
2	E	201	FAD	C2'-C3'-C4'-C5'
2	J	201	FAD	C2'-C3'-C4'-C5'
2	L	201	FAD	C2'-C3'-C4'-C5'
2	E	201	FAD	C2'-C3'-C4'-O4'
2	F	500	FAD	C2'-C3'-C4'-C5'
2	E	201	FAD	O4B-C4B-C5B-O5B
2	K	500	FAD	PA-O3P-P-O5'

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Mol	Chain	Res	Type	Atoms
2	A	201	FAD	O3'-C3'-C4'-O4'
2	I	201	FAD	O4B-C4B-C5B-O5B
2	G	201	FAD	C2'-C3'-C4'-O4'
2	K	500	FAD	C5'-O5'-P-O3P
2	B	201	FAD	C5'-O5'-P-O1P
2	D	201	FAD	C5B-O5B-PA-O2A
2	D	201	FAD	C5'-O5'-P-O1P
2	D	201	FAD	C5'-O5'-P-O2P
2	E	201	FAD	C5B-O5B-PA-O1A
2	E	201	FAD	C5B-O5B-PA-O2A
2	F	500	FAD	C5B-O5B-PA-O2A
2	F	500	FAD	C5'-O5'-P-O1P
2	G	201	FAD	C5B-O5B-PA-O1A
2	J	201	FAD	C5B-O5B-PA-O1A
2	K	500	FAD	C5B-O5B-PA-O1A
2	K	500	FAD	C5B-O5B-PA-O2A
2	L	201	FAD	C5B-O5B-PA-O1A
2	L	201	FAD	C5B-O5B-PA-O2A
2	D	201	FAD	O4'-C4'-C5'-O5'
2	L	201	FAD	O4'-C4'-C5'-O5'
2	A	201	FAD	C2'-C3'-C4'-C5'
2	B	201	FAD	O4B-C4B-C5B-O5B
2	C	201	FAD	C3B-C4B-C5B-O5B
2	G	201	FAD	C3B-C4B-C5B-O5B
2	C	201	FAD	O3'-C3'-C4'-O4'
2	G	201	FAD	PA-O3P-P-O1P
2	F	500	FAD	O4'-C4'-C5'-O5'
2	E	201	FAD	O3'-C3'-C4'-O4'
2	L	201	FAD	O3'-C3'-C4'-C5'
2	B	201	FAD	PA-O3P-P-O2P
2	C	201	FAD	PA-O3P-P-O2P
2	D	201	FAD	PA-O3P-P-O2P
2	G	201	FAD	PA-O3P-P-O2P
2	D	201	FAD	C3'-C4'-C5'-O5'
2	H	201	FAD	C5B-O5B-PA-O1A
2	C	201	FAD	O3'-C3'-C4'-C5'

There are no ring outliers.

19 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	201	FAD	3	0

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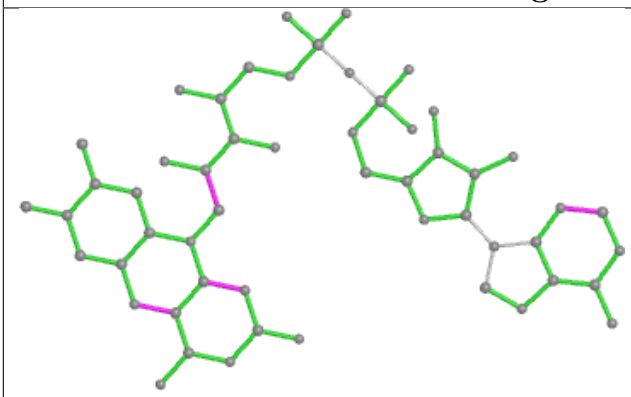
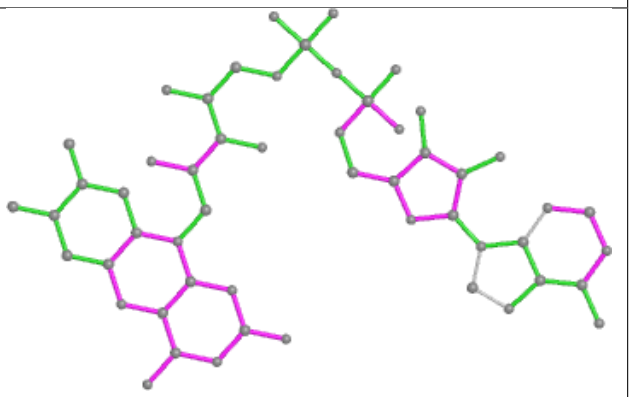
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	201	FAD	2	0
2	H	201	FAD	6	0
2	L	201	FAD	4	0
2	D	201	FAD	2	0
2	E	201	FAD	3	0
4	J	204	SO4	1	0
2	K	500	FAD	4	0
3	D	202	NO3	1	0
3	L	202	NO3	1	0
3	A	202	NO3	1	0
3	J	202	NO3	2	0
2	F	500	FAD	4	0
3	J	203	NO3	1	0
2	C	201	FAD	3	0
2	A	201	FAD	2	0
3	C	202	NO3	1	0
2	G	201	FAD	1	0
3	H	202	NO3	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 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.

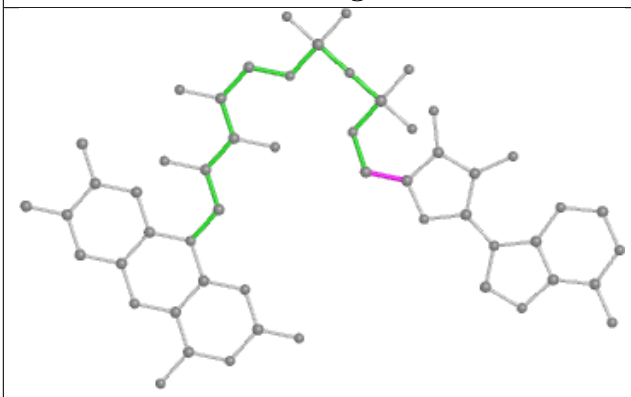
Ligand FAD I 201



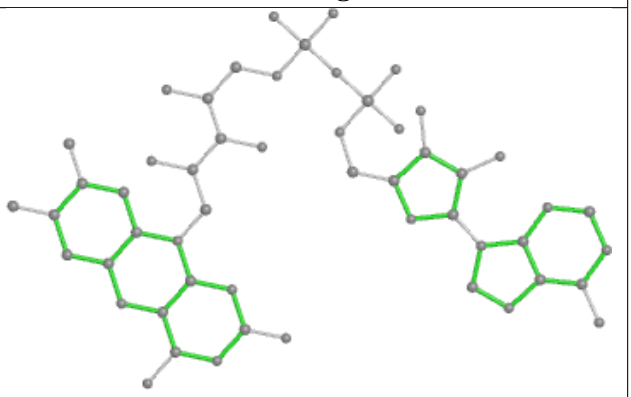
Bond lengths



Bond angles

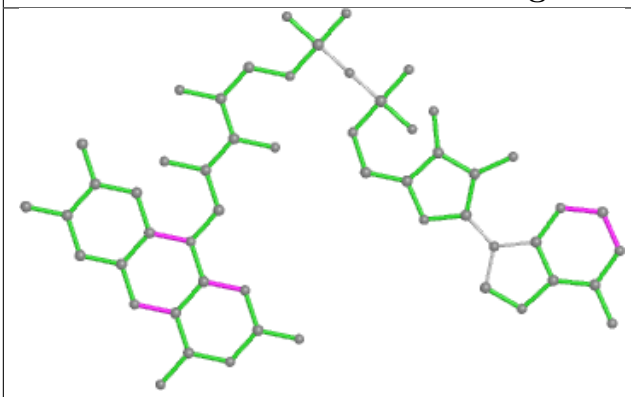


Torsions

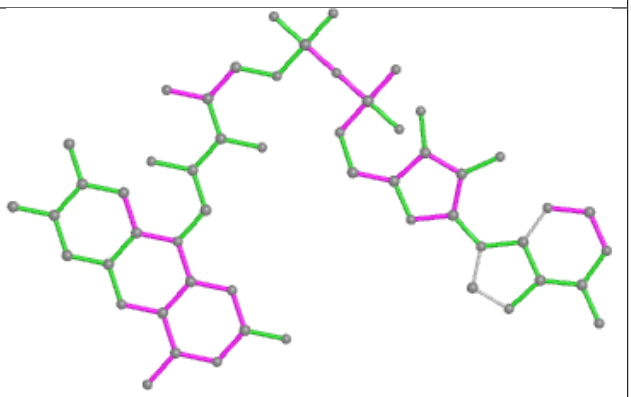


Rings

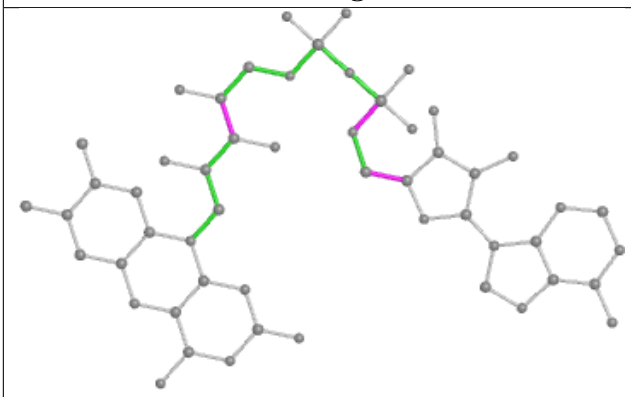
Ligand FAD J 201



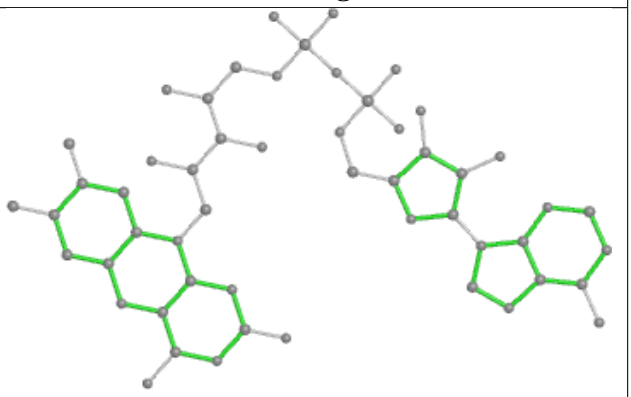
Bond lengths



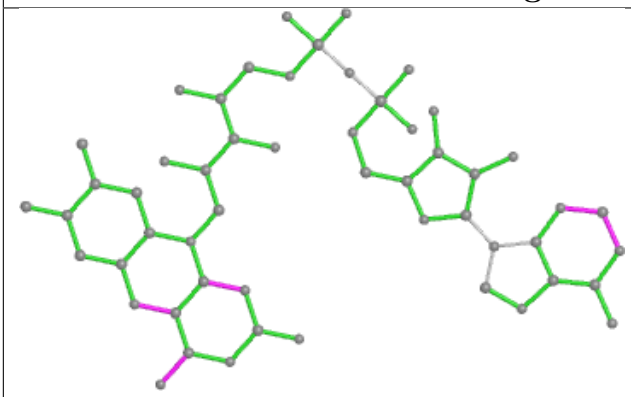
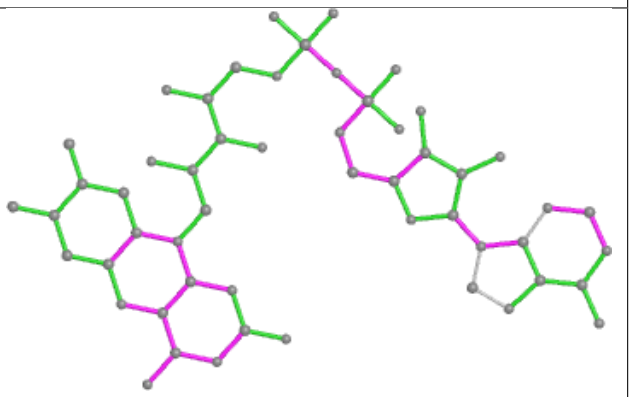
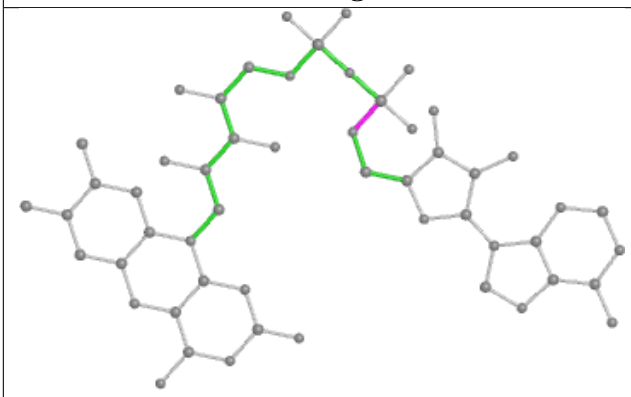
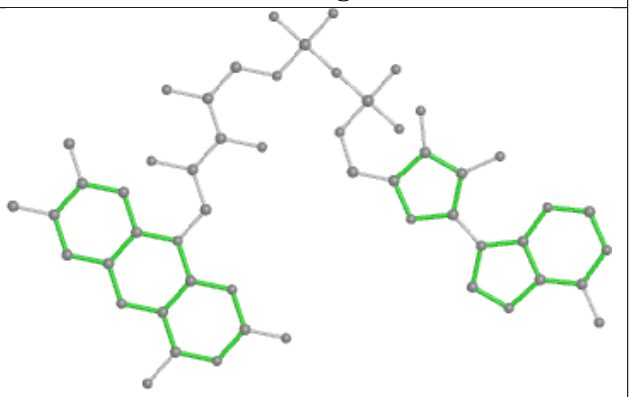
Bond angles



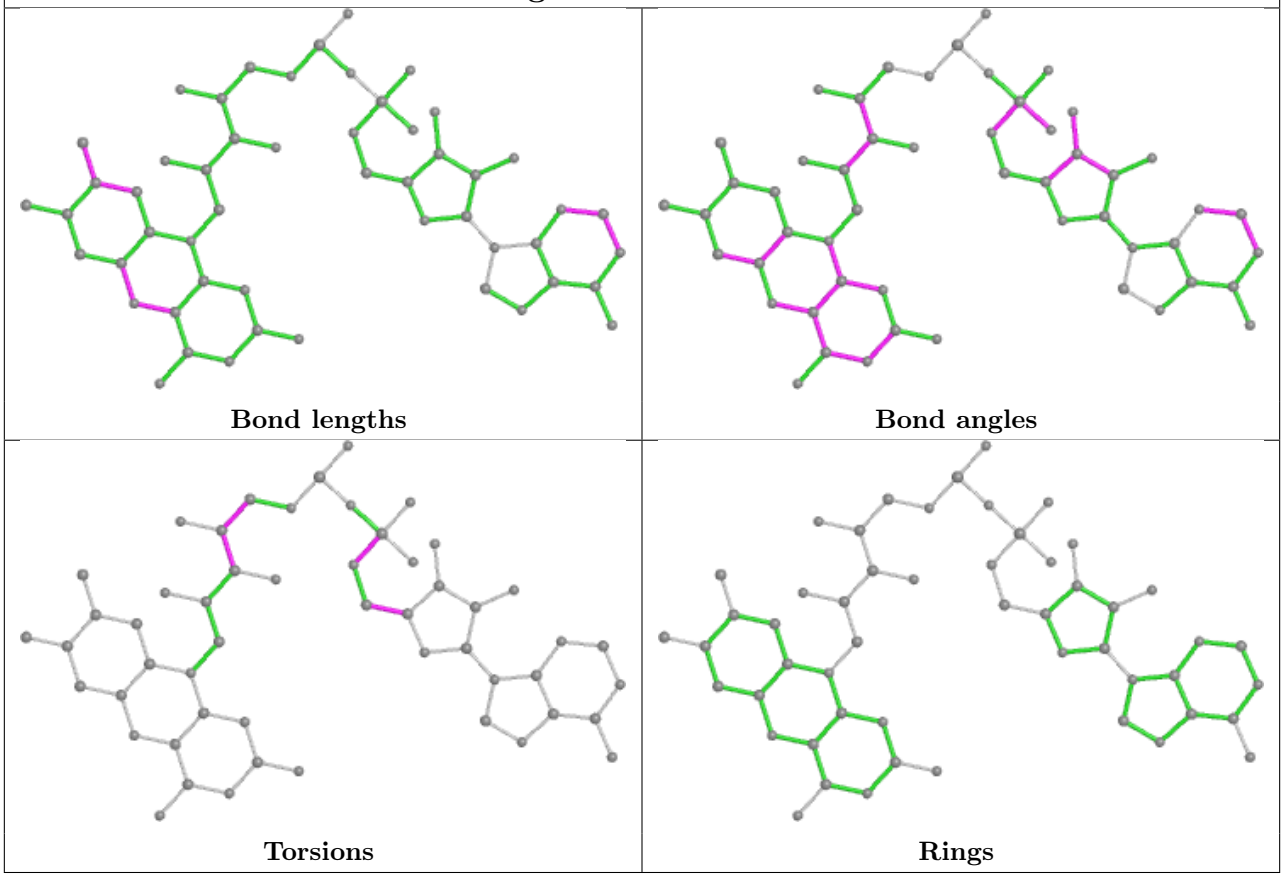
Torsions

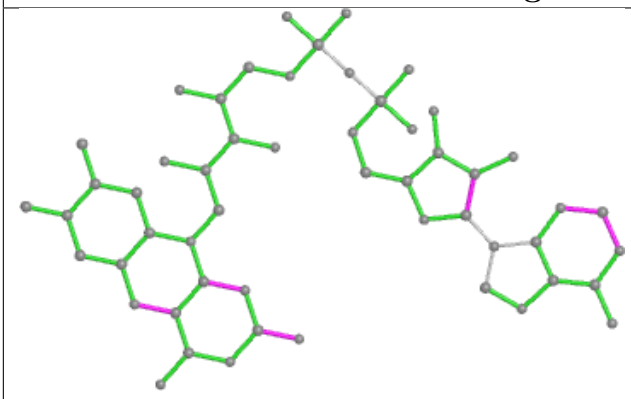
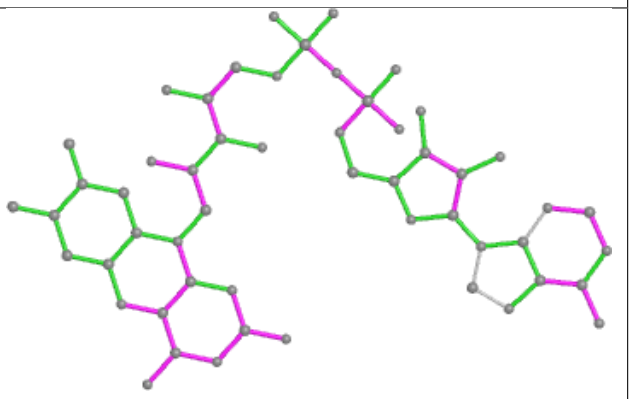
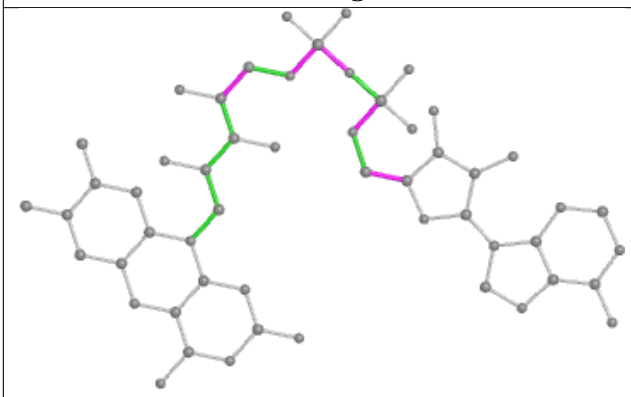
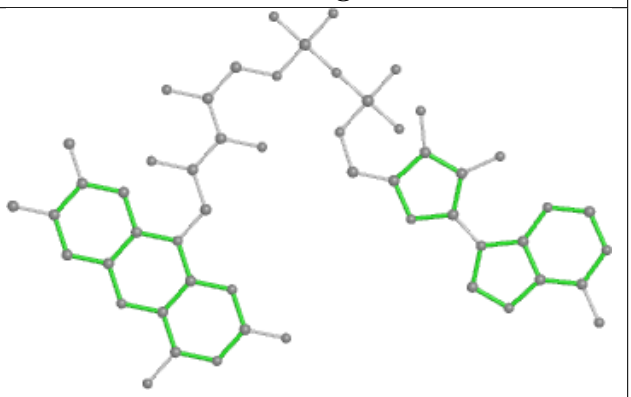


Rings

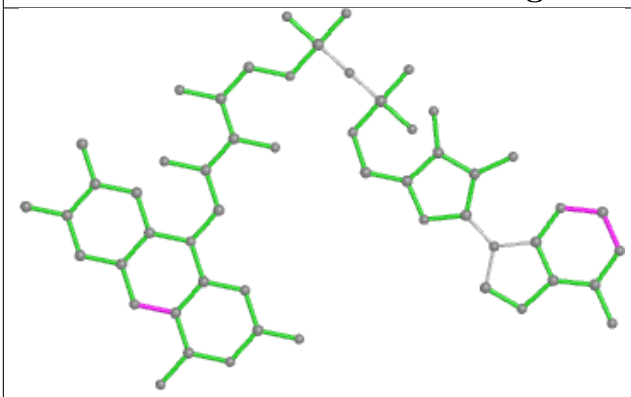
Ligand FAD H 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FAD L 201

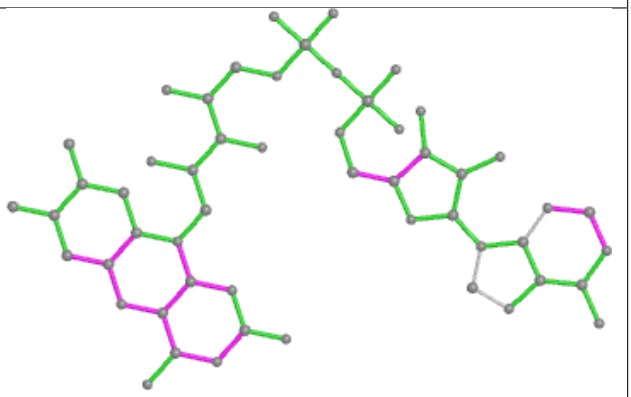


Ligand FAD D 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

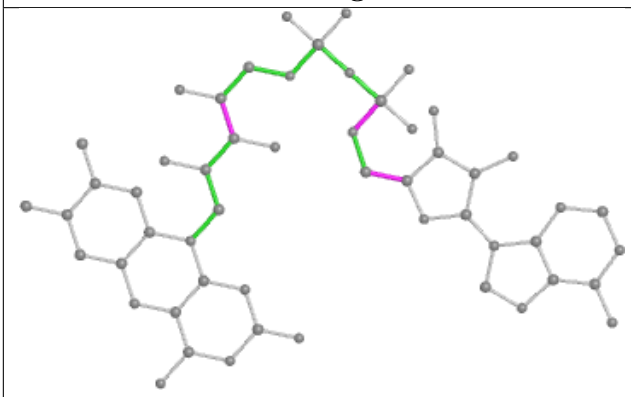
Ligand FAD E 201



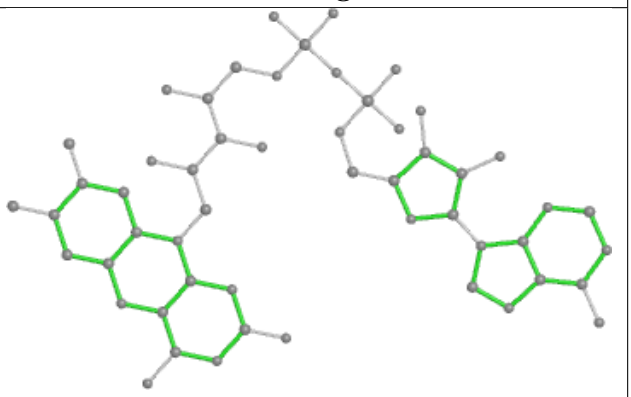
Bond lengths



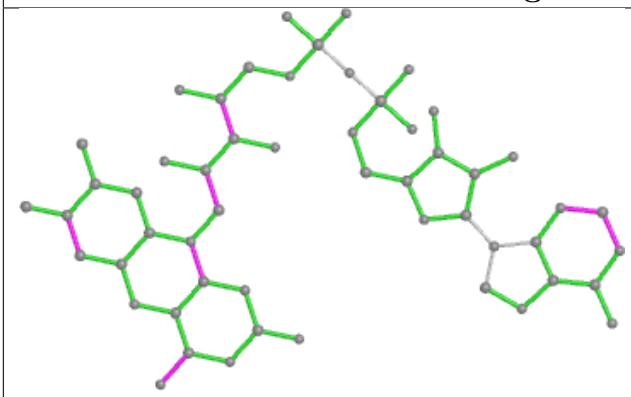
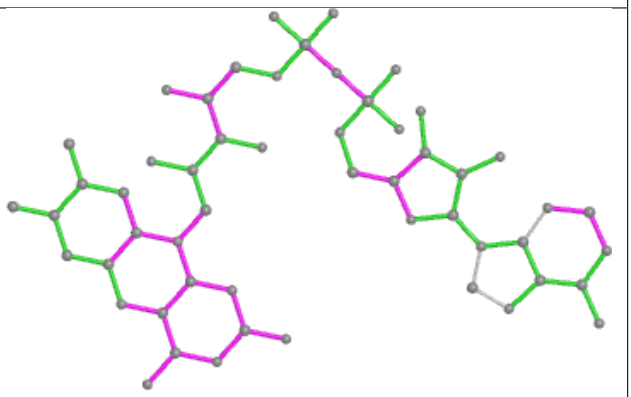
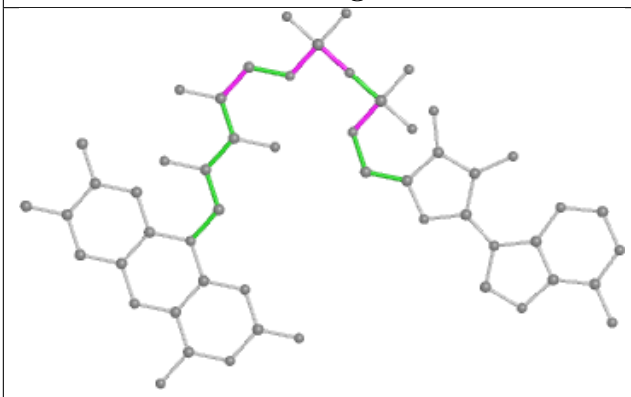
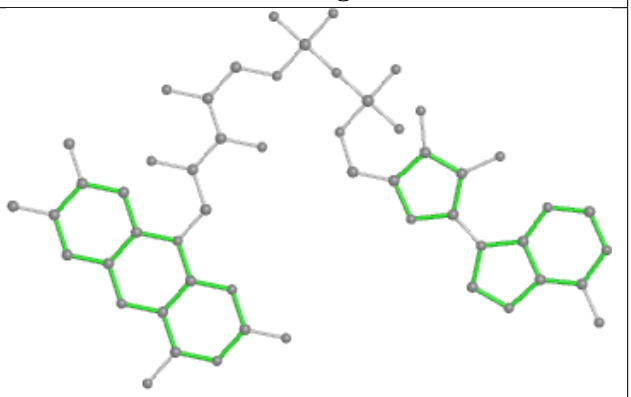
Bond angles

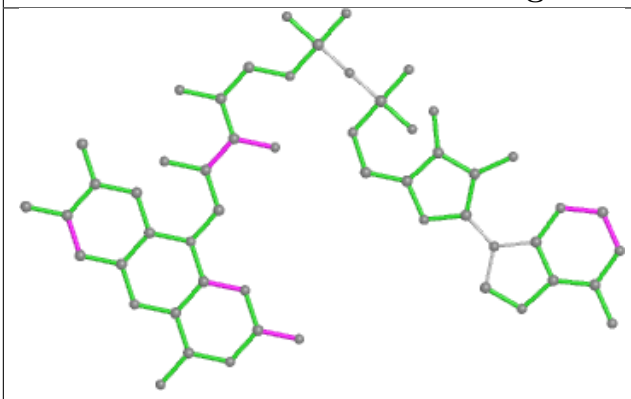
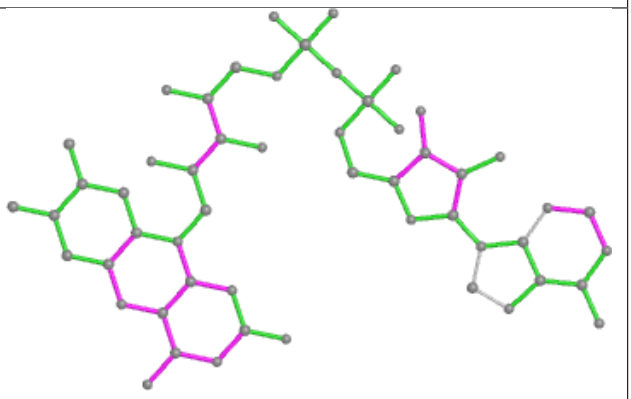
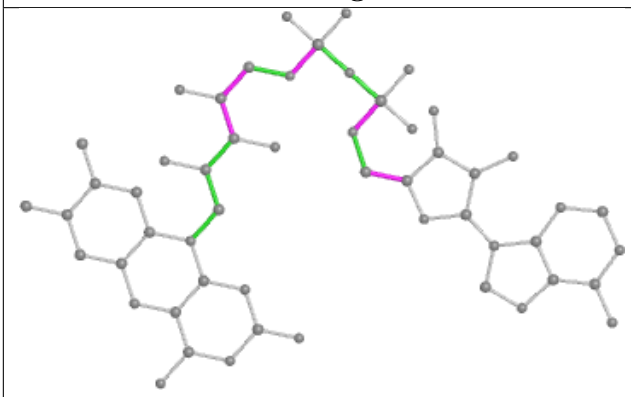
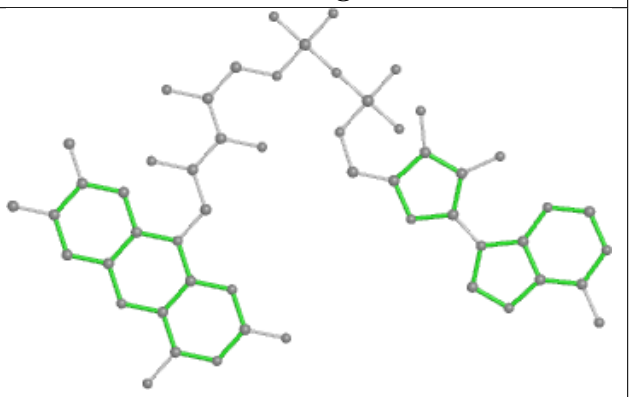


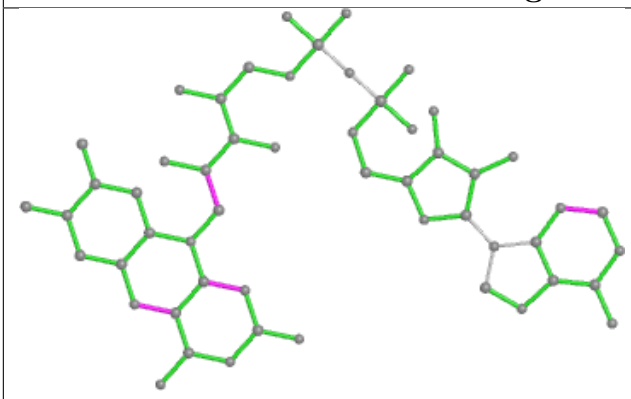
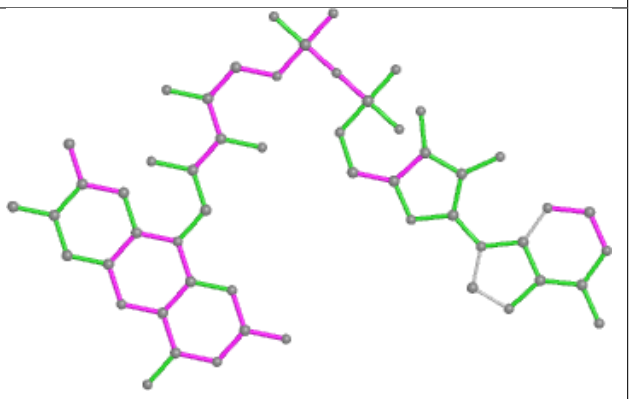
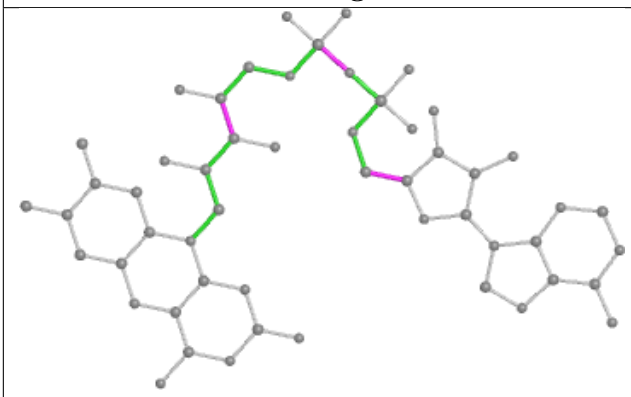
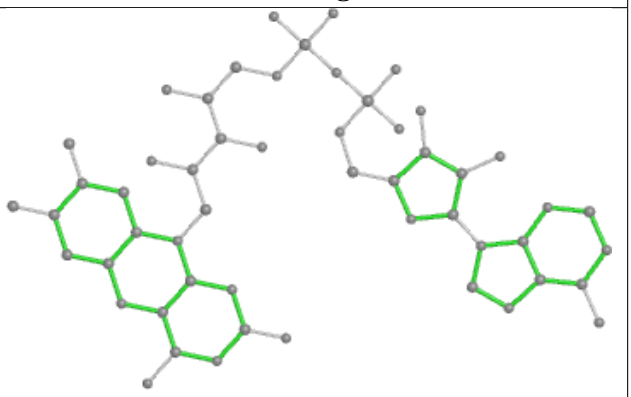
Torsions



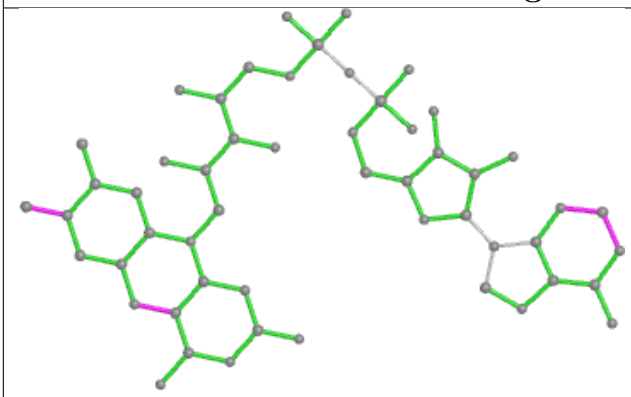
Rings

Ligand FAD K 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

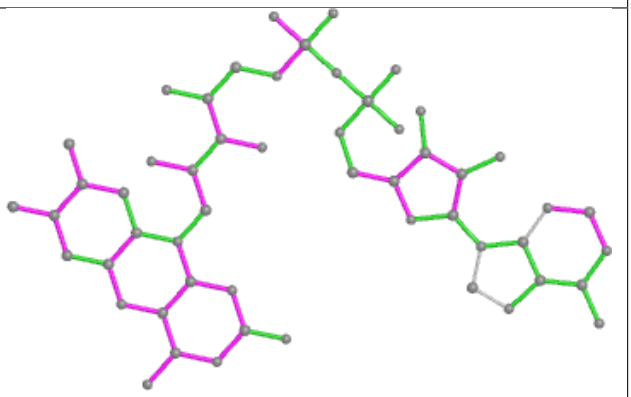
Ligand FAD F 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FAD C 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

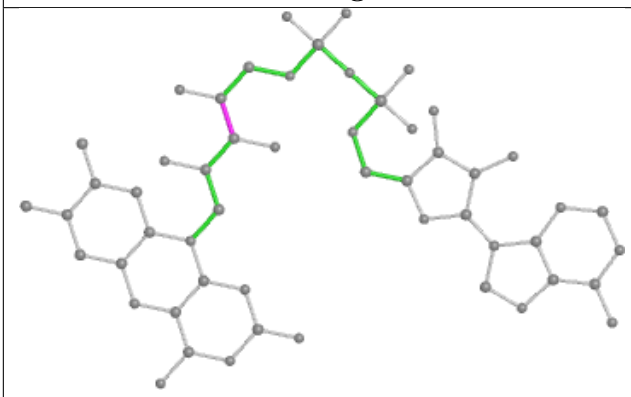
Ligand FAD A 201



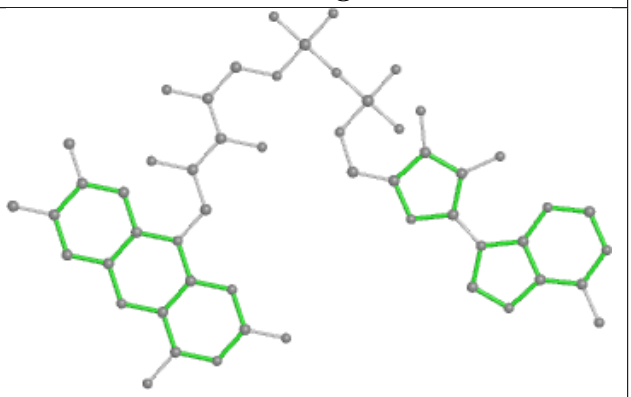
Bond lengths



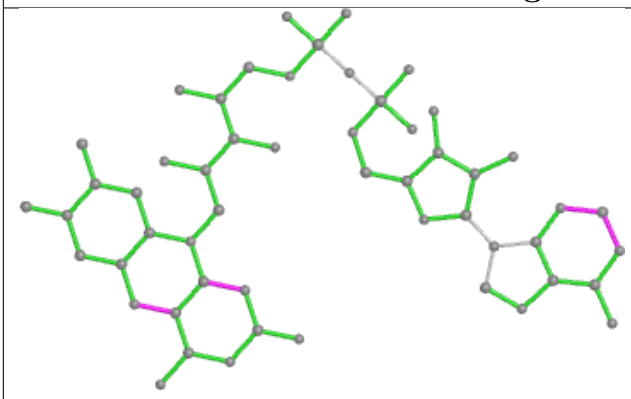
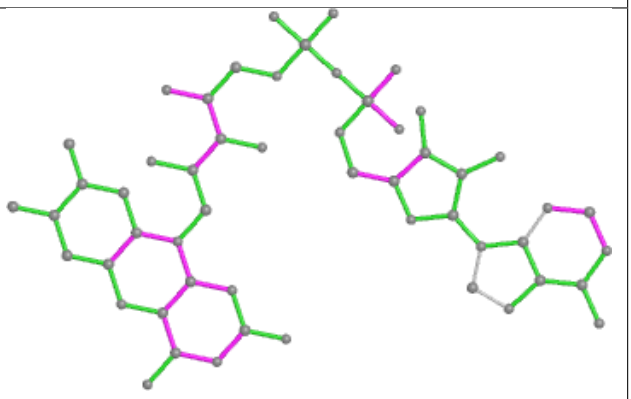
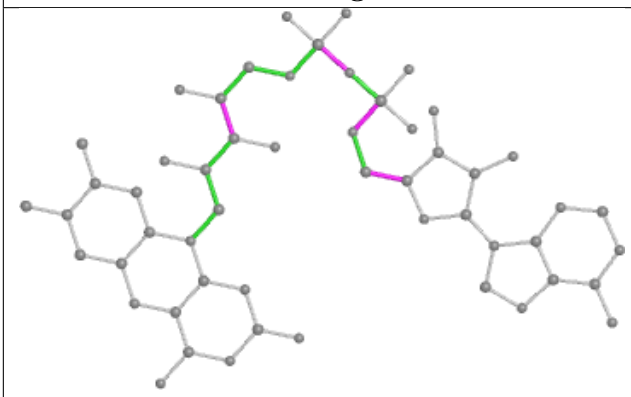
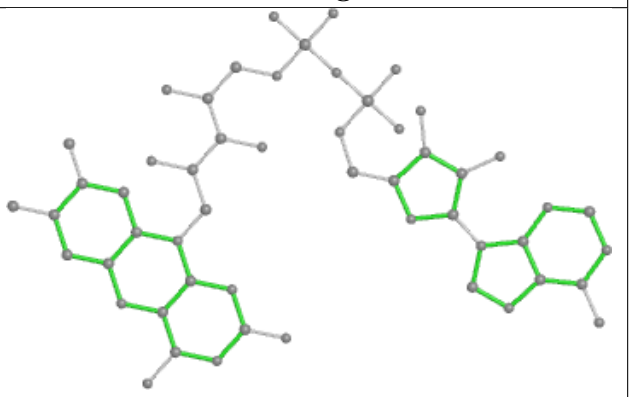
Bond angles



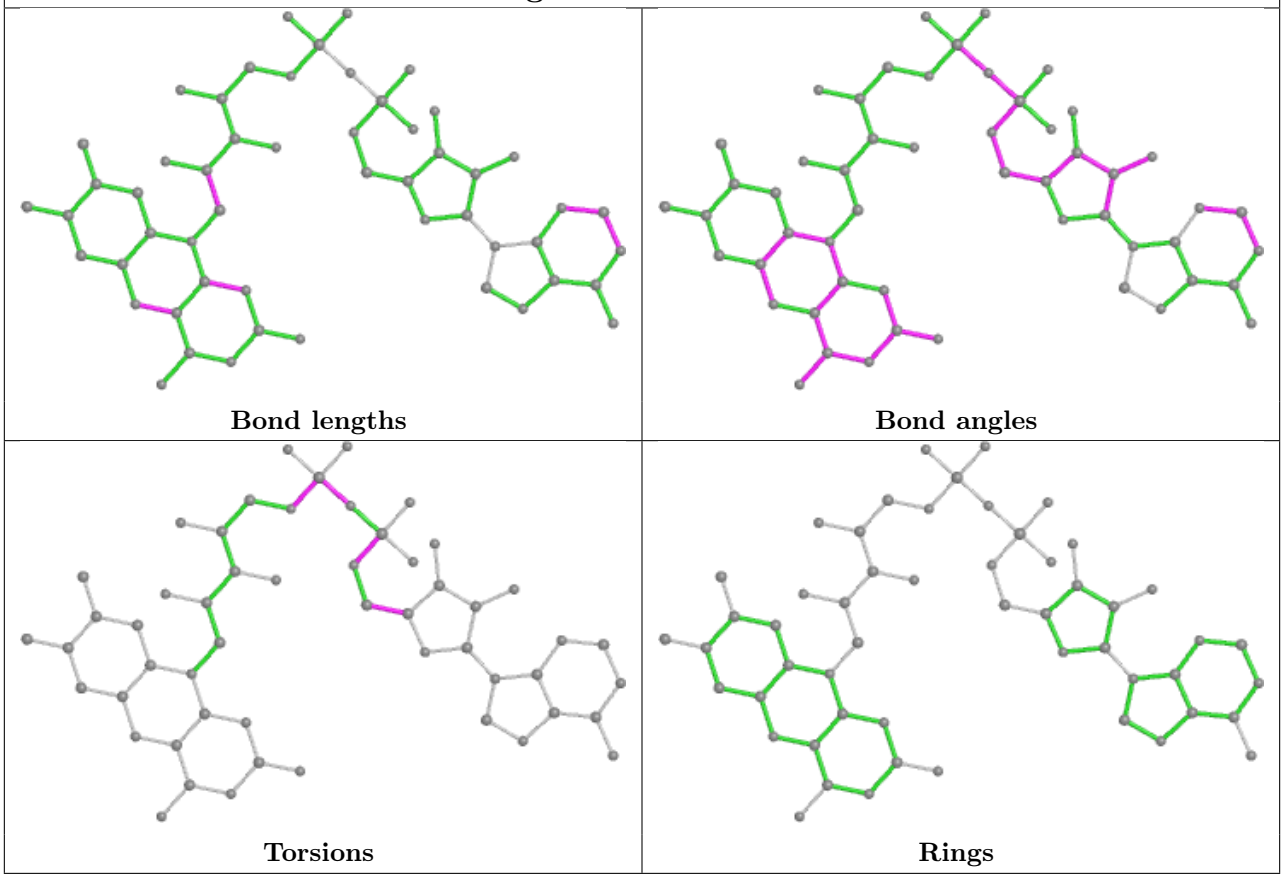
Torsions



Rings

Ligand FAD G 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FAD B 201



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	152/190 (80%)	0.07	5 (3%)	46	53	2, 14, 32, 42	0
1	B	154/190 (81%)	-0.05	4 (2%)	56	63	2, 12, 31, 39	0
1	C	152/190 (80%)	0.07	4 (2%)	56	63	5, 15, 38, 43	0
1	D	153/190 (80%)	0.17	8 (5%)	27	34	3, 17, 35, 45	0
1	E	149/190 (78%)	0.08	5 (3%)	45	52	2, 15, 34, 43	0
1	F	155/190 (81%)	0.02	8 (5%)	27	34	2, 13, 32, 37	0
1	G	153/190 (80%)	0.02	1 (0%)	87	91	2, 14, 30, 39	0
1	H	154/190 (81%)	0.20	10 (6%)	18	24	3, 16, 35, 45	0
1	I	155/190 (81%)	0.01	4 (2%)	56	63	2, 11, 30, 44	0
1	J	155/190 (81%)	0.04	11 (7%)	16	21	2, 11, 35, 42	0
1	K	155/190 (81%)	0.05	3 (1%)	66	73	2, 12, 28, 35	0
1	L	151/190 (79%)	-0.10	4 (2%)	56	63	2, 10, 30, 44	0
All	All	1838/2280 (80%)	0.05	67 (3%)	42	49	2, 14, 33, 45	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	101	PRO	5.6
1	E	36	GLU	5.3
1	H	99	ASP	5.1
1	E	37	GLY	5.0
1	J	14	THR	5.0
1	H	14	THR	4.9
1	D	38	ASP	4.8
1	A	14	THR	4.5
1	D	35	GLU	4.2
1	F	14	THR	4.1
1	F	36	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	K	98	ASP	4.0
1	I	151	THR	3.9
1	J	101	PRO	3.9
1	E	38	ASP	3.7
1	L	100	THR	3.7
1	H	37	GLY	3.6
1	D	33	GLU	3.6
1	J	36	GLU	3.6
1	L	38	ASP	3.4
1	C	14	THR	3.4
1	E	35	GLU	3.3
1	A	36	GLU	3.3
1	B	148	GLU	3.3
1	F	35	GLU	3.2
1	C	100	THR	3.2
1	H	13	SER	3.1
1	A	35	GLU	3.1
1	H	111	LEU	3.0
1	E	105	PHE	3.0
1	H	36	GLU	3.0
1	L	15	ASN	3.0
1	D	100	THR	2.9
1	D	98	ASP	2.8
1	B	14	THR	2.6
1	J	38	ASP	2.6
1	I	36	GLU	2.6
1	F	16	PHE	2.6
1	D	14	THR	2.6
1	G	36	GLU	2.6
1	C	36	GLU	2.5
1	D	36	GLU	2.5
1	H	147	PRO	2.5
1	F	99	ASP	2.5
1	H	35	GLU	2.5
1	J	149	ALA	2.4
1	H	73	GLY	2.4
1	J	37	GLY	2.3
1	H	100	THR	2.3
1	F	39	VAL	2.3
1	K	152	PRO	2.3
1	F	148	GLU	2.3
1	K	112	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	84	SER	2.2
1	B	38	ASP	2.2
1	J	34	THR	2.2
1	B	37	GLY	2.1
1	C	109	ALA	2.1
1	I	152	PRO	2.1
1	A	146	THR	2.1
1	J	100	THR	2.0
1	D	109	ALA	2.0
1	I	34	THR	2.0
1	J	132	HIS	2.0
1	J	148	GLU	2.0
1	J	98	ASP	2.0
1	F	149	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NO3	I	202	4/4	0.72	0.23	13,17,18,20	0
3	NO3	E	202	4/4	0.73	0.24	33,34,35,35	0
3	NO3	J	203	4/4	0.86	0.22	32,35,35,35	0
3	NO3	H	202	4/4	0.88	0.17	22,23,23,25	0
2	FAD	D	201	53/53	0.92	0.13	10,17,28,33	0
3	NO3	C	202	4/4	0.92	0.17	26,27,27,27	0
2	FAD	L	201	52/53	0.93	0.14	2,10,22,26	0
2	FAD	C	201	53/53	0.93	0.12	9,15,27,35	0
2	FAD	B	201	53/53	0.93	0.13	2,14,31,36	0

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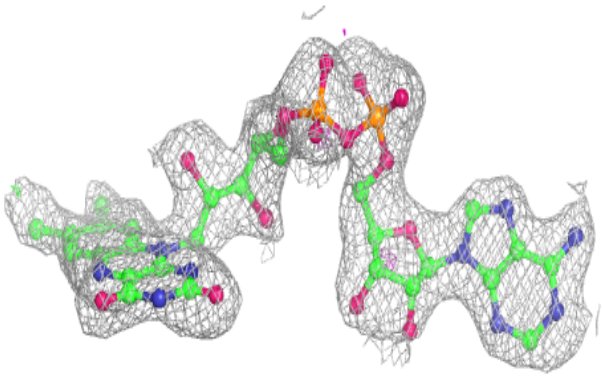
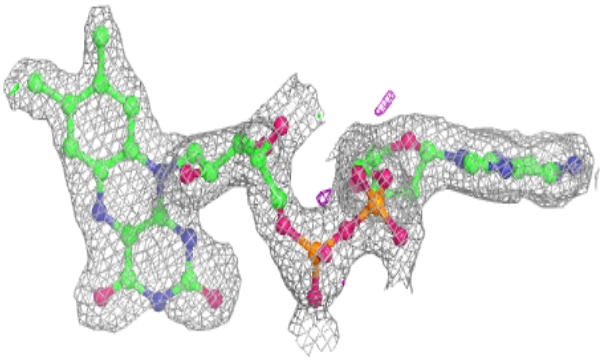
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	D	203	5/5	0.93	0.27	43,46,48,49	0
3	NO3	G	202	4/4	0.94	0.14	27,28,28,28	0
2	FAD	F	500	53/53	0.94	0.13	2,20,35,41	0
3	NO3	A	203	4/4	0.94	0.24	35,35,36,39	0
3	NO3	J	202	4/4	0.94	0.16	22,24,24,27	0
2	FAD	H	201	53/53	0.94	0.12	5,18,32,38	0
3	NO3	L	202	4/4	0.94	0.18	23,24,25,25	0
2	FAD	J	201	53/53	0.94	0.13	2,13,28,30	0
2	FAD	E	201	53/53	0.95	0.12	2,13,24,27	0
2	FAD	I	201	53/53	0.95	0.13	2,20,30,33	0
2	FAD	A	201	53/53	0.95	0.13	2,12,26,36	0
2	FAD	K	500	53/53	0.95	0.12	2,8,22,24	0
2	FAD	G	201	53/53	0.95	0.13	4,15,26,34	0
3	NO3	A	202	4/4	0.96	0.11	24,25,26,29	0
3	NO3	B	202	4/4	0.97	0.14	21,23,24,25	0
3	NO3	D	202	4/4	0.97	0.16	31,32,32,33	0
4	SO4	D	204	5/5	0.97	0.17	48,48,51,51	0
4	SO4	J	204	5/5	0.97	0.14	28,31,32,33	0

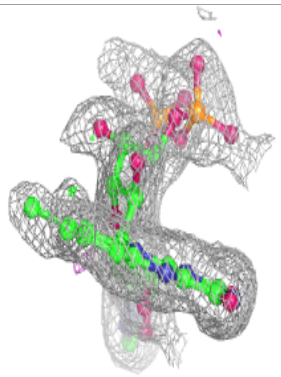
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD D 201:

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

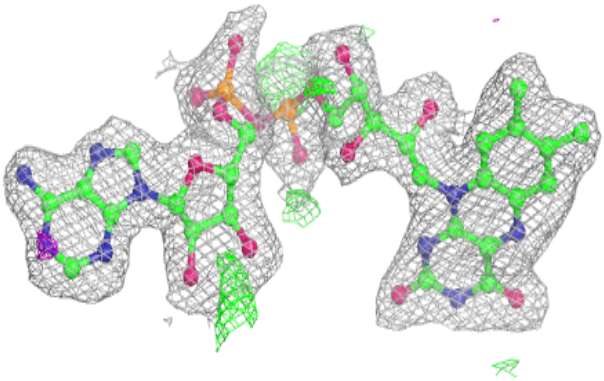


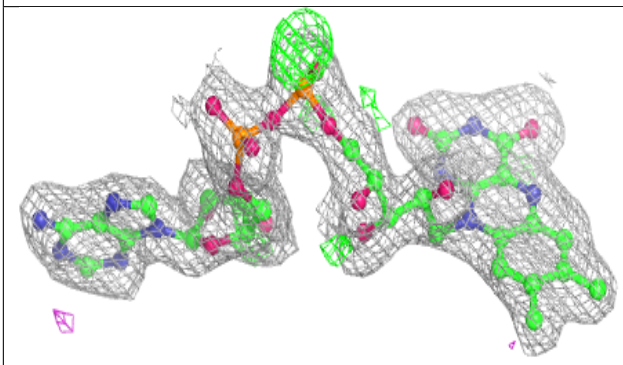


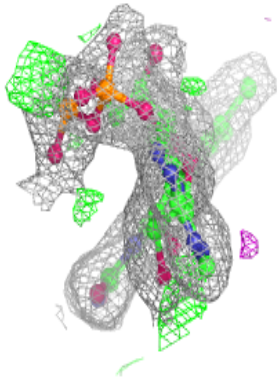


Electron density around FAD L 201:

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

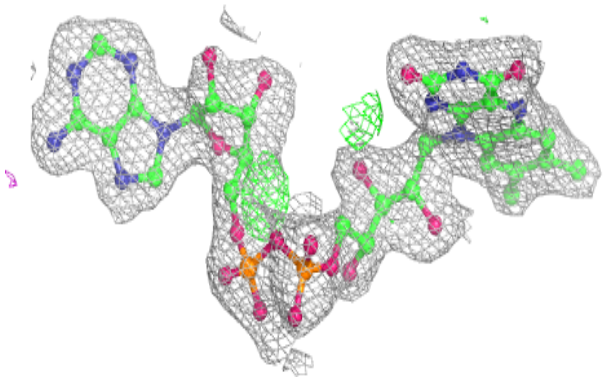


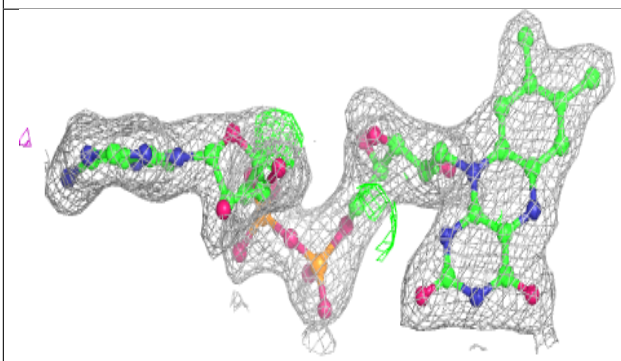


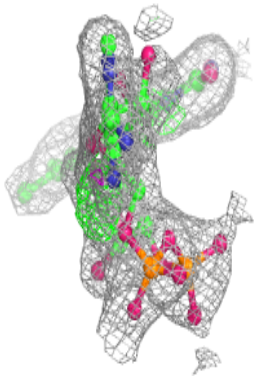


Electron density around FAD C 201:

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

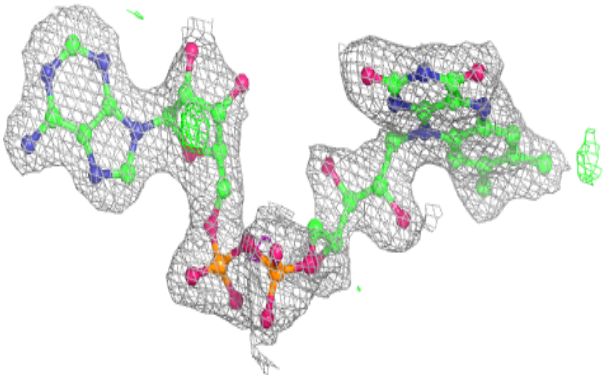


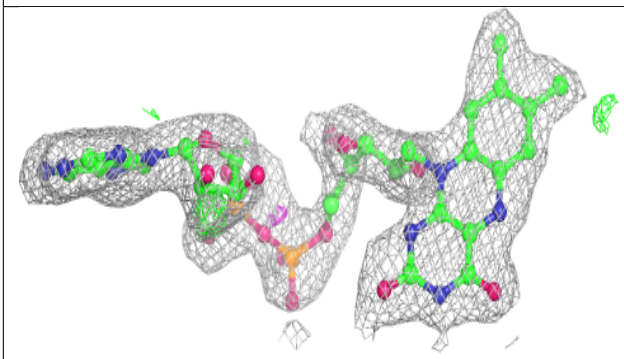


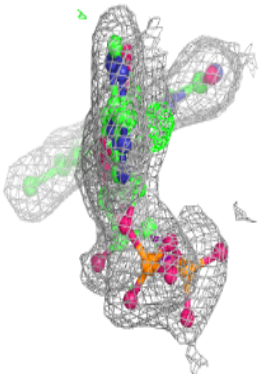


Electron density around FAD B 201:

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

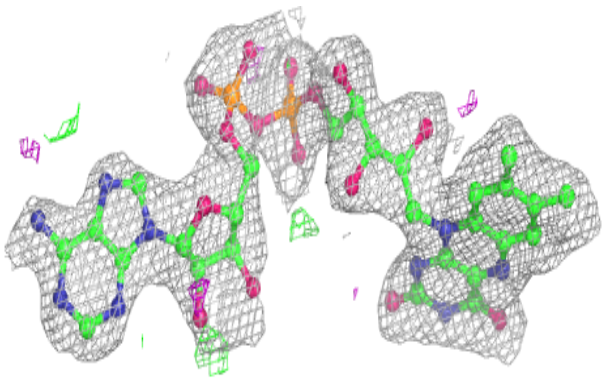


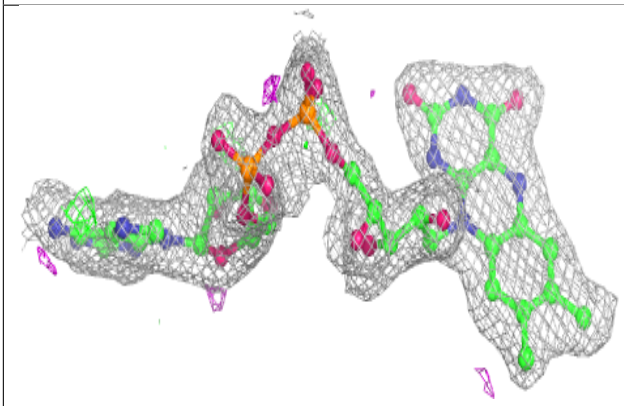


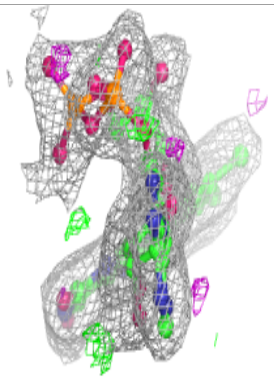


Electron density around FAD F 500:

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

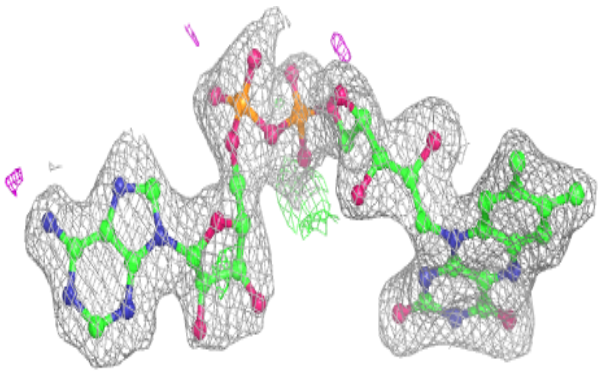


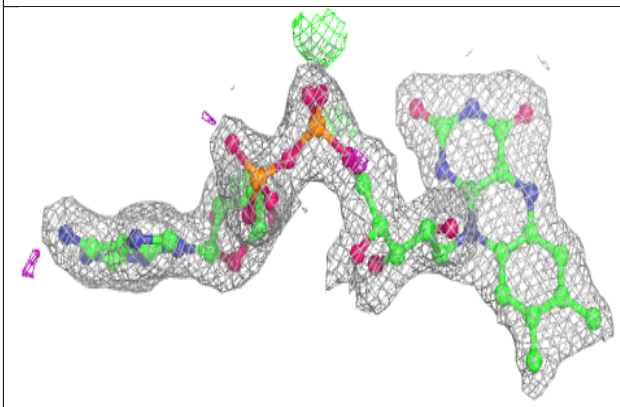


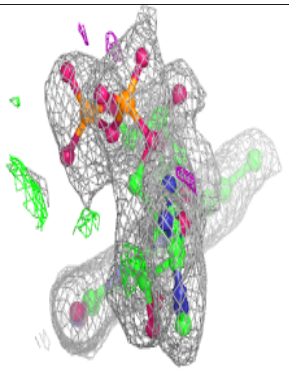


Electron density around FAD H 201:

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

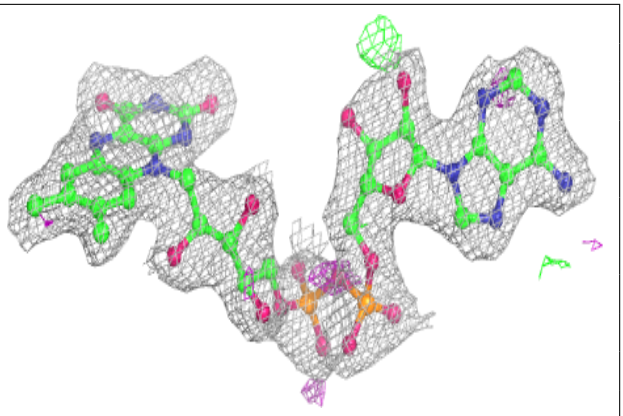


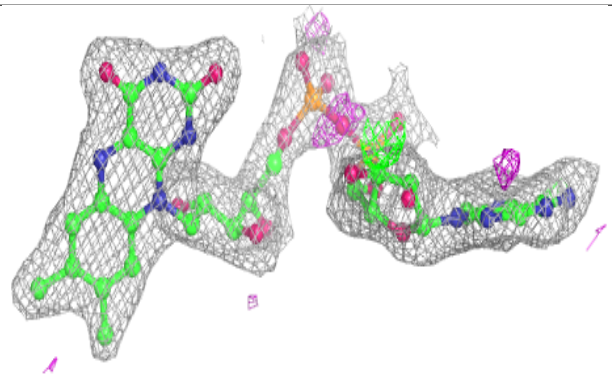


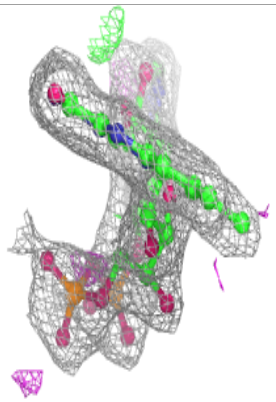


Electron density around FAD J 201:

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

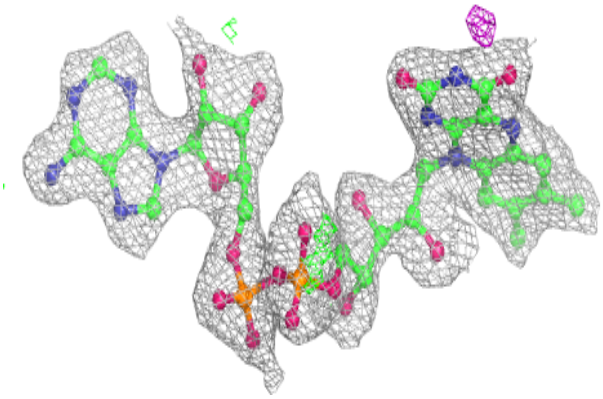


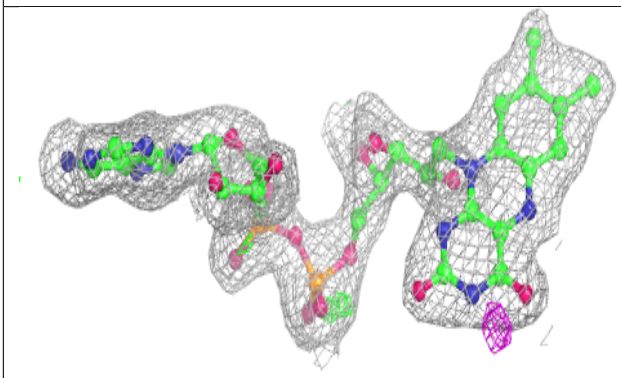


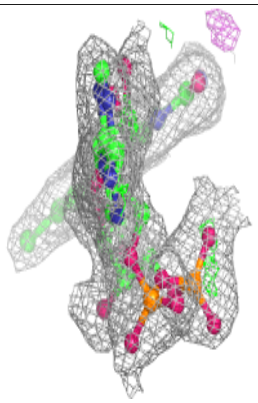


Electron density around FAD E 201:

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

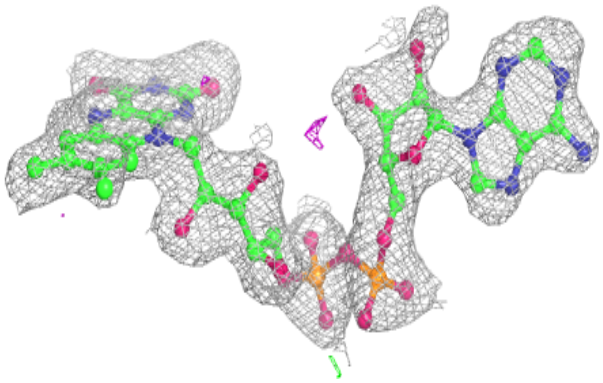


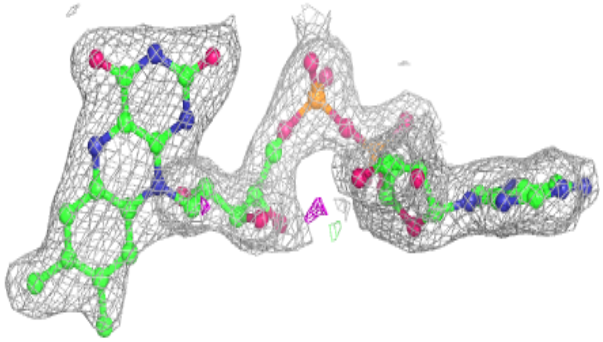




Electron density around FAD I 201:

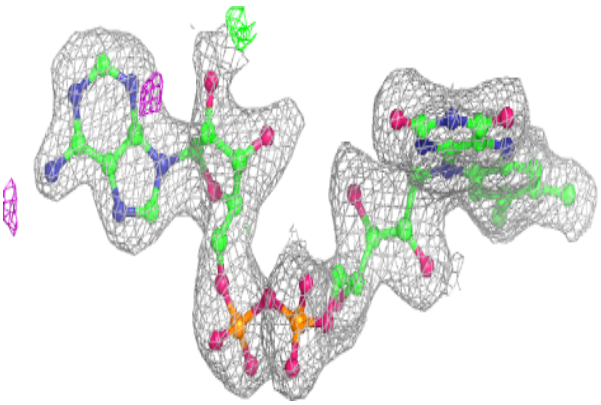
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

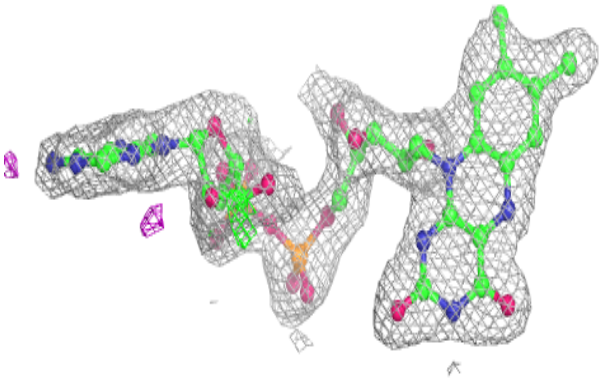


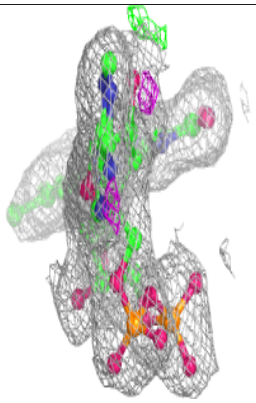


Electron density around FAD A 201:

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

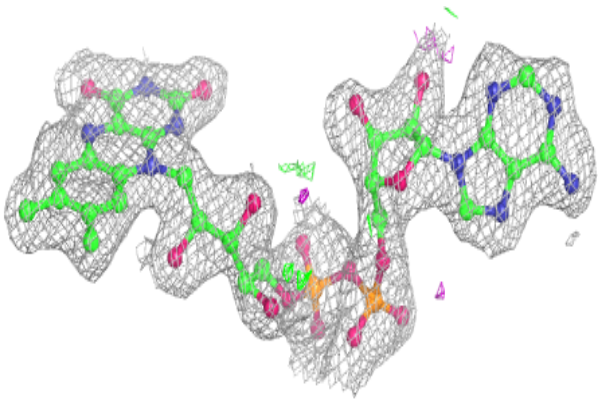


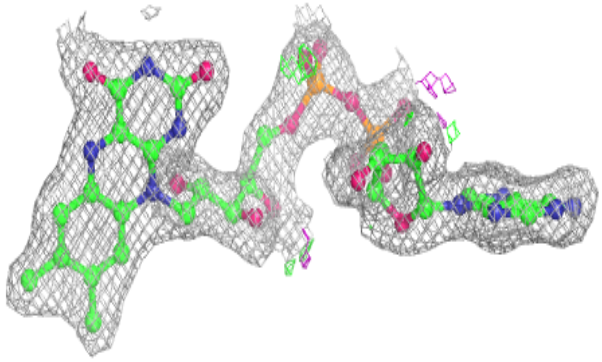


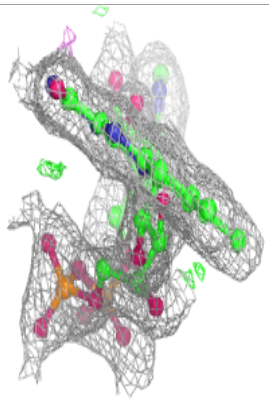


Electron density around FAD K 500:

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

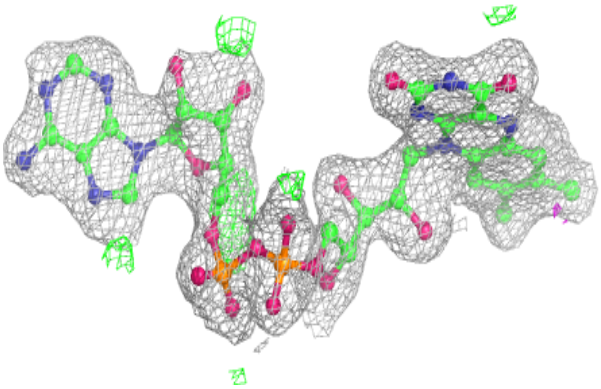


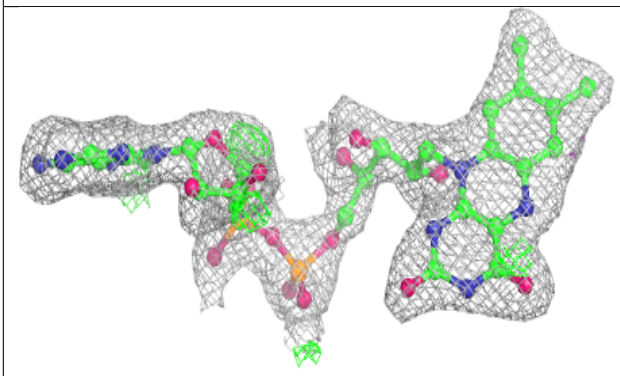


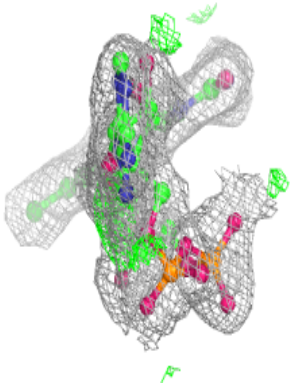


Electron density around FAD G 201:

$2mF_o$-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.