Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 03:02 PM EDT

PDB ID	:	6I4Z
Title	:	Crystal structure of the disease-causing P453L mutant of the human dihydrolipoamide dehydrogenase
Authors	:	Szabo, E.; Wilk, P.; Torocsik, B.; Weiss, M.S.; Adam-Vizi, V.; Ambrus, A.
Deposited on	:	2018-11-12
Resolution	:	2.34 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:

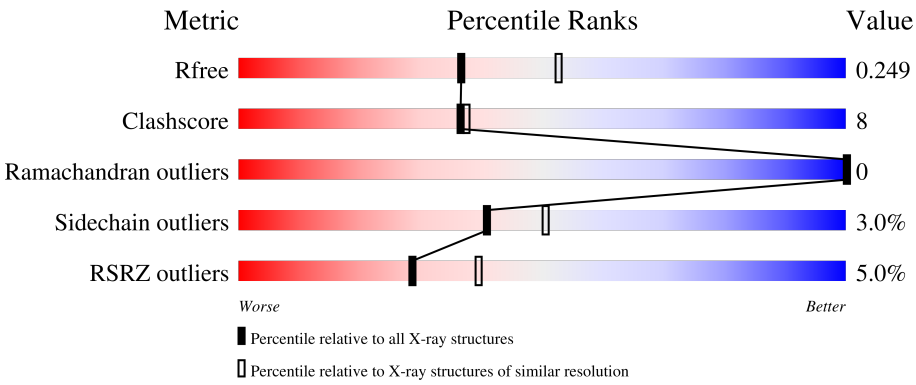
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	496	82% 12% • 5%
1	B	496	6% 77% 18% • 5%
1	C	496	84% 10% • 5%
1	D	496	10% 75% 19% • 5%
1	E	496	6% 77% 18% 5%

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Mol	Chain	Length	Quality of chain
1	F	496	6% 79% 16% • 5%
1	G	496	4% 76% 18% • 5%
1	H	496	6% 83% 12% 5%

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	SO4	C	506	-	-	X	-
3	SO4	E	502	-	-	X	-
3	SO4	G	503	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 57894 atoms, of which 28801 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 Dihydrolipoyl dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	472	7087	2215	3573	607	673	19	0	1	0
1	B	472	7086	2215	3572	607	673	19	0	1	0
1	C	472	7075	2211	3567	607	671	19	0	0	0
1	D	472	7075	2211	3567	607	671	19	0	0	0
1	E	472	7086	2215	3572	607	673	19	0	1	0
1	F	472	7075	2211	3567	607	671	19	0	0	0
1	G	472	7076	2211	3568	607	671	19	0	0	0
1	H	472	7075	2211	3567	607	671	19	0	0	0

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP P09622
A	-20	ALA	-	expression tag	UNP P09622
A	-19	SER	-	expression tag	UNP P09622
A	-18	TRP	-	expression tag	UNP P09622
A	-17	SER	-	expression tag	UNP P09622
A	-16	HIS	-	expression tag	UNP P09622
A	-15	PRO	-	expression tag	UNP P09622
A	-14	GLN	-	expression tag	UNP P09622
A	-13	PHE	-	expression tag	UNP P09622
A	-12	GLU	-	expression tag	UNP P09622
A	-11	LYS	-	expression tag	UNP P09622
A	-10	GLY	-	expression tag	UNP P09622
A	-9	ALA	-	expression tag	UNP P09622

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	LEU	-	expression tag	UNP P09622
A	-7	GLU	-	expression tag	UNP P09622
A	-6	VAL	-	expression tag	UNP P09622
A	-5	LEU	-	expression tag	UNP P09622
A	-4	PHE	-	expression tag	UNP P09622
A	-3	GLN	-	expression tag	UNP P09622
A	-2	GLY	-	expression tag	UNP P09622
A	-1	PRO	-	expression tag	UNP P09622
A	0	GLY	-	expression tag	UNP P09622
A	453	LEU	PRO	engineered mutation	UNP P09622
B	-21	MET	-	initiating methionine	UNP P09622
B	-20	ALA	-	expression tag	UNP P09622
B	-19	SER	-	expression tag	UNP P09622
B	-18	TRP	-	expression tag	UNP P09622
B	-17	SER	-	expression tag	UNP P09622
B	-16	HIS	-	expression tag	UNP P09622
B	-15	PRO	-	expression tag	UNP P09622
B	-14	GLN	-	expression tag	UNP P09622
B	-13	PHE	-	expression tag	UNP P09622
B	-12	GLU	-	expression tag	UNP P09622
B	-11	LYS	-	expression tag	UNP P09622
B	-10	GLY	-	expression tag	UNP P09622
B	-9	ALA	-	expression tag	UNP P09622
B	-8	LEU	-	expression tag	UNP P09622
B	-7	GLU	-	expression tag	UNP P09622
B	-6	VAL	-	expression tag	UNP P09622
B	-5	LEU	-	expression tag	UNP P09622
B	-4	PHE	-	expression tag	UNP P09622
B	-3	GLN	-	expression tag	UNP P09622
B	-2	GLY	-	expression tag	UNP P09622
B	-1	PRO	-	expression tag	UNP P09622
B	0	GLY	-	expression tag	UNP P09622
B	453	LEU	PRO	engineered mutation	UNP P09622
C	-21	MET	-	initiating methionine	UNP P09622
C	-20	ALA	-	expression tag	UNP P09622
C	-19	SER	-	expression tag	UNP P09622
C	-18	TRP	-	expression tag	UNP P09622
C	-17	SER	-	expression tag	UNP P09622
C	-16	HIS	-	expression tag	UNP P09622
C	-15	PRO	-	expression tag	UNP P09622
C	-14	GLN	-	expression tag	UNP P09622
C	-13	PHE	-	expression tag	UNP P09622

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	GLU	-	expression tag	UNP P09622
C	-11	LYS	-	expression tag	UNP P09622
C	-10	GLY	-	expression tag	UNP P09622
C	-9	ALA	-	expression tag	UNP P09622
C	-8	LEU	-	expression tag	UNP P09622
C	-7	GLU	-	expression tag	UNP P09622
C	-6	VAL	-	expression tag	UNP P09622
C	-5	LEU	-	expression tag	UNP P09622
C	-4	PHE	-	expression tag	UNP P09622
C	-3	GLN	-	expression tag	UNP P09622
C	-2	GLY	-	expression tag	UNP P09622
C	-1	PRO	-	expression tag	UNP P09622
C	0	GLY	-	expression tag	UNP P09622
C	453	LEU	PRO	engineered mutation	UNP P09622
D	-21	MET	-	initiating methionine	UNP P09622
D	-20	ALA	-	expression tag	UNP P09622
D	-19	SER	-	expression tag	UNP P09622
D	-18	TRP	-	expression tag	UNP P09622
D	-17	SER	-	expression tag	UNP P09622
D	-16	HIS	-	expression tag	UNP P09622
D	-15	PRO	-	expression tag	UNP P09622
D	-14	GLN	-	expression tag	UNP P09622
D	-13	PHE	-	expression tag	UNP P09622
D	-12	GLU	-	expression tag	UNP P09622
D	-11	LYS	-	expression tag	UNP P09622
D	-10	GLY	-	expression tag	UNP P09622
D	-9	ALA	-	expression tag	UNP P09622
D	-8	LEU	-	expression tag	UNP P09622
D	-7	GLU	-	expression tag	UNP P09622
D	-6	VAL	-	expression tag	UNP P09622
D	-5	LEU	-	expression tag	UNP P09622
D	-4	PHE	-	expression tag	UNP P09622
D	-3	GLN	-	expression tag	UNP P09622
D	-2	GLY	-	expression tag	UNP P09622
D	-1	PRO	-	expression tag	UNP P09622
D	0	GLY	-	expression tag	UNP P09622
D	453	LEU	PRO	engineered mutation	UNP P09622
E	-21	MET	-	initiating methionine	UNP P09622
E	-20	ALA	-	expression tag	UNP P09622
E	-19	SER	-	expression tag	UNP P09622
E	-18	TRP	-	expression tag	UNP P09622
E	-17	SER	-	expression tag	UNP P09622

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-16	HIS	-	expression tag	UNP P09622
E	-15	PRO	-	expression tag	UNP P09622
E	-14	GLN	-	expression tag	UNP P09622
E	-13	PHE	-	expression tag	UNP P09622
E	-12	GLU	-	expression tag	UNP P09622
E	-11	LYS	-	expression tag	UNP P09622
E	-10	GLY	-	expression tag	UNP P09622
E	-9	ALA	-	expression tag	UNP P09622
E	-8	LEU	-	expression tag	UNP P09622
E	-7	GLU	-	expression tag	UNP P09622
E	-6	VAL	-	expression tag	UNP P09622
E	-5	LEU	-	expression tag	UNP P09622
E	-4	PHE	-	expression tag	UNP P09622
E	-3	GLN	-	expression tag	UNP P09622
E	-2	GLY	-	expression tag	UNP P09622
E	-1	PRO	-	expression tag	UNP P09622
E	0	GLY	-	expression tag	UNP P09622
E	453	LEU	PRO	engineered mutation	UNP P09622
F	-21	MET	-	initiating methionine	UNP P09622
F	-20	ALA	-	expression tag	UNP P09622
F	-19	SER	-	expression tag	UNP P09622
F	-18	TRP	-	expression tag	UNP P09622
F	-17	SER	-	expression tag	UNP P09622
F	-16	HIS	-	expression tag	UNP P09622
F	-15	PRO	-	expression tag	UNP P09622
F	-14	GLN	-	expression tag	UNP P09622
F	-13	PHE	-	expression tag	UNP P09622
F	-12	GLU	-	expression tag	UNP P09622
F	-11	LYS	-	expression tag	UNP P09622
F	-10	GLY	-	expression tag	UNP P09622
F	-9	ALA	-	expression tag	UNP P09622
F	-8	LEU	-	expression tag	UNP P09622
F	-7	GLU	-	expression tag	UNP P09622
F	-6	VAL	-	expression tag	UNP P09622
F	-5	LEU	-	expression tag	UNP P09622
F	-4	PHE	-	expression tag	UNP P09622
F	-3	GLN	-	expression tag	UNP P09622
F	-2	GLY	-	expression tag	UNP P09622
F	-1	PRO	-	expression tag	UNP P09622
F	0	GLY	-	expression tag	UNP P09622
F	453	LEU	PRO	engineered mutation	UNP P09622
G	-21	MET	-	initiating methionine	UNP P09622

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-20	ALA	-	expression tag	UNP P09622
G	-19	SER	-	expression tag	UNP P09622
G	-18	TRP	-	expression tag	UNP P09622
G	-17	SER	-	expression tag	UNP P09622
G	-16	HIS	-	expression tag	UNP P09622
G	-15	PRO	-	expression tag	UNP P09622
G	-14	GLN	-	expression tag	UNP P09622
G	-13	PHE	-	expression tag	UNP P09622
G	-12	GLU	-	expression tag	UNP P09622
G	-11	LYS	-	expression tag	UNP P09622
G	-10	GLY	-	expression tag	UNP P09622
G	-9	ALA	-	expression tag	UNP P09622
G	-8	LEU	-	expression tag	UNP P09622
G	-7	GLU	-	expression tag	UNP P09622
G	-6	VAL	-	expression tag	UNP P09622
G	-5	LEU	-	expression tag	UNP P09622
G	-4	PHE	-	expression tag	UNP P09622
G	-3	GLN	-	expression tag	UNP P09622
G	-2	GLY	-	expression tag	UNP P09622
G	-1	PRO	-	expression tag	UNP P09622
G	0	GLY	-	expression tag	UNP P09622
G	453	LEU	PRO	engineered mutation	UNP P09622
H	-21	MET	-	initiating methionine	UNP P09622
H	-20	ALA	-	expression tag	UNP P09622
H	-19	SER	-	expression tag	UNP P09622
H	-18	TRP	-	expression tag	UNP P09622
H	-17	SER	-	expression tag	UNP P09622
H	-16	HIS	-	expression tag	UNP P09622
H	-15	PRO	-	expression tag	UNP P09622
H	-14	GLN	-	expression tag	UNP P09622
H	-13	PHE	-	expression tag	UNP P09622
H	-12	GLU	-	expression tag	UNP P09622
H	-11	LYS	-	expression tag	UNP P09622
H	-10	GLY	-	expression tag	UNP P09622
H	-9	ALA	-	expression tag	UNP P09622
H	-8	LEU	-	expression tag	UNP P09622
H	-7	GLU	-	expression tag	UNP P09622
H	-6	VAL	-	expression tag	UNP P09622
H	-5	LEU	-	expression tag	UNP P09622
H	-4	PHE	-	expression tag	UNP P09622
H	-3	GLN	-	expression tag	UNP P09622
H	-2	GLY	-	expression tag	UNP P09622

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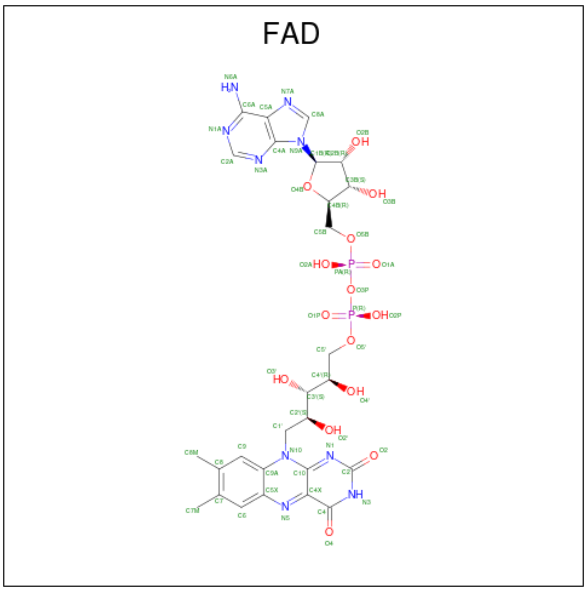
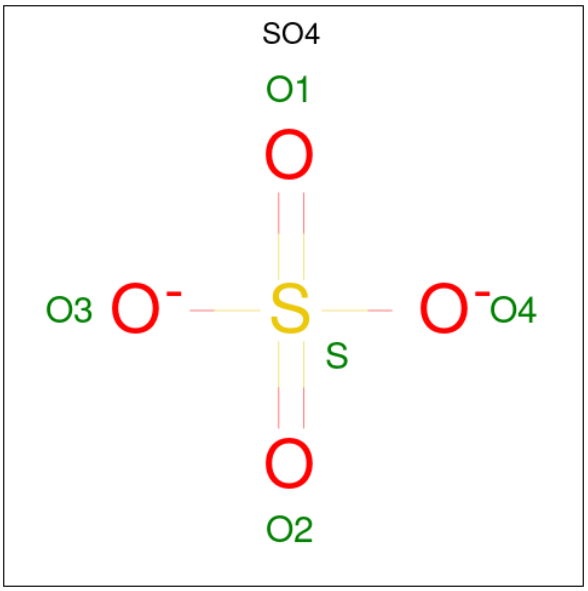
Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	PRO	-	expression tag	UNP P09622
H	0	GLY	-	expression tag	UNP P09622
H	453	LEU	PRO	engineered mutation	UNP P09622

- 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	H	N	O	P		
2	A	1	84	27	31	9	15	2	0	0
2	B	1	84	27	31	9	15	2	0	0
2	C	1	84	27	31	9	15	2	0	0
2	D	1	84	27	31	9	15	2	0	0
2	E	1	84	27	31	9	15	2	0	0
2	F	1	84	27	31	9	15	2	0	0
2	G	1	84	27	31	9	15	2	0	0
2	H	1	84	27	31	9	15	2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	D	1	5	4	1		0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	124	Total O 124 124	0	0
4	B	32	Total O 32 32	0	0
4	C	120	Total O 120 120	0	0
4	D	28	Total O 28 28	0	0
4	E	41	Total O 41 41	0	0
4	F	33	Total O 33 33	0	0

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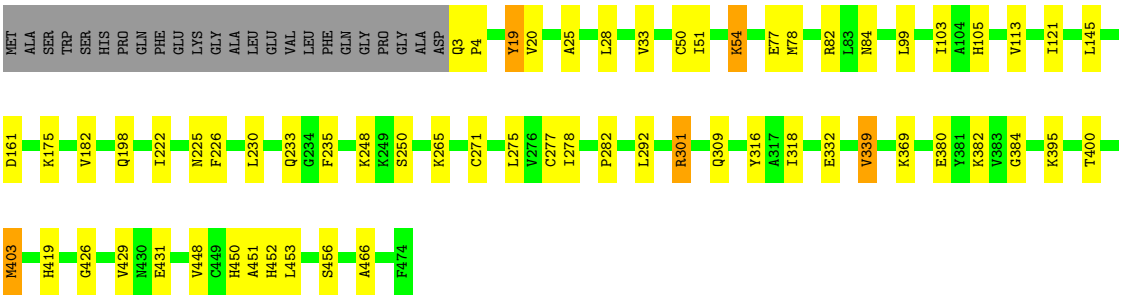
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	G	40	40	40	0	0
			Total	O		
4	H	34	34	34	0	0

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.

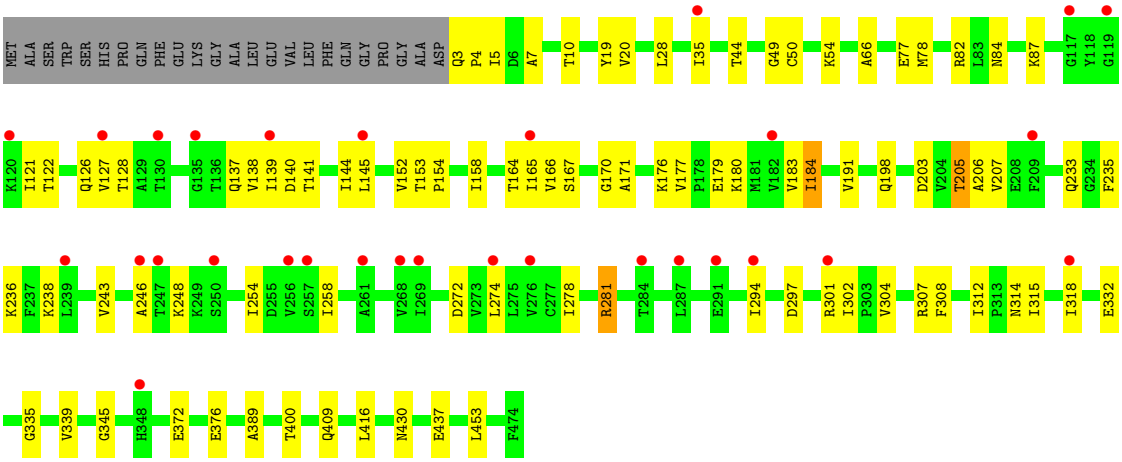
• Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

Chain A: 82% 12% • 5%



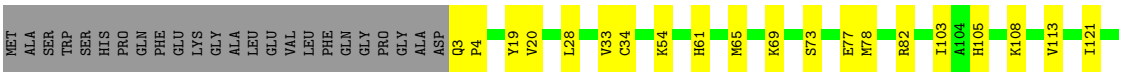
• Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

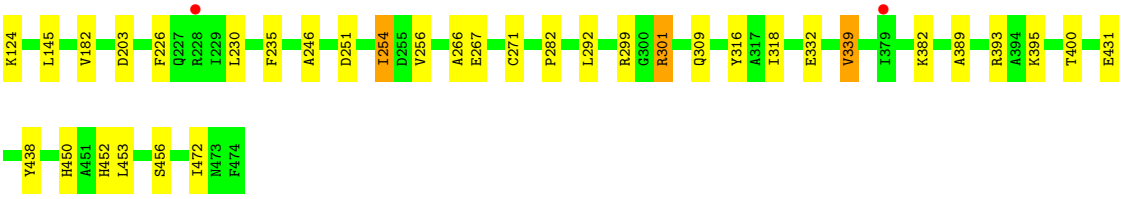
Chain B: 6% 77% 18% • 5%



• Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

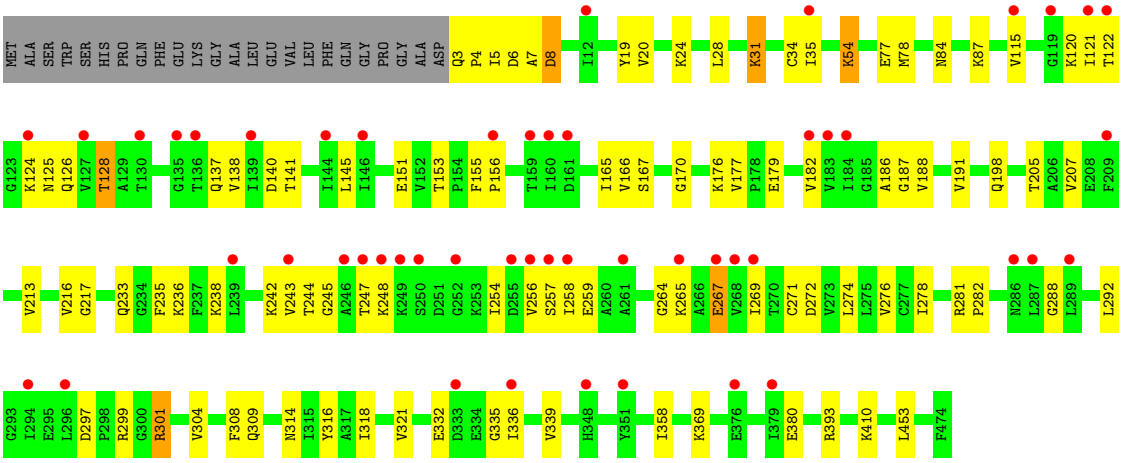
Chain C: 84% 10% • 5%





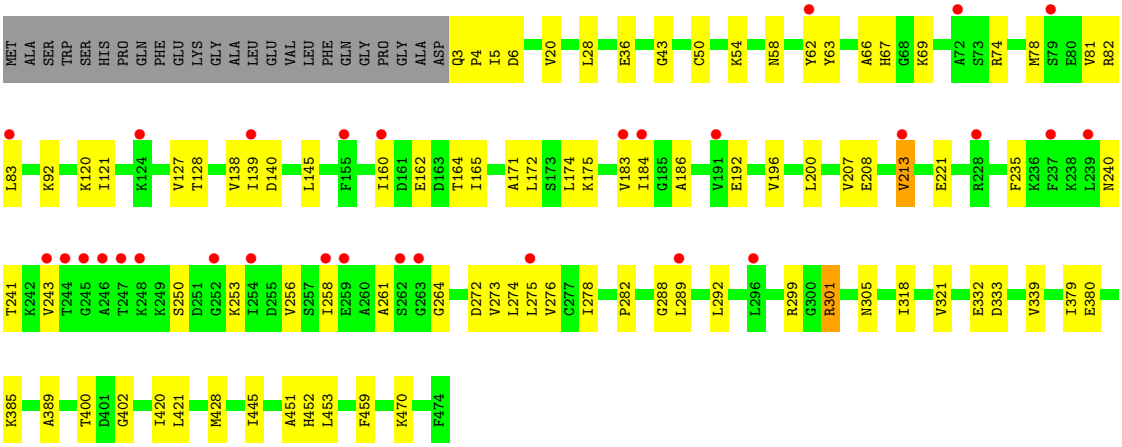
• Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

Chain D:



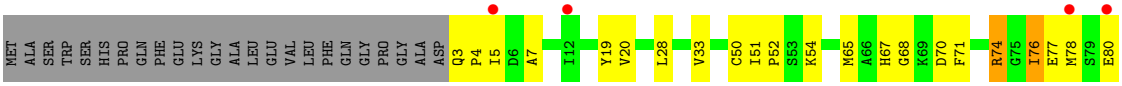
• Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

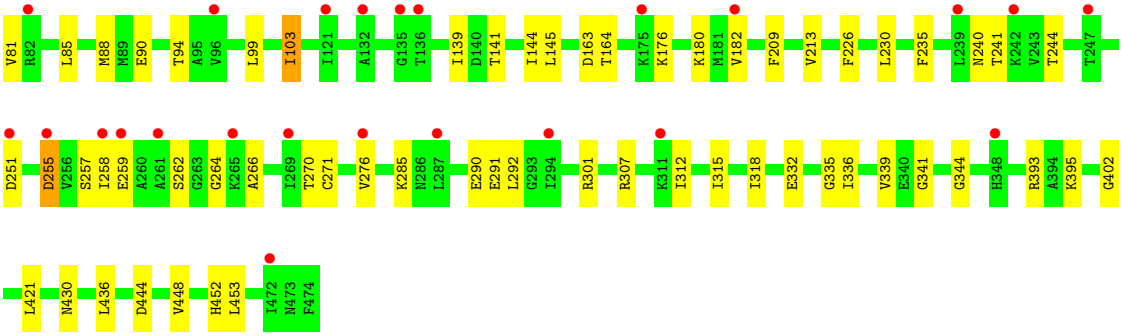
Chain E:



• Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

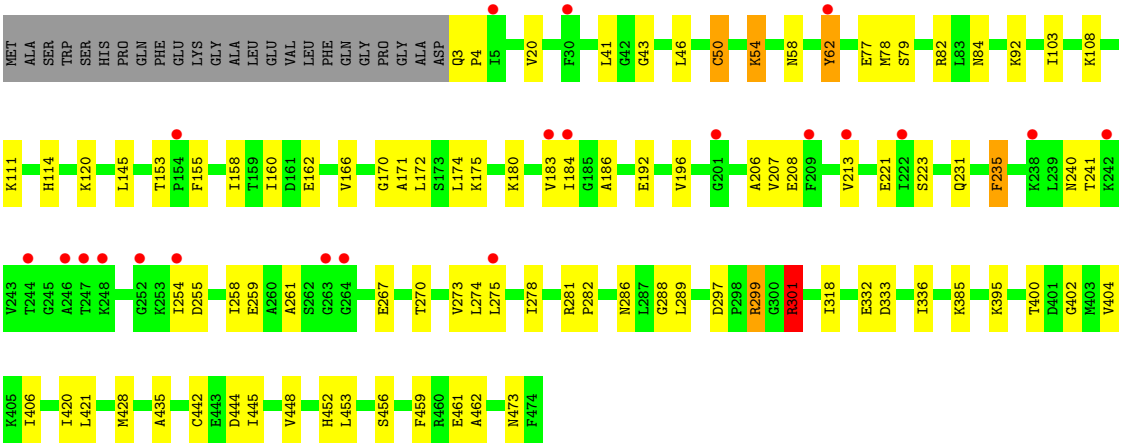
Chain F:





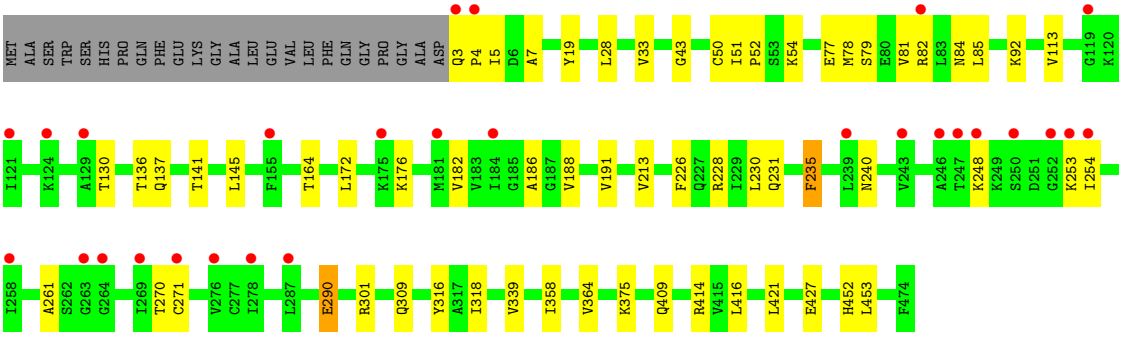
• Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

Chain G:



• Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.56Å 123.39Å 158.41Å 105.95° 91.31° 90.00°	Depositor
Resolution (Å)	46.57 – 2.34 46.57 – 2.34	Depositor EDS
% Data completeness (in resolution range)	96.6 (46.57-2.34) 96.6 (46.57-2.34)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.227 , 0.249 0.228 , 0.249	Depositor DCC
R_{free} test set	2468 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 32.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.104 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	57894	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: 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	0.61	1/3571 (0.0%)	0.63	0/4821
1	B	0.58	2/3571 (0.1%)	0.68	3/4821 (0.1%)
1	C	0.62	1/3562 (0.0%)	0.65	0/4809
1	D	0.54	0/3562	0.63	1/4809 (0.0%)
1	E	0.45	0/3571	0.61	1/4821 (0.0%)
1	F	0.51	1/3562 (0.0%)	0.69	2/4809 (0.0%)
1	G	0.52	1/3562 (0.0%)	0.64	4/4809 (0.1%)
1	H	0.51	2/3562 (0.1%)	0.62	2/4809 (0.0%)
All	All	0.55	8/28523 (0.0%)	0.64	13/38508 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	281	ARG	CZ-NH2	-12.86	1.16	1.33
1	F	255	ASP	CG-OD1	-8.87	1.04	1.25
1	G	442	CYS	CB-SG	7.36	1.94	1.82
1	A	277	CYS	CB-SG	-6.59	1.71	1.82
1	H	82	ARG	CZ-NH1	-5.93	1.25	1.33
1	H	375	LYS	CE-NZ	-5.21	1.36	1.49
1	B	281	ARG	CZ-NH1	-5.17	1.26	1.33
1	C	34	CYS	CB-SG	-5.09	1.73	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	255	ASP	CB-CG-OD2	21.13	137.32	118.30
1	B	281	ARG	NE-CZ-NH1	20.04	130.32	120.30
1	F	255	ASP	CB-CG-OD1	-13.69	105.98	118.30
1	G	301	ARG	NE-CZ-NH2	-12.26	114.17	120.30
1	H	82	ARG	NE-CZ-NH2	11.86	126.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	82	ARG	NE-CZ-NH1	-9.56	115.52	120.30
1	B	281	ARG	NH1-CZ-NH2	-7.29	111.38	119.40
1	G	62	TYR	CB-CG-CD1	6.53	124.92	121.00
1	E	301	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	D	267	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	G	62	TYR	CB-CG-CD2	-5.73	117.56	121.00
1	B	281	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	G	299	ARG	NE-CZ-NH1	5.01	122.80	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	3514	3573	3572	43	0
1	B	3514	3572	3572	72	0
1	C	3508	3567	3566	32	0
1	D	3508	3567	3566	97	0
1	E	3514	3572	3572	67	0
1	F	3508	3567	3566	54	0
1	G	3508	3568	3566	77	0
1	H	3508	3567	3566	41	0
2	A	53	31	31	0	0
2	B	53	31	31	1	0
2	C	53	31	31	1	0
2	D	53	31	31	1	0
2	E	53	31	31	2	0
2	F	53	31	31	0	0
2	G	53	31	31	1	0
2	H	53	31	31	2	0
3	A	25	0	0	1	0
3	B	10	0	0	0	0
3	C	30	0	0	3	0
3	D	20	0	0	0	0
3	E	15	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	10	0	0	1	0
3	G	15	0	0	2	0
3	H	10	0	0	1	0
4	A	124	0	0	0	0
4	B	32	0	0	3	0
4	C	120	0	0	1	0
4	D	28	0	0	2	0
4	E	41	0	0	3	0
4	F	33	0	0	3	0
4	G	40	0	0	0	0
4	H	34	0	0	1	0
All	All	29093	28801	28794	453	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 8.

All (453) 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:F:259:GLU:HG2	1:F:266:ALA:HA	1.48	0.92
1:D:176:LYS:HD3	1:D:177:VAL:N	1.91	0.86
1:D:176:LYS:HD3	1:D:177:VAL:H	1.41	0.84
1:D:128:THR:HG22	1:D:138:VAL:HG22	1.63	0.80
1:E:164:THR:HG23	1:E:165:ILE:HD12	1.65	0.79
1:G:166:VAL:HG21	1:G:170:GLY:HA3	1.64	0.79
1:E:288:GLY:O	1:E:292:LEU:HD13	1.85	0.75
1:B:158:ILE:HD12	1:B:246:ALA:HB3	1.65	0.75
1:A:105:HIS:ND1	3:A:506:SO4:O3	2.20	0.75
1:G:184:ILE:HG22	1:G:278:ILE:HG23	1.68	0.74
1:G:162:GLU:HA	1:G:166:VAL:HG23	1.68	0.74
1:H:164:THR:OG1	1:H:248:LYS:NZ	2.21	0.73
1:C:266:ALA:HB2	4:C:644:HOH:O	1.87	0.73
1:E:128:THR:HG22	1:E:138:VAL:HG22	1.71	0.72
1:G:288:GLY:N	3:G:503:SO4:O1	2.21	0.72
1:B:128:THR:HG22	1:B:138:VAL:HG23	1.71	0.72
1:D:8:ASP:OD1	1:D:8:ASP:N	2.21	0.72
1:F:5:ILE:HB	1:F:139:ILE:HD13	1.71	0.71
1:G:192:GLU:O	1:G:196:VAL:HG23	1.90	0.71
1:F:259:GLU:HG2	1:F:266:ALA:CA	2.21	0.71
1:G:120:LYS:HE2	1:G:286:ASN:O	1.89	0.70
1:C:105:HIS:ND1	3:C:506:SO4:O1	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:ARG:HH21	1:D:301:ARG:HH12	1.38	0.70
1:A:161:ASP:OD2	1:A:248:LYS:NZ	2.24	0.70
1:F:3:GLN:N	1:F:4:PRO:HD3	2.06	0.70
1:E:184:ILE:HG23	1:E:278:ILE:HG23	1.74	0.69
1:F:20:VAL:HG21	1:F:332:GLU:HG2	1.72	0.69
1:G:255:ASP:OD1	1:G:270:THR:HG22	1.92	0.69
1:A:395:LYS:HD2	1:A:400:THR:HG21	1.74	0.69
1:B:184:ILE:HD13	1:B:243:VAL:HG21	1.74	0.69
1:G:78:MET:HG2	1:H:81:VAL:HG12	1.75	0.68
1:D:121:ILE:CG2	1:D:292:LEU:HD21	2.23	0.68
1:G:108:LYS:O	1:G:111:LYS:HD3	1.93	0.68
1:G:153:THR:HG22	1:G:281:ARG:HG2	1.74	0.68
1:B:409:GLN:HG2	1:B:416:LEU:HD11	1.76	0.68
1:B:164:THR:HG23	1:B:254:ILE:HD11	1.76	0.67
1:E:186:ALA:HB1	1:E:213:VAL:HG22	1.75	0.67
1:E:288:GLY:N	3:E:502:SO4:O3	2.28	0.67
1:G:79:SER:HG	1:H:79:SER:HG	1.41	0.67
1:B:154:PRO:HD2	1:B:281:ARG:NH2	2.10	0.66
1:C:82:ARG:NH2	1:D:77:GLU:OE1	2.29	0.66
1:D:299:ARG:HE	1:D:301:ARG:NH2	1.94	0.65
1:A:3:GLN:N	1:A:4:PRO:HD3	2.12	0.65
1:H:92:LYS:NZ	1:H:172:LEU:O	2.28	0.65
1:B:121:ILE:HD12	1:B:144:ILE:CD1	2.26	0.65
1:F:290:GLU:HG3	3:F:503:SO4:S	2.37	0.64
1:B:5:ILE:HB	1:B:139:ILE:CD1	2.27	0.64
1:C:3:GLN:N	1:C:4:PRO:HD3	2.12	0.64
1:D:145:LEU:HD11	1:D:318:ILE:HG12	1.78	0.64
1:D:28:LEU:HD12	1:D:339:VAL:HG12	1.80	0.64
1:E:20:VAL:HG21	1:E:332[B]:GLU:HG3	1.80	0.64
1:E:264:GLY:HA3	4:E:611:HOH:O	1.97	0.64
1:F:291:GLU:N	1:F:291:GLU:OE1	2.29	0.64
1:F:244:THR:HG1	1:F:257:SER:HG	1.45	0.63
1:B:153:THR:OG1	1:B:281:ARG:HG3	1.97	0.63
1:D:3:GLN:N	1:D:4:PRO:HD3	2.13	0.63
1:A:77:GLU:OE1	1:B:82:ARG:NH1	2.32	0.63
1:A:403:MET:SD	1:A:403:MET:N	2.71	0.63
1:E:175:LYS:HD2	1:E:175:LYS:N	2.13	0.62
1:G:282:PRO:HG3	1:G:301:ARG:HG3	1.81	0.62
1:D:258:ILE:C	1:D:258:ILE:HD12	2.20	0.62
1:A:51:ILE:HG21	1:A:99:LEU:HD12	1.82	0.62
1:G:456:SER:N	1:H:427:GLU:OE1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:LYS:CD	1:H:453:LEU:HD13	2.30	0.61
1:E:28:LEU:HD12	1:E:339:VAL:HG12	1.82	0.61
1:G:258:ILE:HD11	1:G:267:GLU:HG2	1.81	0.61
1:A:145:LEU:HD11	1:A:318:ILE:HG12	1.82	0.61
1:B:166:VAL:HG22	1:B:167:SER:O	2.00	0.61
1:H:240:ASN:C	1:H:261:ALA:HB2	2.21	0.61
1:C:124:LYS:NZ	3:C:507:SO4:O4	2.34	0.61
1:F:5:ILE:HB	1:F:139:ILE:CD1	2.30	0.61
1:A:28:LEU:HD12	1:A:339:VAL:HG13	1.82	0.61
1:D:297:ASP:OD1	1:D:301:ARG:N	2.32	0.61
1:C:73:SER:O	1:D:87:LYS:NZ	2.34	0.60
1:B:372:GLU:N	4:B:601:HOH:O	2.35	0.60
1:G:184:ILE:HG22	1:G:278:ILE:CG2	2.32	0.60
1:D:274:LEU:CD2	1:D:276:VAL:HG13	2.32	0.60
1:G:274:LEU:HD23	1:G:275:LEU:N	2.16	0.60
1:B:3:GLN:N	1:B:4:PRO:CD	2.65	0.60
1:C:33:VAL:HG22	1:C:113:VAL:HB	1.83	0.60
1:H:28:LEU:HD12	1:H:339:VAL:HG12	1.84	0.60
1:F:436:LEU:HD23	4:F:616:HOH:O	2.01	0.59
1:D:35:ILE:HD12	1:D:115:VAL:HB	1.84	0.59
1:A:222:ILE:HD12	1:A:419:HIS:HB3	1.84	0.59
1:E:3:GLN:N	1:E:4:PRO:CD	2.65	0.59
1:B:28:LEU:HD12	1:B:339:VAL:HG12	1.83	0.59
1:B:307:ARG:NH2	1:B:345:GLY:O	2.33	0.59
1:D:20:VAL:HG21	1:D:332:GLU:HG2	1.85	0.59
1:E:74:ARG:O	1:F:88:MET:HG3	2.02	0.59
1:G:82:ARG:HG2	1:G:82:ARG:HH11	1.68	0.59
1:H:186:ALA:HB1	1:H:213:VAL:HG22	1.85	0.59
1:D:166:VAL:CG2	1:D:170:GLY:HA3	2.33	0.58
1:E:184:ILE:HG22	1:E:276:VAL:HA	1.84	0.58
1:E:253:LYS:NZ	1:E:272:ASP:OD1	2.36	0.58
1:E:240:ASN:C	1:E:261:ALA:HB2	2.23	0.58
1:E:299:ARG:HH21	1:E:301:ARG:HH22	1.50	0.58
1:G:406:ILE:HD13	1:G:462:ALA:CB	2.34	0.58
1:D:244:THR:OG1	1:D:257:SER:OG	2.22	0.58
1:D:24:LYS:HB2	1:D:336:ILE:CD1	2.35	0.57
1:C:182:VAL:HG13	1:C:271:CYS:SG	2.44	0.57
1:C:251:ASP:OD1	1:C:251:ASP:O	2.22	0.57
1:E:165:ILE:HG23	1:E:274:LEU:HD22	1.85	0.57
1:B:126:GLN:NE2	1:B:140:ASP:OD1	2.33	0.57
1:H:452:HIS:O	1:H:453:LEU:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:THR:OG1	1:E:272:ASP:O	2.22	0.57
1:F:255:ASP:OD1	1:F:270:THR:HG22	2.03	0.57
1:D:122:THR:HG21	1:D:128:THR:HG23	1.87	0.57
1:D:153:THR:HG23	1:D:281:ARG:HD3	1.85	0.57
1:B:184:ILE:HG22	1:B:278:ILE:HG23	1.86	0.57
1:G:213:VAL:O	1:G:223:SER:OG	2.20	0.57
1:B:198:GLN:NE2	1:B:233:GLN:O	2.38	0.56
1:D:380:GLU:HG2	1:D:410:LYS:CE	2.35	0.56
1:B:3:GLN:O	1:B:137:GLN:NE2	2.31	0.56
1:G:171:ALA:HB2	1:G:275:LEU:HD13	1.88	0.56
1:G:420:ILE:HD13	1:G:428:MET:HB3	1.87	0.56
1:A:33:VAL:HG22	1:A:113:VAL:HB	1.87	0.56
1:F:276:VAL:HG23	1:F:276:VAL:O	2.05	0.56
1:G:186:ALA:HB3	1:G:208:GLU:HG2	1.86	0.56
1:D:5:ILE:HG22	1:D:6:ASP:N	2.20	0.56
1:D:288:GLY:O	1:D:292:LEU:HD13	2.05	0.56
1:E:82:ARG:NH2	1:F:77:GLU:OE1	2.38	0.56
1:B:314:ASN:OD1	1:B:315:ILE:HD12	2.05	0.56
1:B:121:ILE:HD12	1:B:144:ILE:HD12	1.87	0.55
1:G:221:GLU:OE2	1:G:385:LYS:NZ	2.39	0.55
1:D:128:THR:HG22	1:D:138:VAL:CG2	2.34	0.55
1:G:3:GLN:N	1:G:4:PRO:HD3	2.21	0.55
1:H:290:GLU:N	3:H:503:SO4:O1	2.33	0.55
1:E:289:LEU:N	3:E:502:SO4:O3	2.40	0.55
1:F:5:ILE:HG21	1:F:33:VAL:HG21	1.88	0.55
1:D:245:GLY:N	1:D:257:SER:OG	2.40	0.55
1:A:282:PRO:HG3	1:A:301:ARG:HG3	1.88	0.54
1:E:192:GLU:O	1:E:196:VAL:HG23	2.07	0.54
1:B:66:ALA:HB1	1:B:78:MET:CE	2.38	0.54
1:D:155:PHE:CD1	1:D:156:PRO:HD2	2.43	0.54
1:G:166:VAL:CG2	1:G:170:GLY:HA3	2.36	0.54
1:G:180:LYS:HD3	1:G:270:THR:O	2.08	0.54
1:H:130:THR:HG22	1:H:136:THR:HG22	1.89	0.54
1:B:180:LYS:HG2	1:B:203:ASP:HB3	1.89	0.54
1:H:226:PHE:CZ	1:H:230:LEU:HD11	2.43	0.54
1:F:99:LEU:O	1:F:103:ILE:HD13	2.08	0.54
1:B:258:ILE:HD12	1:B:258:ILE:C	2.28	0.54
1:D:304:VAL:CG1	1:D:308:PHE:HA	2.38	0.54
1:G:406:ILE:HD13	1:G:462:ALA:HB1	1.90	0.54
1:G:175:LYS:HD2	1:G:175:LYS:N	2.23	0.54
1:B:5:ILE:HB	1:B:139:ILE:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:GLU:CA	4:B:601:HOH:O	2.56	0.53
1:G:46:LEU:HD22	1:G:103:ILE:HD11	1.89	0.53
1:A:51:ILE:CG2	1:A:99:LEU:HD12	2.38	0.53
1:D:7:ALA:O	1:D:141:THR:HA	2.09	0.53
1:D:24:LYS:HG2	1:D:336:ILE:HG23	1.89	0.53
1:D:205:THR:HG22	1:D:236:LYS:CB	2.38	0.53
1:F:28:LEU:HD12	1:F:339:VAL:HG12	1.90	0.53
1:F:259:GLU:OE2	1:F:266:ALA:HB2	2.08	0.53
1:G:20:VAL:HG21	1:G:332:GLU:HG2	1.90	0.53
1:A:25:ALA:HB2	1:A:339:VAL:HG21	1.91	0.53
1:B:35:ILE:HG22	2:B:501:FAD:H2A	1.91	0.53
1:C:145:LEU:HD11	1:C:318:ILE:HG12	1.91	0.53
1:G:54:LYS:HD3	1:H:453:LEU:HD13	1.91	0.53
1:G:395:LYS:HD2	1:G:400:THR:HG21	1.91	0.53
1:E:184:ILE:HG21	1:E:276:VAL:HG13	1.91	0.53
1:E:380:GLU:HA	4:E:605:HOH:O	2.09	0.53
1:G:58:ASN:O	1:G:62:TYR:CD2	2.62	0.52
1:H:364:VAL:HG22	1:H:421:LEU:HD13	1.91	0.52
1:H:409:GLN:HG2	1:H:416:LEU:HD11	1.91	0.52
1:A:182:VAL:HG23	1:A:271:CYS:HB3	1.91	0.52
1:B:372:GLU:HA	4:B:601:HOH:O	2.08	0.52
1:B:297:ASP:OD1	1:B:301:ARG:N	2.36	0.52
1:D:3:GLN:N	1:D:4:PRO:CD	2.73	0.52
1:H:145:LEU:HD11	1:H:318:ILE:HG12	1.91	0.52
1:A:3:GLN:N	1:A:4:PRO:CD	2.73	0.52
1:B:294:ILE:HD11	1:B:312:ILE:HD13	1.92	0.52
1:G:183:VAL:HG22	1:G:206:ALA:HA	1.91	0.52
1:G:452:HIS:ND1	1:G:453:LEU:HD23	2.24	0.52
1:F:145:LEU:HD11	1:F:318:ILE:HG12	1.92	0.52
1:D:299:ARG:HH21	1:D:301:ARG:NH1	2.07	0.51
1:H:414:ARG:HH21	1:H:416:LEU:HD23	1.75	0.51
1:B:318:ILE:HD13	1:B:335:GLY:HA2	1.91	0.51
1:D:166:VAL:HG21	1:D:170:GLY:HA3	1.92	0.51
1:E:299:ARG:NH2	1:E:301:ARG:HH22	2.07	0.51
1:D:34:CYS:C	1:D:35:ILE:HD13	2.30	0.51
1:G:461:GLU:OE2	1:G:473:ASN:ND2	2.42	0.51
1:F:68:GLY:HA3	4:F:604:HOH:O	2.10	0.51
1:D:242:LYS:HD2	1:D:243:VAL:H	1.75	0.51
1:E:288:GLY:CA	3:E:502:SO4:O3	2.57	0.51
1:G:174:LEU:HD11	1:G:273:VAL:HG11	1.92	0.51
1:D:54:LYS:HD3	1:D:54:LYS:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:240:ASN:C	1:G:261:ALA:HB2	2.31	0.51
1:E:160:ILE:O	1:E:160:ILE:HG13	2.11	0.51
1:G:41:LEU:HD21	1:G:114:HIS:NE2	2.26	0.51
1:B:145:LEU:HD11	1:B:318:ILE:HG12	1.93	0.50
1:B:164:THR:CG2	1:B:254:ILE:HD11	2.42	0.50
1:F:3:GLN:N	1:F:4:PRO:CD	2.73	0.50
1:B:121:ILE:HD12	1:B:144:ILE:HD13	1.93	0.50
1:G:241:THR:HG23	1:G:259:GLU:O	2.12	0.50
1:E:186:ALA:N	1:E:208:GLU:OE1	2.40	0.50
1:H:85:LEU:HD23	1:H:176:LYS:HA	1.94	0.50
1:E:127:VAL:HB	1:E:139:ILE:CG2	2.42	0.50
1:E:321:VAL:HG22	1:E:321:VAL:O	2.12	0.50
1:E:6:ASP:OD1	1:E:140:ASP:HB2	2.11	0.50
1:B:166:VAL:HG21	1:B:171:ALA:N	2.26	0.50
1:B:7:ALA:O	1:B:141:THR:HA	2.12	0.49
1:E:184:ILE:O	1:E:184:ILE:CG2	2.60	0.49
1:D:205:THR:HG22	1:D:236:LYS:HB3	1.94	0.49
1:D:258:ILE:HD11	1:D:267:GLU:OE2	2.13	0.49
1:D:4:PRO:HB3	1:D:138:VAL:O	2.13	0.49
1:E:43:GLY:HA2	2:E:501:FAD:O3B	2.13	0.49
1:G:299:ARG:HH21	1:G:301:ARG:HH22	1.61	0.49
1:D:128:THR:CG2	1:D:138:VAL:HG22	2.39	0.49
1:E:66:ALA:HB2	1:F:71:PHE:HE2	1.78	0.49
1:E:69:LYS:O	1:E:69:LYS:HG3	2.12	0.49
1:H:51:ILE:HB	1:H:52:PRO:HD3	1.95	0.49
1:A:451:ALA:H	1:B:430:ASN:HD21	1.60	0.49
1:H:3:GLN:CG	1:H:4:PRO:HD3	2.43	0.49
1:D:120:LYS:NZ	4:D:601:HOH:O	2.24	0.49
1:D:304:VAL:HG12	1:D:308:PHE:HA	1.93	0.49
1:F:259:GLU:HB3	1:F:264:GLY:O	2.12	0.49
1:A:452:HIS:O	1:A:453:LEU:HB2	2.13	0.49
1:A:309:GLN:HG2	1:A:316:TYR:CE2	2.48	0.49
1:C:393:ARG:HD3	1:C:453:LEU:O	2.13	0.49
1:F:103:ILE:CD1	1:F:103:ILE:N	2.76	0.49
1:D:166:VAL:HG22	1:D:167:SER:O	2.12	0.49
1:E:58:ASN:O	1:E:62:TYR:CD2	2.65	0.49
1:F:5:ILE:HD12	1:F:139:ILE:HD11	1.95	0.49
1:G:186:ALA:H	1:G:208:GLU:HG2	1.78	0.49
1:C:61:HIS:NE2	1:C:65:MET:SD	2.86	0.48
1:E:221:GLU:OE2	1:E:385:LYS:NZ	2.31	0.48
1:C:246:ALA:HB1	1:C:254:ILE:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:LYS:HE3	2:D:501:FAD:O4	2.13	0.48
1:D:155:PHE:CZ	1:D:243:VAL:HB	2.49	0.48
1:D:165:ILE:HG23	1:D:274:LEU:HD22	1.95	0.48
1:B:176:LYS:HG3	1:B:177:VAL:N	2.29	0.48
1:D:6:ASP:OD1	1:D:6:ASP:O	2.32	0.48
1:D:207:VAL:HG22	1:D:238:LYS:HB2	1.94	0.48
1:E:20:VAL:HG11	1:E:332[B]:GLU:HG3	1.96	0.48
1:D:217:GLY:HA3	4:D:612:HOH:O	2.14	0.48
1:G:155:PHE:CD1	1:G:158:ILE:CD1	2.97	0.48
1:C:28:LEU:HD12	1:C:339:VAL:CG1	2.44	0.48
1:A:452:HIS:NE2	1:B:332[A]:GLU:OE2	2.47	0.48
1:G:3:GLN:N	1:G:4:PRO:CD	2.77	0.48
1:F:241:THR:HG21	1:F:258:ILE:HD12	1.96	0.48
1:H:3:GLN:N	1:H:4:PRO:CD	2.77	0.48
1:F:258:ILE:O	1:F:259:GLU:HG3	2.14	0.48
1:G:186:ALA:HB3	1:G:208:GLU:CG	2.44	0.48
1:G:445:ILE:HG21	1:G:459:PHE:CE2	2.49	0.47
1:D:5:ILE:HG22	1:D:6:ASP:H	1.79	0.47
1:E:5:ILE:O	1:E:139:ILE:HD12	2.14	0.47
1:H:309:GLN:HG2	1:H:316:TYR:CE2	2.49	0.47
1:E:121:ILE:HG21	1:E:292:LEU:HD21	1.97	0.47
1:D:380:GLU:HG2	1:D:410:LYS:HE3	1.96	0.47
1:F:67:HIS:HA	1:F:81:VAL:HG21	1.97	0.47
1:F:144:ILE:HB	1:F:315:ILE:HG12	1.96	0.47
1:G:207:VAL:HG13	1:G:241:THR:HB	1.97	0.47
1:A:222:ILE:CD1	1:A:419:HIS:HB3	2.44	0.47
1:C:20:VAL:HG21	1:C:332:GLU:HG3	1.97	0.47
1:D:198:GLN:NE2	1:D:233:GLN:O	2.47	0.47
1:C:254:ILE:HD11	1:C:256:VAL:HG22	1.97	0.47
1:E:83:LEU:HD22	1:E:200:LEU:HD22	1.96	0.47
1:E:183:VAL:HG13	1:E:275:LEU:HD23	1.96	0.47
1:H:186:ALA:CB	1:H:213:VAL:HG22	2.45	0.47
1:D:121:ILE:HG21	1:D:292:LEU:HD21	1.95	0.47
1:D:265:LYS:CD	1:D:265:LYS:N	2.78	0.47
1:F:318:ILE:HD13	1:F:335:GLY:HA2	1.97	0.47
1:B:166:VAL:CG2	1:B:170:GLY:HA3	2.45	0.47
1:D:137:GLN:HA	1:D:137:GLN:NE2	2.30	0.46
1:E:127:VAL:O	1:E:139:ILE:HG22	2.15	0.46
1:G:254:ILE:O	1:G:270:THR:HA	2.15	0.46
1:H:253:LYS:HD3	1:H:270:THR:HG21	1.97	0.46
1:B:183:VAL:CG2	1:B:206:ALA:HA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:LYS:O	1:C:69:LYS:HG2	2.15	0.46
1:G:46:LEU:HD22	1:G:103:ILE:CD1	2.44	0.46
1:G:58:ASN:CG	1:G:62:TYR:HE2	2.18	0.46
1:H:188:VAL:HG13	1:H:358:ILE:HG12	1.97	0.46
1:B:165:ILE:HG23	1:B:274:LEU:HD23	1.97	0.46
1:C:77:GLU:OE2	1:D:84:ASN:ND2	2.42	0.46
1:G:145:LEU:HD11	1:G:318:ILE:HG12	1.98	0.46
1:H:191:VAL:HG21	1:H:213:VAL:CG1	2.45	0.46
1:A:448:VAL:HG22	1:B:437:GLU:HG2	1.97	0.46
1:D:121:ILE:HG22	1:D:292:LEU:HD21	1.97	0.46
1:E:171:ALA:HB2	1:E:275:LEU:HD13	1.97	0.46
1:F:90:GLU:OE2	1:F:94:THR:OG1	2.33	0.46
1:D:24:LYS:CG	1:D:336:ILE:HD12	2.46	0.46
1:C:452:HIS:O	1:C:453:LEU:HB2	2.16	0.46
1:D:259:GLU:HB2	1:D:264:GLY:O	2.15	0.46
1:G:289:LEU:N	3:G:503:SO4:O1	2.47	0.46
1:D:122:THR:HG21	1:D:128:THR:CG2	2.45	0.46
1:H:33:VAL:HG22	1:H:113:VAL:CG2	2.46	0.46
1:B:304:VAL:CG1	1:B:308:PHE:HA	2.46	0.45
1:C:3:GLN:N	1:C:4:PRO:CD	2.78	0.45
1:D:126:GLN:OE1	1:D:140:ASP:OD1	2.34	0.45
1:F:51:ILE:HB	1:F:52:PRO:HD3	1.98	0.45
1:E:139:ILE:HG23	1:E:139:ILE:O	2.16	0.45
1:E:282:PRO:HG3	1:E:301:ARG:HG3	1.98	0.45
1:E:445:ILE:HG21	1:E:459:PHE:CE2	2.52	0.45
1:A:77:GLU:OE1	1:B:82:ARG:NH2	2.48	0.45
1:C:121:ILE:HG21	1:C:292:LEU:HD11	1.98	0.45
1:E:36:GLU:OE2	2:E:501:FAD:O2B	2.25	0.45
1:B:158:ILE:HD11	1:B:246:ALA:N	2.32	0.45
1:E:420:ILE:HD13	1:E:428:MET:HB3	1.98	0.45
1:F:226:PHE:CZ	1:F:230:LEU:HD11	2.51	0.45
1:G:46:LEU:CD2	1:G:103:ILE:HD11	2.46	0.45
1:G:153:THR:HG22	1:G:281:ARG:CG	2.45	0.45
1:G:258:ILE:HD12	1:G:258:ILE:C	2.37	0.45
1:B:166:VAL:HG23	1:B:170:GLY:HA3	1.99	0.45
1:D:187:GLY:O	1:D:191:VAL:HG23	2.17	0.45
1:F:251:ASP:OD1	1:F:251:ASP:O	2.34	0.45
1:D:165:ILE:HG12	1:D:254:ILE:HD13	1.98	0.45
1:B:166:VAL:HG21	1:B:170:GLY:C	2.37	0.45
1:B:207:VAL:HG22	1:B:238:LYS:HB2	1.98	0.45
1:D:122:THR:HG23	1:D:128:THR:OG1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:452:HIS:O	1:E:453:LEU:HB2	2.15	0.45
1:A:431:GLU:OE2	1:A:450:HIS:HE1	1.99	0.44
1:A:175:LYS:N	1:A:175:LYS:HD2	2.33	0.44
1:A:20:VAL:HG11	1:A:332[B]:GLU:HG3	1.98	0.44
1:A:84:ASN:ND2	1:B:77:GLU:OE2	2.45	0.44
1:B:158:ILE:HD11	1:B:246:ALA:H	1.82	0.44
1:E:452:HIS:ND1	1:E:453:LEU:HD23	2.32	0.44
1:F:292:LEU:HB3	1:F:312:ILE:HD11	1.99	0.44
1:A:25:ALA:HB2	1:A:339:VAL:CG2	2.48	0.44
1:G:274:LEU:HD23	1:G:274:LEU:C	2.38	0.44
1:E:174:LEU:HD11	1:E:273:VAL:HG11	1.99	0.44
1:A:451:ALA:H	1:B:430:ASN:ND2	2.15	0.44
1:D:166:VAL:HG21	1:D:170:GLY:CA	2.48	0.44
1:D:243:VAL:HG22	1:D:258:ILE:HG22	2.00	0.44
1:D:256:VAL:HB	1:D:269:ILE:HG13	1.98	0.44
1:D:122:THR:CG2	1:D:128:THR:HG23	2.48	0.44
1:F:452:HIS:ND1	1:F:453:LEU:HD23	2.32	0.44
1:H:7:ALA:O	1:H:141:THR:HA	2.18	0.44
1:H:231:GLN:HA	1:H:235:PHE:O	2.18	0.44
1:D:186:ALA:HB1	1:D:213:VAL:HG22	2.00	0.43
1:F:180:LYS:NZ	4:F:603:HOH:O	2.49	0.43
1:G:82:ARG:HB2	1:H:77:GLU:HB2	2.00	0.43
1:B:205:THR:HG23	1:B:236:LYS:HB2	2.00	0.43
1:B:304:VAL:HG12	1:B:308:PHE:HA	2.00	0.43
1:D:182:VAL:HG23	1:D:271:CYS:HB3	2.00	0.43
1:D:258:ILE:HD11	1:D:267:GLU:CD	2.38	0.43
1:E:145:LEU:HD11	1:E:318:ILE:HG12	1.99	0.43
1:F:70:ASP:OD1	1:F:74:ARG:NH2	2.51	0.43
1:F:182:VAL:HG23	1:F:271:CYS:HB3	1.99	0.43
1:F:444:ASP:O	1:F:448:VAL:HG23	2.19	0.43
1:A:77:GLU:HB3	1:B:82:ARG:NH2	2.34	0.43
1:E:451:ALA:H	1:F:430:ASN:HD21	1.65	0.43
1:G:92:LYS:NZ	1:G:172:LEU:O	2.45	0.43
2:H:501:FAD:HM83	4:H:607:HOH:O	2.17	0.43
1:A:225:ASN:N	1:A:225:ASN:HD22	2.17	0.43
1:D:265:LYS:H	1:D:265:LYS:HD3	1.83	0.43
1:E:299:ARG:NH2	3:E:503:SO4:O1	2.50	0.43
1:F:163:ASP:OD1	1:F:164:THR:HG23	2.18	0.43
1:G:78:MET:SD	1:H:78:MET:SD	3.16	0.43
1:B:158:ILE:CD1	1:B:246:ALA:HB3	2.43	0.43
1:D:137:GLN:OE1	1:D:138:VAL:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:THR:HG22	1:D:236:LYS:HB2	2.00	0.43
1:D:265:LYS:CD	1:D:265:LYS:H	2.32	0.43
1:E:120:LYS:HG2	1:E:121:ILE:N	2.33	0.43
1:E:389:ALA:HA	1:E:400:THR:HB	2.00	0.43
1:H:5:ILE:HD12	1:H:137:GLN:NE2	2.33	0.43
1:B:44:THR:O	1:B:49:GLY:N	2.52	0.43
1:D:125:ASN:OD1	1:D:314:ASN:ND2	2.51	0.43
1:E:63:TYR:HB2	1:F:76:ILE:HD13	2.01	0.43
1:G:166:VAL:HG21	1:G:170:GLY:CA	2.41	0.43
1:D:124:LYS:HD2	1:D:124:LYS:N	2.34	0.43
1:D:321:VAL:O	1:D:321:VAL:HG22	2.19	0.43
1:B:312:ILE:HG22	1:B:314:ASN:OD1	2.19	0.43
1:E:92:LYS:NZ	1:E:172:LEU:O	2.39	0.43
1:G:406:ILE:HD13	1:G:462:ALA:HB3	2.01	0.43
1:A:382:LYS:CE	1:A:466:ALA:O	2.67	0.42
1:A:384:GLY:HA3	1:A:466:ALA:HB2	2.01	0.42
1:F:85:LEU:HD23	1:F:176:LYS:HA	2.01	0.42
1:G:77:GLU:OE1	1:H:84:ASN:ND2	2.39	0.42
1:E:402:GLY:HA3	1:E:421:LEU:O	2.18	0.42
1:G:50:CYS:HB3	1:H:453:LEU:HD12	2.00	0.42
1:G:406:ILE:N	1:G:406:ILE:HD12	2.34	0.42
1:A:19:TYR:CE1	1:A:103:ILE:HD12	2.55	0.42
1:G:452:HIS:O	1:G:453:LEU:HB2	2.19	0.42
1:A:426:GLY:O	1:A:429:VAL:HG12	2.18	0.42
1:C:472:ILE:HG21	1:D:20:VAL:HG22	2.02	0.42
1:D:188:VAL:HG23	1:D:358:ILE:HG12	2.00	0.42
1:E:207:VAL:HG23	1:E:241:THR:HB	2.02	0.42
1:H:43:GLY:HA2	2:H:501:FAD:O3B	2.19	0.42
1:D:179:GLU:HB2	1:D:272:ASP:OD2	2.19	0.42
1:E:4:PRO:HA	1:E:138:VAL:O	2.20	0.42
1:E:67:HIS:HA	1:E:81:VAL:HG21	2.02	0.42
1:F:7:ALA:O	1:F:141:THR:HA	2.19	0.42
1:F:20:VAL:CG1	1:F:336:ILE:HD11	2.50	0.42
1:A:382:LYS:HE3	1:A:466:ALA:O	2.19	0.42
1:B:302:ILE:O	1:B:304:VAL:HG23	2.20	0.42
1:D:247:THR:HG22	1:D:248:LYS:N	2.35	0.42
1:F:209:PHE:O	1:F:240:ASN:HA	2.20	0.42
1:F:258:ILE:C	1:F:259:GLU:HG3	2.39	0.42
1:B:144:ILE:HB	1:B:315:ILE:HG13	2.02	0.41
1:D:24:LYS:HB2	1:D:336:ILE:HD12	2.00	0.41
1:E:184:ILE:HD11	1:E:243:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:PRO:HB3	1:D:321:VAL:HA	2.01	0.41
1:C:452:HIS:ND1	1:C:453:LEU:HD23	2.36	0.41
1:D:245:GLY:C	1:D:257:SER:HG	2.23	0.41
1:D:393:ARG:HD3	1:D:453:LEU:O	2.19	0.41
1:A:121:ILE:HG21	1:A:292:LEU:HD11	2.02	0.41
1:D:125:ASN:HB3	1:D:141:THR:O	2.20	0.41
1:G:186:ALA:CB	1:G:208:GLU:HG2	2.51	0.41
1:G:299:ARG:NH2	1:G:301:ARG:HH22	2.18	0.41
1:B:183:VAL:HG23	1:B:206:ALA:HA	2.02	0.41
1:D:258:ILE:CD1	1:D:267:GLU:HG2	2.51	0.41
1:G:435:ALA:HB1	1:G:445:ILE:HD11	2.02	0.41
1:A:54:LYS:HG2	1:B:453:LEU:HD13	2.02	0.41
1:B:122:THR:OG1	1:B:128:THR:HG23	2.21	0.41
1:B:164:THR:HG21	1:B:248:LYS:HD2	2.03	0.41
1:B:318:ILE:HD13	1:B:335:GLY:CA	2.50	0.41
1:D:5:ILE:CG2	1:D:6:ASP:N	2.81	0.41
1:G:84:ASN:HB2	1:H:77:GLU:OE2	2.20	0.41
1:H:33:VAL:HG22	1:H:113:VAL:HG22	2.02	0.41
1:H:182:VAL:HG23	1:H:271:CYS:HB3	2.02	0.41
1:A:250:SER:OG	1:F:344:GLY:O	2.24	0.41
1:C:108:LYS:NZ	3:C:506:SO4:O4	2.32	0.41
1:C:431:GLU:OE2	1:C:450:HIS:HE1	2.04	0.41
1:F:80:GLU:O	1:F:80:GLU:HG3	2.21	0.41
1:F:402:GLY:HA3	1:F:421:LEU:O	2.21	0.41
1:F:452:HIS:O	1:F:453:LEU:HB2	2.19	0.41
1:C:472:ILE:HD12	1:D:20:VAL:HG13	2.03	0.41
1:D:5:ILE:CG2	1:D:6:ASP:H	2.33	0.41
1:D:8:ASP:OD1	1:D:31:LYS:CB	2.69	0.41
1:E:256:VAL:HG22	1:E:274:LEU:HD12	2.02	0.41
1:A:198:GLN:NE2	1:A:233:GLN:O	2.54	0.41
1:A:226:PHE:CZ	1:A:230:LEU:HD11	2.56	0.41
1:B:179:GLU:HB3	1:B:272:ASP:OD2	2.21	0.41
1:F:393:ARG:HD3	1:F:453:LEU:O	2.20	0.41
1:G:231:GLN:HA	1:G:235:PHE:O	2.21	0.41
1:G:402:GLY:HA3	1:G:421:LEU:O	2.20	0.41
1:G:444:ASP:O	1:G:448:VAL:HG23	2.21	0.41
1:A:51:ILE:HD12	1:A:99:LEU:CD1	2.51	0.41
1:A:77:GLU:OE2	1:B:84:ASN:ND2	2.39	0.41
1:B:10:THR:HG21	1:B:127:VAL:HG21	2.02	0.41
2:C:501:FAD:H9	2:C:501:FAD:H1'1	1.88	0.41
1:F:307:ARG:HH21	1:F:341:GLY:C	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:409:GLN:HG2	1:H:416:LEU:HD21	2.02	0.41
1:B:389:ALA:HA	1:B:400:THR:HB	2.03	0.40
1:C:19:TYR:CE1	1:C:103:ILE:HD12	2.56	0.40
1:C:226:PHE:CZ	1:C:230:LEU:HD11	2.56	0.40
1:D:318:ILE:HD13	1:D:335:GLY:HA2	2.03	0.40
1:E:160:ILE:HG23	4:E:608:HOH:O	2.21	0.40
1:G:153:THR:OG1	1:G:278:ILE:CD1	2.69	0.40
1:H:164:THR:HB	1:H:254:ILE:HD11	2.02	0.40
1:C:282:PRO:HG3	1:C:301:ARG:HG3	2.03	0.40
1:E:5:ILE:HG22	1:E:6:ASP:N	2.36	0.40
1:G:43:GLY:HA2	2:G:501:FAD:O3B	2.21	0.40
1:G:160:ILE:HG23	1:G:166:VAL:HA	2.02	0.40
1:B:20:VAL:HG21	1:B:332[B]:GLU:HG3	2.03	0.40
1:C:389:ALA:HA	1:C:400:THR:HB	2.03	0.40
1:G:404:VAL:HG12	1:G:406:ILE:CD1	2.51	0.40
1:B:10:THR:HB	1:B:141:THR:HG21	2.04	0.40
1:C:309:GLN:HG2	1:C:316:TYR:CE2	2.56	0.40
1:D:309:GLN:HG2	1:D:316:TYR:CE2	2.57	0.40
1:B:205:THR:CG2	1:B:236:LYS:HB2	2.51	0.40
1:C:438:TYR:O	1:E:305:ASN:HB2	2.21	0.40
1:D:166:VAL:HG21	1:D:170:GLY:C	2.41	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	471/496 (95%)	464 (98%)	7 (2%)	0	100	100
1	B	471/496 (95%)	464 (98%)	7 (2%)	0	100	100
1	C	470/496 (95%)	461 (98%)	9 (2%)	0	100	100
1	D	470/496 (95%)	459 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	471/496 (95%)	459 (98%)	12 (2%)	0	100	100
1	F	470/496 (95%)	461 (98%)	9 (2%)	0	100	100
1	G	470/496 (95%)	459 (98%)	11 (2%)	0	100	100
1	H	470/496 (95%)	458 (97%)	12 (3%)	0	100	100
All	All	3763/3968 (95%)	3685 (98%)	78 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	373/390 (96%)	358 (96%)	15 (4%)	31	40
1	B	373/390 (96%)	363 (97%)	10 (3%)	44	55
1	C	372/390 (95%)	360 (97%)	12 (3%)	39	47
1	D	372/390 (95%)	360 (97%)	12 (3%)	39	47
1	E	373/390 (96%)	362 (97%)	11 (3%)	42	52
1	F	372/390 (95%)	358 (96%)	14 (4%)	33	41
1	G	372/390 (95%)	365 (98%)	7 (2%)	57	68
1	H	372/390 (95%)	365 (98%)	7 (2%)	57	68
All	All	2979/3120 (96%)	2891 (97%)	88 (3%)	41	50

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	TYR
1	A	50	CYS
1	A	54	LYS
1	A	78	MET
1	A	82	ARG
1	A	235	PHE

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Mol	Chain	Res	Type
1	A	265	LYS
1	A	275	LEU
1	A	278	ILE
1	A	301	ARG
1	A	339	VAL
1	A	369	LYS
1	A	380	GLU
1	A	403	MET
1	A	456	SER
1	B	19	TYR
1	B	50	CYS
1	B	54	LYS
1	B	87	LYS
1	B	152	VAL
1	B	184	ILE
1	B	191	VAL
1	B	205	THR
1	B	235	PHE
1	B	376	GLU
1	C	54	LYS
1	C	78	MET
1	C	203	ASP
1	C	235	PHE
1	C	254	ILE
1	C	267	GLU
1	C	299	ARG
1	C	301	ARG
1	C	339	VAL
1	C	382	LYS
1	C	395	LYS
1	C	456	SER
1	D	8	ASP
1	D	19	TYR
1	D	31	LYS
1	D	54	LYS
1	D	78	MET
1	D	128	THR
1	D	151	GLU
1	D	216	VAL
1	D	235	PHE
1	D	278	ILE
1	D	301	ARG

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Mol	Chain	Res	Type
1	D	369	LYS
1	E	50	CYS
1	E	54	LYS
1	E	78	MET
1	E	162	GLU
1	E	213	VAL
1	E	235	PHE
1	E	250	SER
1	E	258	ILE
1	E	333	ASP
1	E	379	ILE
1	E	470	LYS
1	F	19	TYR
1	F	50	CYS
1	F	54	LYS
1	F	65	MET
1	F	74	ARG
1	F	76	ILE
1	F	78	MET
1	F	103	ILE
1	F	213	VAL
1	F	235	PHE
1	F	262	SER
1	F	285	LYS
1	F	301	ARG
1	F	395	LYS
1	G	50	CYS
1	G	54	LYS
1	G	235	PHE
1	G	297	ASP
1	G	301	ARG
1	G	333	ASP
1	G	336	ILE
1	H	19	TYR
1	H	50	CYS
1	H	54	LYS
1	H	228	ARG
1	H	235	PHE
1	H	290	GLU
1	H	301	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	430	ASN
1	C	231	GLN
1	F	137	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

35 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	SO4	A	504	-	4,4,4	0.23	0	6,6,6	0.07	0
2	FAD	C	501	-	53,58,58	0.66	0	68,89,89	0.69	1 (1%)
2	FAD	F	501	-	53,58,58	0.56	0	68,89,89	0.60	1 (1%)
3	SO4	H	502	-	4,4,4	0.13	0	6,6,6	0.06	0
2	FAD	H	501	-	53,58,58	0.64	1 (1%)	68,89,89	0.60	1 (1%)
3	SO4	F	503	-	4,4,4	0.83	0	6,6,6	1.28	0
2	FAD	A	501	-	53,58,58	0.63	0	68,89,89	0.58	1 (1%)
3	SO4	C	502	-	4,4,4	0.26	0	6,6,6	0.30	0
3	SO4	C	506	-	4,4,4	0.33	0	6,6,6	0.28	0
3	SO4	B	502	-	4,4,4	0.13	0	6,6,6	0.11	0
3	SO4	H	503	-	4,4,4	0.08	0	6,6,6	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	D	502	-	4,4,4	0.16	0	6,6,6	0.11	0
3	SO4	G	504	-	4,4,4	0.17	0	6,6,6	0.17	0
3	SO4	D	505	-	4,4,4	0.13	0	6,6,6	0.14	0
3	SO4	D	504	-	4,4,4	0.20	0	6,6,6	0.08	0
3	SO4	E	502	-	4,4,4	0.16	0	6,6,6	0.11	0
3	SO4	A	506	-	4,4,4	0.16	0	6,6,6	0.10	0
3	SO4	E	503	-	4,4,4	0.17	0	6,6,6	0.16	0
2	FAD	B	501	-	53,58,58	0.56	0	68,89,89	0.63	2 (2%)
2	FAD	D	501	-	53,58,58	0.58	0	68,89,89	0.58	0
3	SO4	C	505	-	4,4,4	0.10	0	6,6,6	0.10	0
3	SO4	F	502	-	4,4,4	0.14	0	6,6,6	0.18	0
2	FAD	G	501	-	53,58,58	0.56	0	68,89,89	0.61	1 (1%)
3	SO4	C	507	-	4,4,4	0.18	0	6,6,6	0.12	0
2	FAD	E	501	-	53,58,58	0.55	0	68,89,89	0.55	0
3	SO4	C	504	-	4,4,4	0.17	0	6,6,6	0.13	0
3	SO4	C	503	-	4,4,4	0.13	0	6,6,6	0.11	0
3	SO4	B	503	-	4,4,4	0.20	0	6,6,6	0.14	0
3	SO4	G	502	-	4,4,4	0.15	0	6,6,6	0.20	0
3	SO4	D	503	-	4,4,4	0.12	0	6,6,6	0.09	0
3	SO4	E	504	-	4,4,4	0.21	0	6,6,6	0.07	0
3	SO4	A	502	-	4,4,4	0.12	0	6,6,6	0.34	0
3	SO4	A	503	-	4,4,4	0.21	0	6,6,6	0.22	0
3	SO4	A	505	-	4,4,4	0.17	0	6,6,6	0.15	0
3	SO4	G	503	-	4,4,4	0.15	0	6,6,6	0.09	0

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	C	501	-	-	2/30/50/50	0/6/6/6
2	FAD	B	501	-	-	2/30/50/50	0/6/6/6
2	FAD	F	501	-	-	2/30/50/50	0/6/6/6
2	FAD	D	501	-	-	2/30/50/50	0/6/6/6
2	FAD	H	501	-	-	4/30/50/50	0/6/6/6
2	FAD	G	501	-	-	3/30/50/50	0/6/6/6
2	FAD	E	501	-	-	3/30/50/50	0/6/6/6
2	FAD	A	501	-	-	2/30/50/50	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	FAD	P-O2P	-2.09	1.45	1.55

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FAD	C5A-C6A-N6A	2.85	124.69	120.35
2	B	501	FAD	P-O3P-PA	-2.65	123.73	132.83
2	F	501	FAD	C5A-C6A-N6A	2.18	123.67	120.35
2	C	501	FAD	O2'-C2'-C1'	2.13	114.95	109.80
2	B	501	FAD	C5A-C6A-N6A	2.10	123.54	120.35
2	G	501	FAD	C4'-C3'-C2'	-2.05	109.09	113.36
2	H	501	FAD	C5A-C6A-N6A	2.01	123.41	120.35

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	501	FAD	O4B-C4B-C5B-O5B
2	H	501	FAD	C5'-O5'-P-O1P
2	B	501	FAD	O4B-C4B-C5B-O5B
2	G	501	FAD	O4B-C4B-C5B-O5B
2	G	501	FAD	C3B-C4B-C5B-O5B
2	H	501	FAD	O4B-C4B-C5B-O5B
2	E	501	FAD	C3B-C4B-C5B-O5B
2	H	501	FAD	C3B-C4B-C5B-O5B
2	B	501	FAD	C3B-C4B-C5B-O5B
2	G	501	FAD	O4'-C4'-C5'-O5'
2	A	501	FAD	PA-O3P-P-O5'
2	C	501	FAD	PA-O3P-P-O5'
2	E	501	FAD	PA-O3P-P-O5'
2	F	501	FAD	O4B-C4B-C5B-O5B
2	H	501	FAD	C5'-O5'-P-O3P
2	C	501	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	O4B-C4B-C5B-O5B
2	F	501	FAD	C3B-C4B-C5B-O5B
2	D	501	FAD	C3B-C4B-C5B-O5B

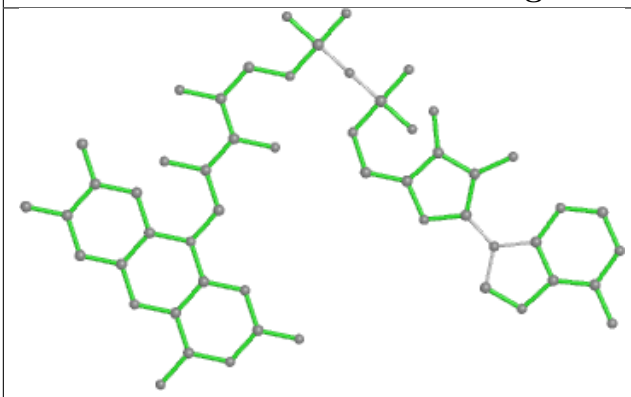
There are no ring outliers.

14 monomers are involved in 20 short contacts:

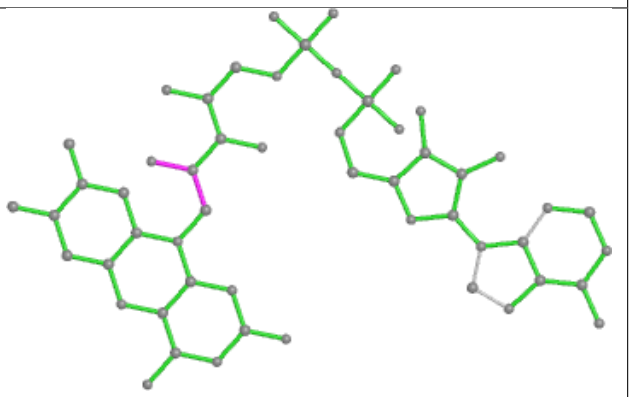
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	FAD	1	0
2	H	501	FAD	2	0
3	F	503	SO4	1	0
3	C	506	SO4	2	0
3	H	503	SO4	1	0
3	E	502	SO4	3	0
3	A	506	SO4	1	0
3	E	503	SO4	1	0
2	B	501	FAD	1	0
2	D	501	FAD	1	0
2	G	501	FAD	1	0
3	C	507	SO4	1	0
2	E	501	FAD	2	0
3	G	503	SO4	2	0

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.

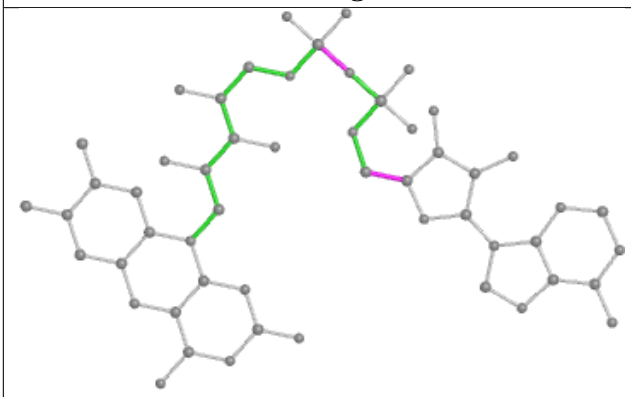
Ligand FAD C 501



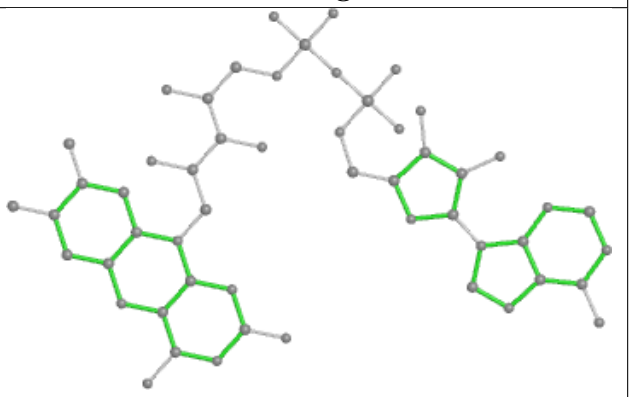
Bond lengths



Bond angles

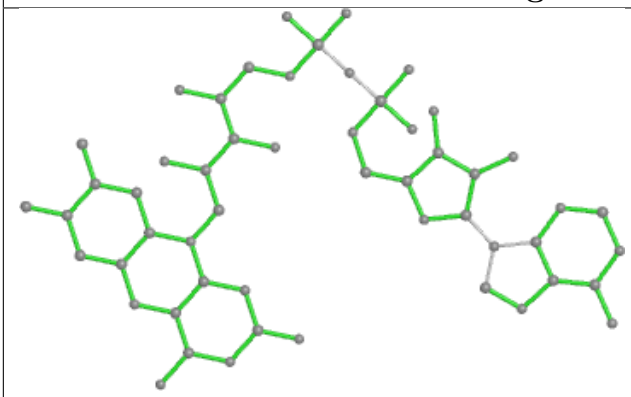


Torsions

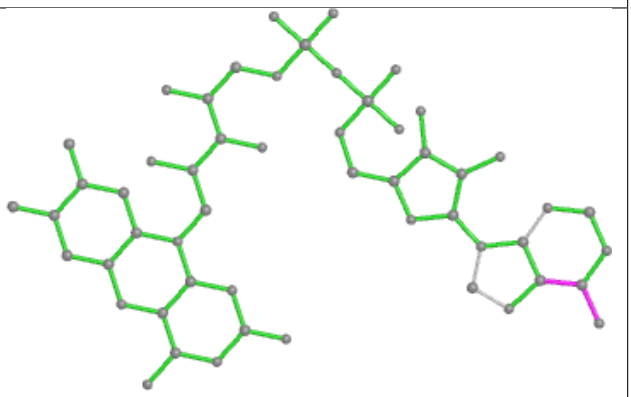


Rings

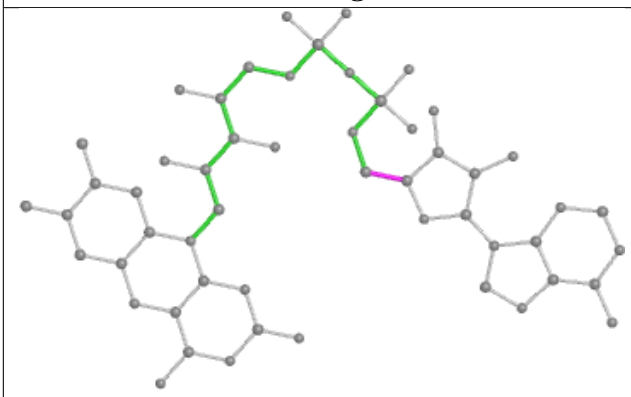
Ligand FAD F 501



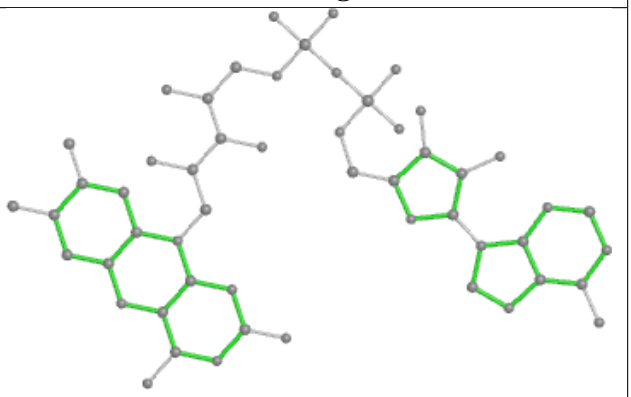
Bond lengths



Bond angles

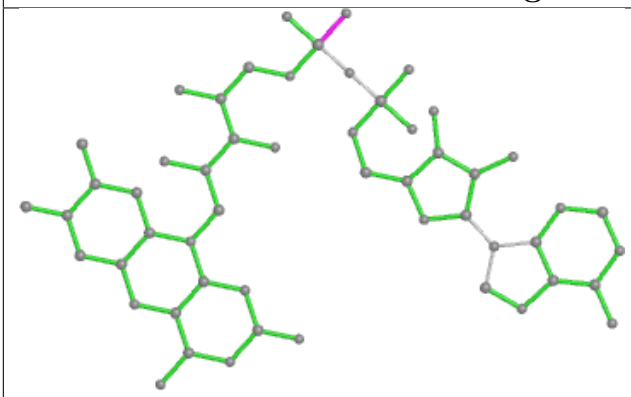


Torsions

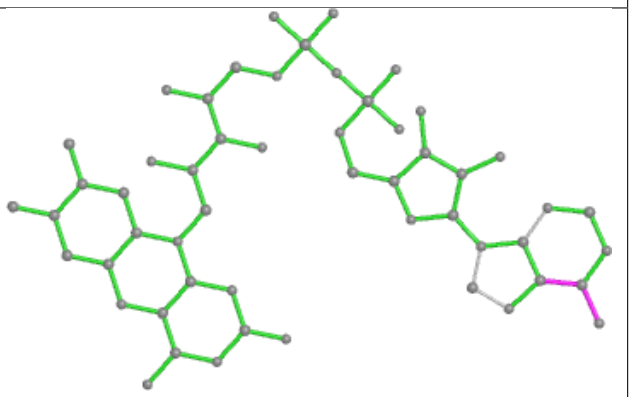


Rings

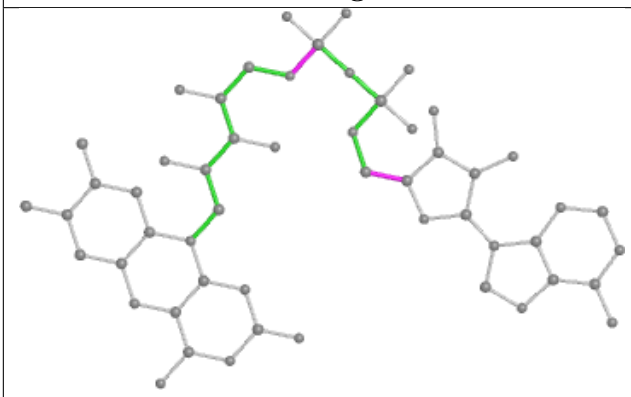
Ligand FAD H 501



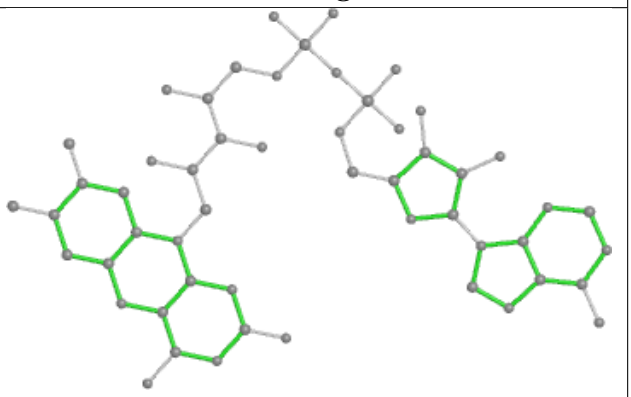
Bond lengths



Bond angles

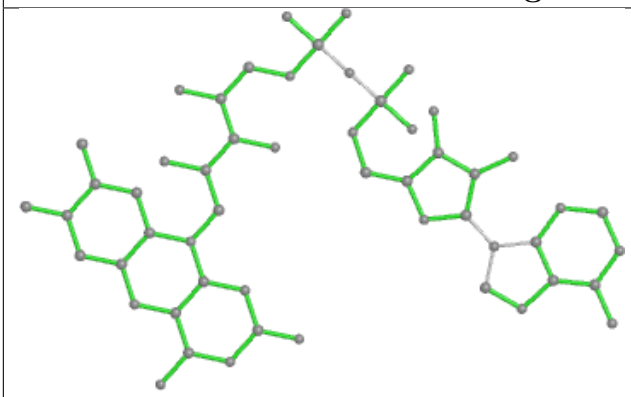


Torsions

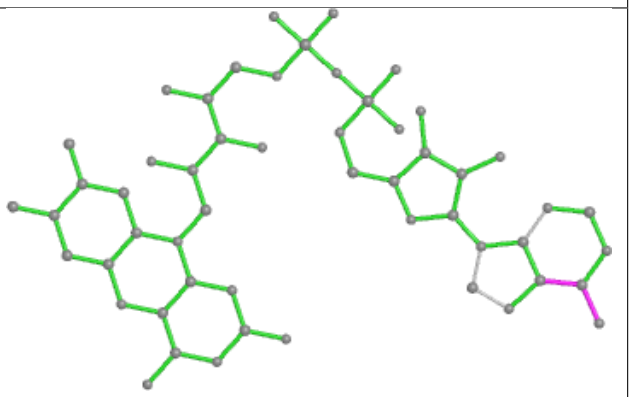


Rings

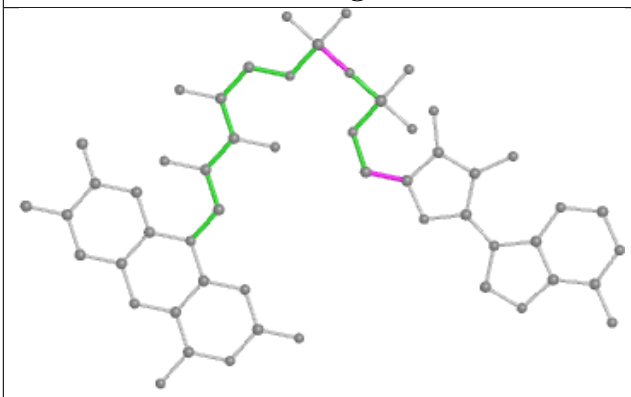
Ligand FAD A 501



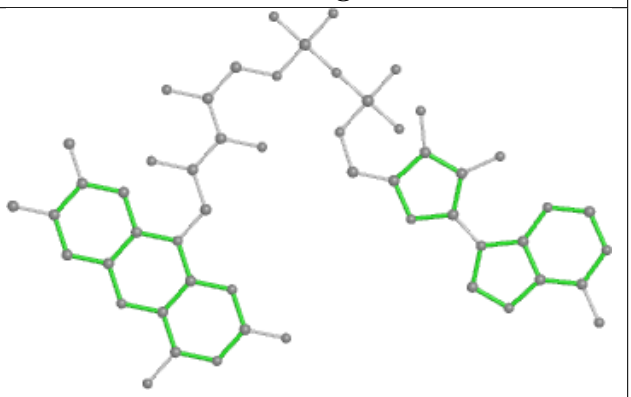
Bond lengths



Bond angles

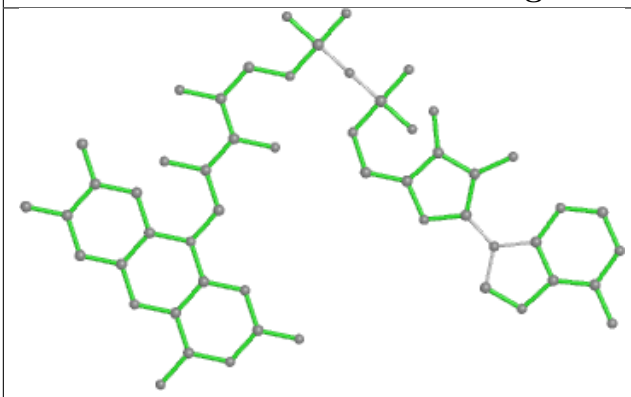


Torsions

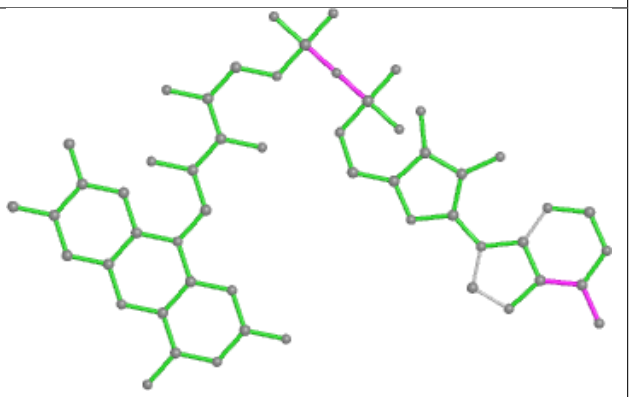


Rings

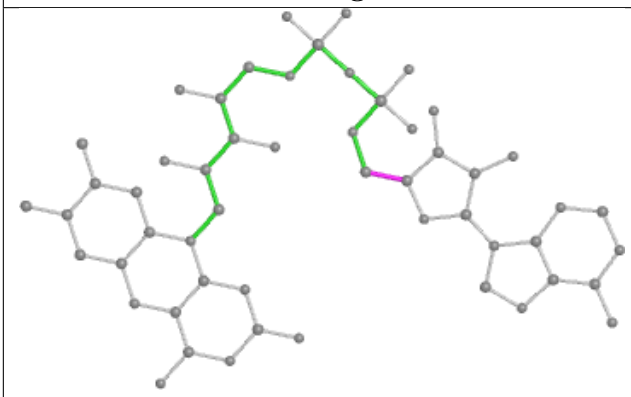
Ligand FAD B 501



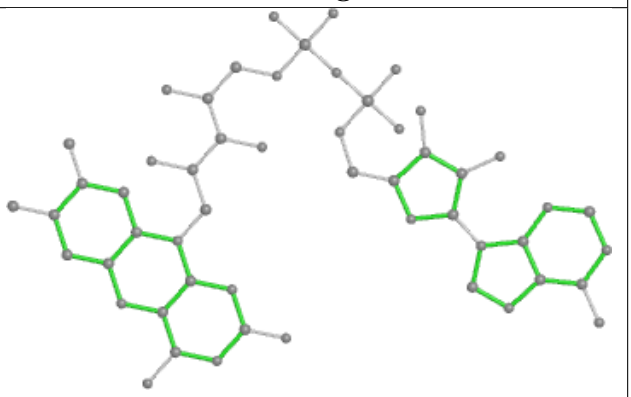
Bond lengths



Bond angles

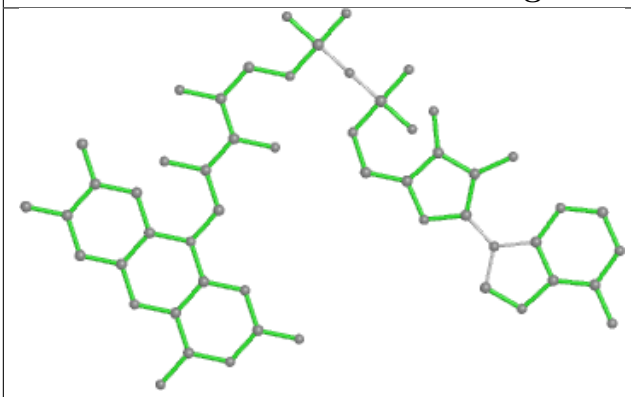


Torsions

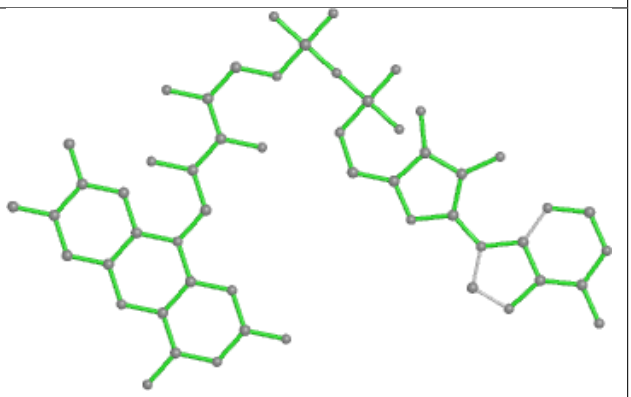


Rings

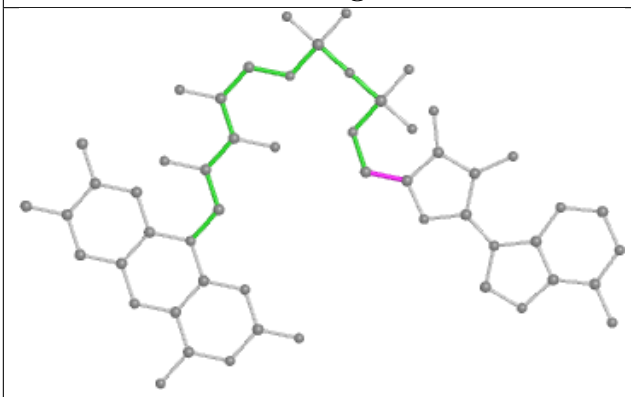
Ligand FAD D 501



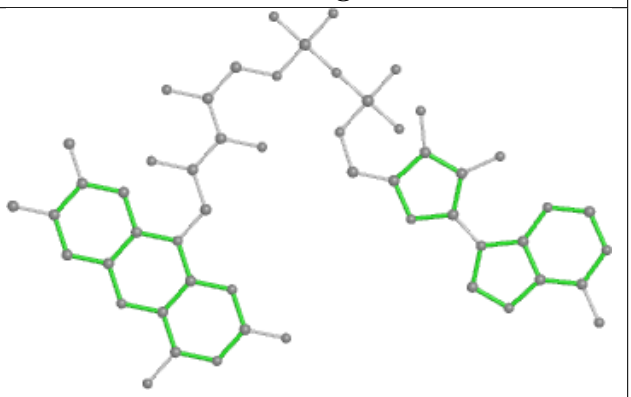
Bond lengths



Bond angles

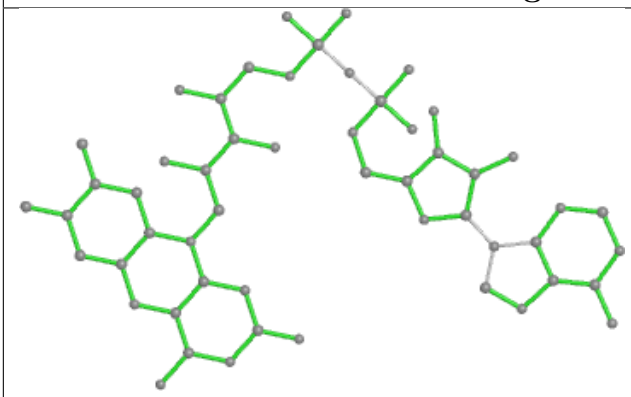


Torsions

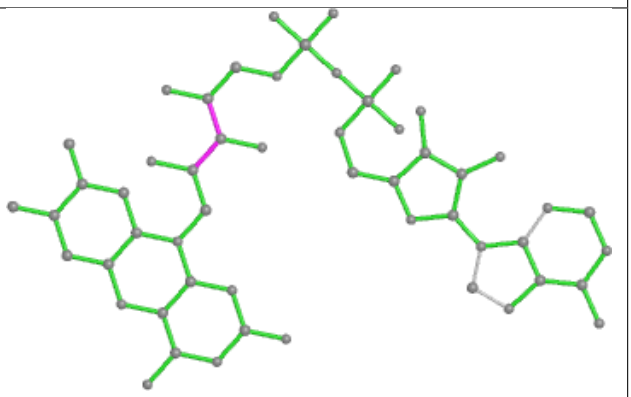


Rings

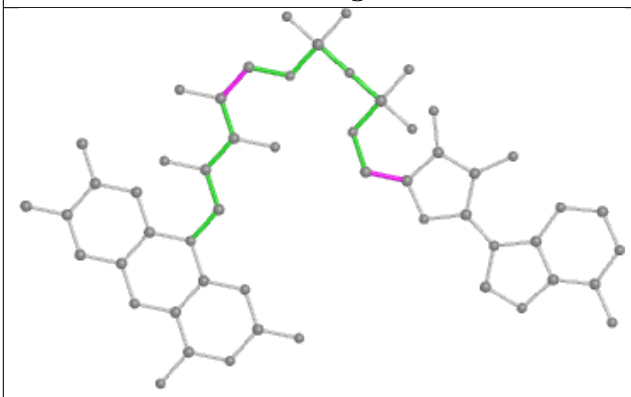
Ligand FAD G 501



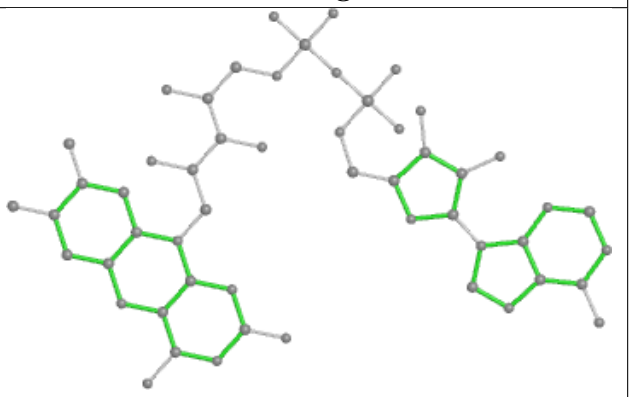
Bond lengths



Bond angles

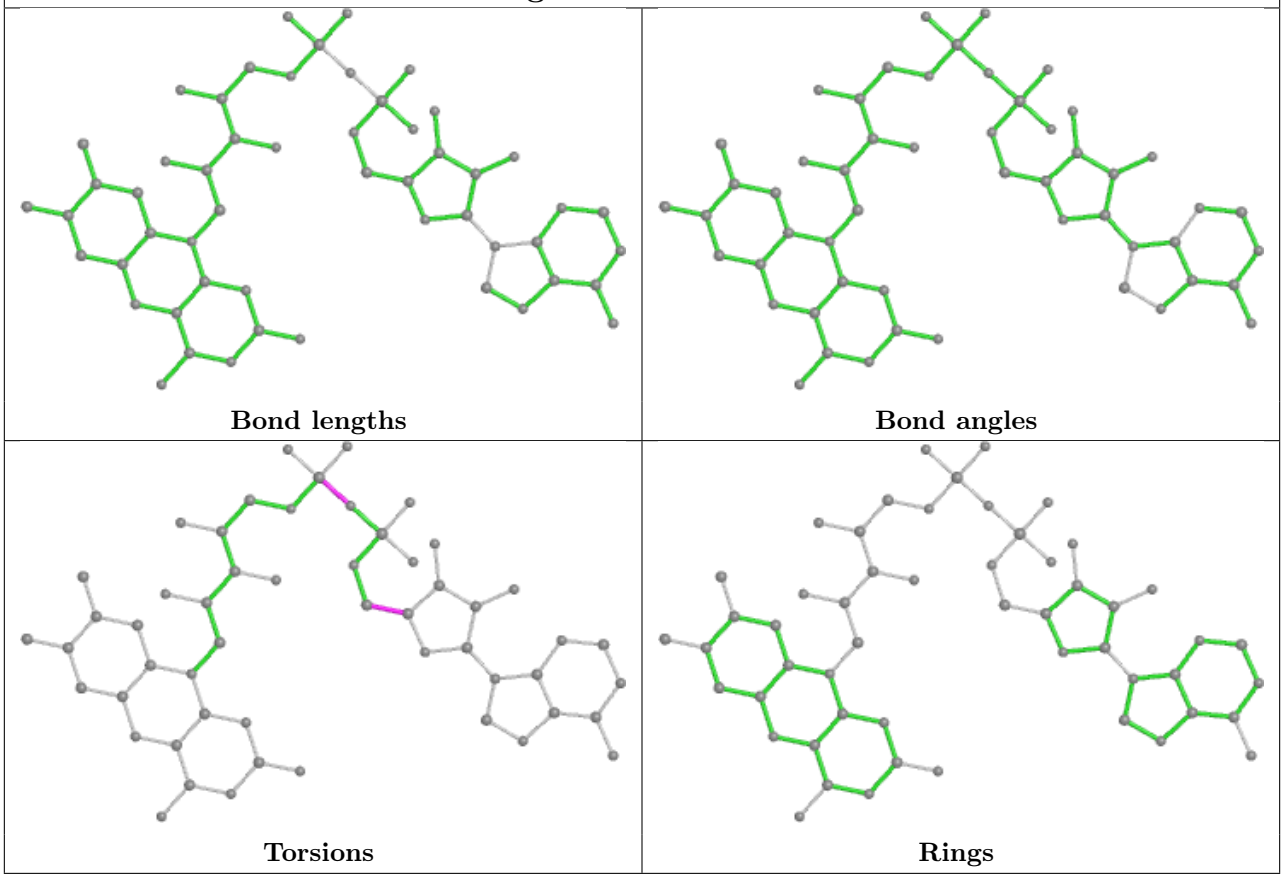


Torsions



Rings

Ligand FAD E 501



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	472/496 (95%)	0.08	0	100	100	23, 35, 58, 85	0
1	B	472/496 (95%)	0.53	30 (6%)	19	27	28, 64, 102, 132	0
1	C	472/496 (95%)	0.16	2 (0%)	92	96	23, 37, 61, 83	0
1	D	472/496 (95%)	0.68	50 (10%)	6	10	29, 67, 109, 134	0
1	E	472/496 (95%)	0.49	30 (6%)	19	27	32, 62, 97, 124	0
1	F	472/496 (95%)	0.52	28 (5%)	22	31	37, 61, 94, 124	0
1	G	472/496 (95%)	0.46	21 (4%)	34	45	32, 61, 97, 123	0
1	H	472/496 (95%)	0.51	28 (5%)	22	31	32, 59, 97, 130	0
All	All	3776/3968 (95%)	0.43	189 (5%)	28	39	23, 56, 97, 134	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	268	VAL	7.6
1	F	132	ALA	7.1
1	D	246	ALA	5.9
1	D	247	THR	5.3
1	F	259	GLU	5.0
1	E	243	VAL	4.7
1	D	139	ILE	4.6
1	H	252	GLY	4.4
1	D	252	GLY	4.2
1	F	287	LEU	4.2
1	D	294	ILE	4.1
1	E	183	VAL	4.1
1	D	159	THR	4.0
1	D	250	SER	4.0
1	B	294	ILE	4.0
1	D	287	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	239	LEU	3.9
1	H	124	LYS	3.9
1	B	246	ALA	3.8
1	G	209	PHE	3.7
1	D	256	VAL	3.7
1	E	259	GLU	3.7
1	D	12	ILE	3.6
1	H	82	ARG	3.6
1	B	119	GLY	3.6
1	H	264	GLY	3.6
1	E	252	GLY	3.5
1	B	291	GLU	3.5
1	G	254	ILE	3.4
1	D	184	ILE	3.4
1	G	183	VAL	3.4
1	F	276	VAL	3.4
1	E	263	GLY	3.4
1	B	247	THR	3.4
1	F	12	ILE	3.4
1	G	62	TYR	3.3
1	E	160	ILE	3.3
1	B	145	LEU	3.3
1	H	278	ILE	3.2
1	H	269	ILE	3.2
1	B	256	VAL	3.1
1	D	265	LYS	3.1
1	D	119	GLY	3.1
1	D	267	GLU	3.1
1	B	250	SER	3.1
1	H	243	VAL	3.1
1	D	289	LEU	3.1
1	G	244	THR	3.1
1	H	247	THR	3.1
1	F	258	ILE	3.1
1	E	246	ALA	3.1
1	D	182	VAL	3.0
1	H	3	GLN	3.0
1	B	274	LEU	3.0
1	B	284	THR	3.0
1	D	296	LEU	3.0
1	F	261	ALA	3.0
1	E	254	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	287	LEU	2.9
1	D	257	SER	2.9
1	E	244	THR	2.9
1	G	238	LYS	2.9
1	E	184	ILE	2.9
1	H	175	LYS	2.9
1	B	139	ILE	2.8
1	B	120	LYS	2.8
1	B	35	ILE	2.8
1	D	136	THR	2.8
1	F	5	ILE	2.8
1	F	247	THR	2.8
1	G	154	PRO	2.8
1	E	239	LEU	2.8
1	B	182	VAL	2.8
1	G	246	ALA	2.8
1	D	286	ASN	2.8
1	F	136	THR	2.8
1	D	122	THR	2.8
1	D	35	ILE	2.8
1	C	228	ARG	2.8
1	H	271	CYS	2.7
1	G	263	GLY	2.7
1	E	83	LEU	2.7
1	D	130	THR	2.7
1	E	247	THR	2.7
1	D	336	ILE	2.7
1	B	318	ILE	2.7
1	E	62	TYR	2.7
1	E	237	PHE	2.7
1	F	96	VAL	2.7
1	H	155	PHE	2.7
1	E	79	SER	2.6
1	D	333	ASP	2.6
1	F	121	ILE	2.6
1	D	243	VAL	2.6
1	G	252	GLY	2.6
1	D	269	ILE	2.6
1	E	258	ILE	2.6
1	F	269	ILE	2.6
1	B	301	ARG	2.6
1	H	253	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	144	ILE	2.6
1	H	254	ILE	2.6
1	D	255	ASP	2.6
1	B	257	SER	2.6
1	B	269	ILE	2.6
1	C	379	ILE	2.6
1	D	146	ILE	2.6
1	F	294	ILE	2.6
1	F	175	LYS	2.5
1	G	248	LYS	2.5
1	H	4	PRO	2.5
1	B	135	GLY	2.5
1	D	156	PRO	2.5
1	D	248	LYS	2.5
1	F	135	GLY	2.5
1	H	239	LEU	2.5
1	F	182	VAL	2.4
1	D	249	LYS	2.4
1	F	265	LYS	2.4
1	E	296	LEU	2.4
1	D	115	VAL	2.4
1	D	121	ILE	2.4
1	G	275	LEU	2.4
1	B	268	VAL	2.4
1	H	248	LYS	2.4
1	E	228	ARG	2.4
1	F	242	LYS	2.4
1	G	30	PHE	2.4
1	G	213	VAL	2.4
1	E	248	LYS	2.4
1	D	127	VAL	2.4
1	E	155	PHE	2.4
1	G	184	ILE	2.3
1	D	261	ALA	2.3
1	H	246	ALA	2.3
1	H	263	GLY	2.3
1	B	165	ILE	2.3
1	H	258	ILE	2.3
1	D	239	LEU	2.3
1	E	275	LEU	2.3
1	H	181	MET	2.3
1	B	348	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	276	VAL	2.3
1	E	124	LYS	2.2
1	E	262	SER	2.2
1	D	160	ILE	2.2
1	F	82	ARG	2.2
1	G	264	GLY	2.2
1	F	348	HIS	2.2
1	H	276	VAL	2.2
1	D	135	GLY	2.2
1	E	191	VAL	2.2
1	E	213	VAL	2.2
1	B	117	GLY	2.2
1	D	209	PHE	2.2
1	B	261	ALA	2.2
1	H	121	ILE	2.2
1	H	184	ILE	2.2
1	D	161	ASP	2.2
1	F	80	GLU	2.1
1	F	239	LEU	2.1
1	E	245	GLY	2.1
1	B	127	VAL	2.1
1	D	376	GLU	2.1
1	B	130	THR	2.1
1	D	124	LYS	2.1
1	F	255	ASP	2.1
1	G	247	THR	2.1
1	H	129	ALA	2.1
1	H	287	LEU	2.1
1	D	348	HIS	2.1
1	E	289	LEU	2.1
1	F	311	LYS	2.1
1	F	251	ASP	2.1
1	G	242	LYS	2.1
1	E	139	ILE	2.0
1	F	472	ILE	2.0
1	G	5	ILE	2.0
1	E	72	ALA	2.0
1	G	201	GLY	2.0
1	H	250	SER	2.0
1	D	183	VAL	2.0
1	D	351	TYR	2.0
1	D	258	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	379	ILE	2.0
1	H	119	GLY	2.0
1	B	209	PHE	2.0
1	G	222	ILE	2.0
1	F	78	MET	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	SO4	E	503	5/5	0.78	0.16	105,105,106,108	0
3	SO4	G	504	5/5	0.82	0.17	94,94,96,96	0
3	SO4	C	506	5/5	0.84	0.21	56,63,70,70	0
3	SO4	A	505	5/5	0.87	0.17	80,82,83,83	0
3	SO4	G	502	5/5	0.89	0.19	89,89,92,93	0
3	SO4	F	503	5/5	0.89	0.15	50,53,57,57	5
3	SO4	C	503	5/5	0.90	0.17	74,75,76,77	0
3	SO4	C	507	5/5	0.90	0.17	41,42,44,46	5
3	SO4	D	505	5/5	0.91	0.14	51,53,56,57	5
3	SO4	B	503	5/5	0.91	0.13	96,97,98,99	0
3	SO4	G	503	5/5	0.91	0.15	90,105,107,108	0
3	SO4	E	504	5/5	0.91	0.13	84,84,86,87	0
3	SO4	D	502	5/5	0.92	0.14	100,100,101,101	0
3	SO4	A	506	5/5	0.92	0.12	75,88,90,90	0
3	SO4	E	502	5/5	0.92	0.10	80,97,99,99	0
3	SO4	B	502	5/5	0.93	0.14	97,98,98,100	0
2	FAD	D	501	53/53	0.93	0.16	42,64,81,84	0
2	FAD	B	501	53/53	0.94	0.15	42,58,74,78	0

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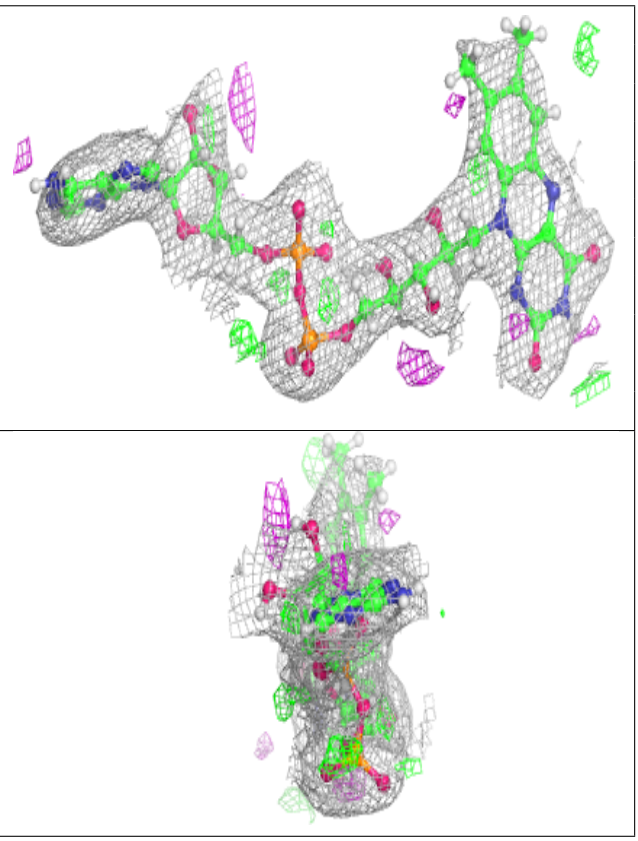
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	E	501	53/53	0.94	0.15	28,56,84,88	0
2	FAD	F	501	53/53	0.94	0.15	36,54,68,76	0
2	FAD	H	501	53/53	0.94	0.14	39,55,67,71	0
3	SO4	D	503	5/5	0.94	0.10	98,98,98,99	0
3	SO4	D	504	5/5	0.94	0.14	82,83,85,85	0
3	SO4	C	502	5/5	0.94	0.18	66,66,67,67	0
2	FAD	G	501	53/53	0.95	0.13	29,53,66,68	0
3	SO4	A	503	5/5	0.95	0.13	64,64,65,67	0
3	SO4	C	504	5/5	0.95	0.12	82,82,84,84	0
3	SO4	F	502	5/5	0.95	0.12	83,84,84,85	0
3	SO4	H	502	5/5	0.95	0.14	90,91,93,93	0
2	FAD	C	501	53/53	0.97	0.16	17,26,36,38	0
2	FAD	A	501	53/53	0.97	0.16	15,26,34,40	0
3	SO4	C	505	5/5	0.97	0.10	73,74,76,78	0
3	SO4	H	503	5/5	0.97	0.12	49,53,55,60	5
3	SO4	A	502	5/5	0.99	0.15	47,48,49,51	0
3	SO4	A	504	5/5	0.99	0.10	65,67,70,72	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.

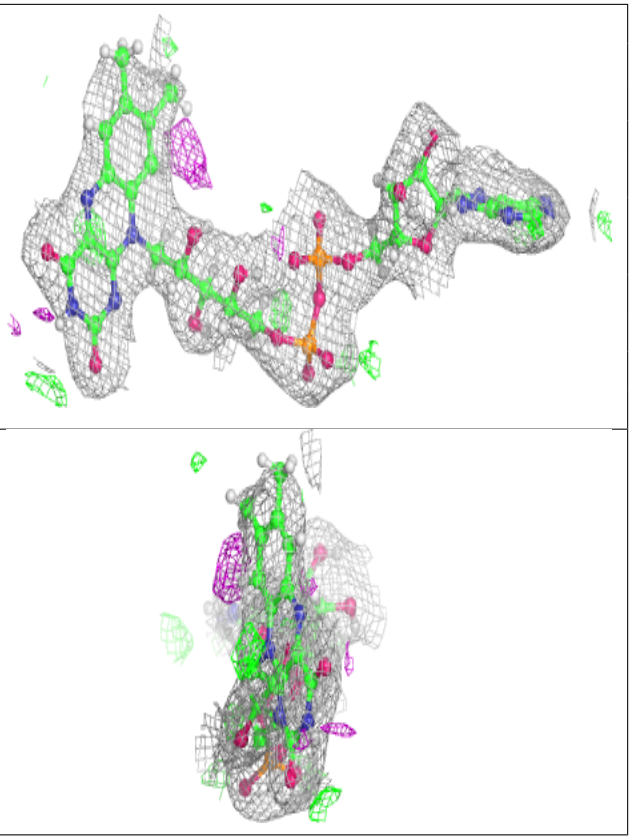
Electron density around FAD D 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



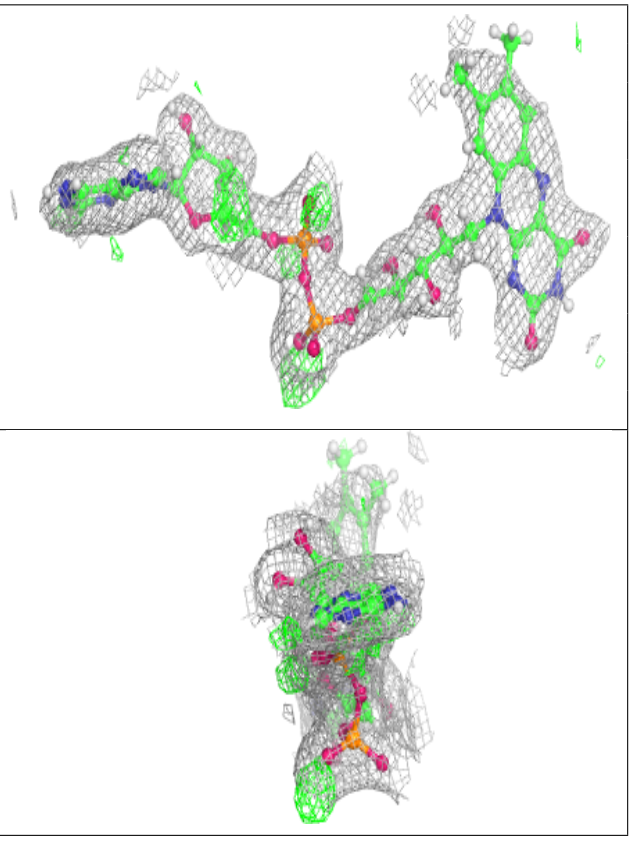
Electron density around FAD B 501:

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



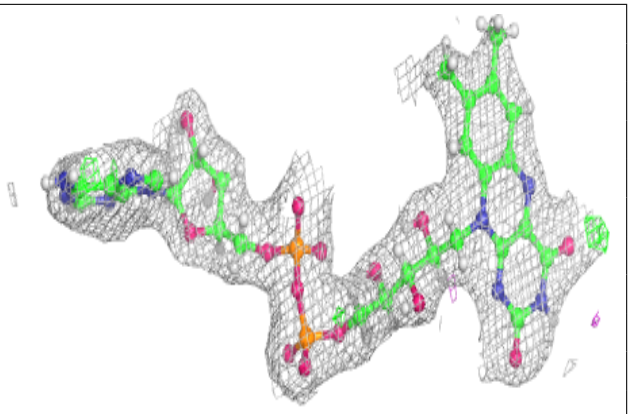
Electron density around FAD E 501:

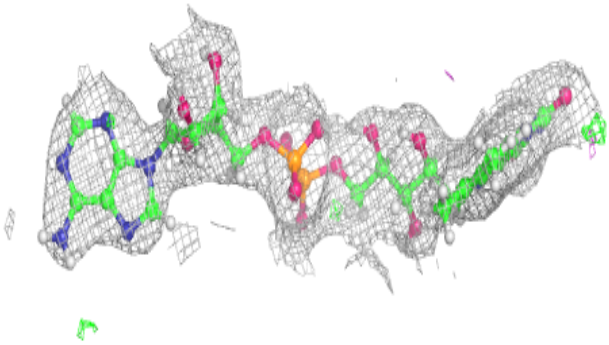
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

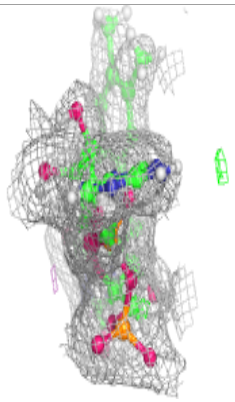


Electron density around FAD F 501:

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

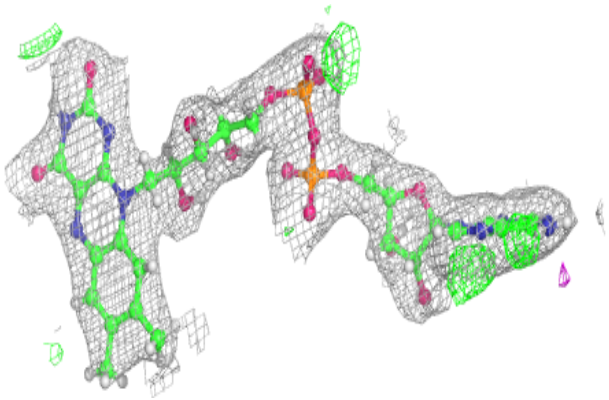


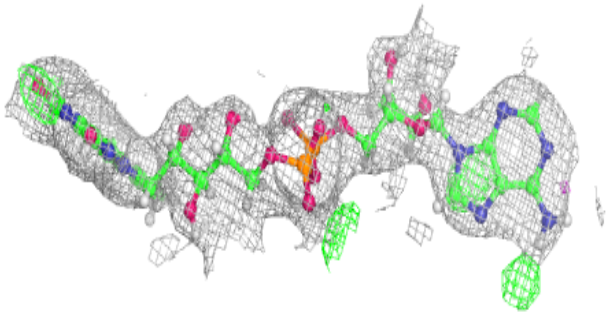


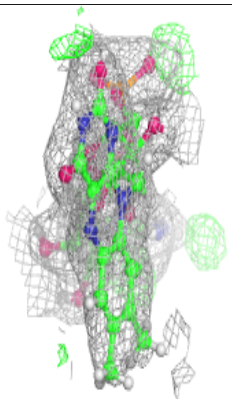


Electron density around FAD H 501:

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

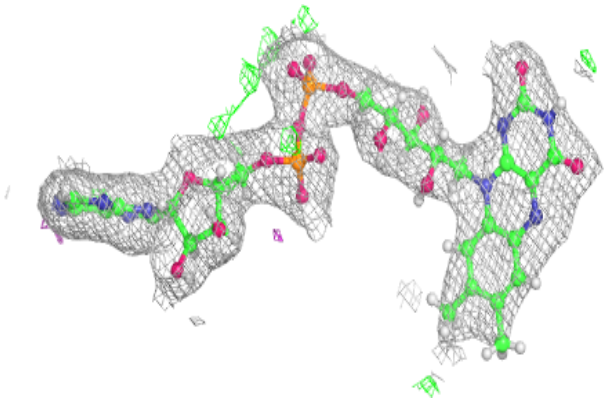


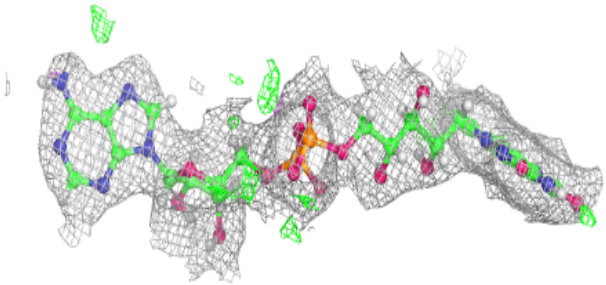


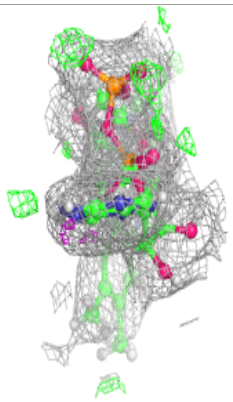


Electron density around FAD G 501:

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

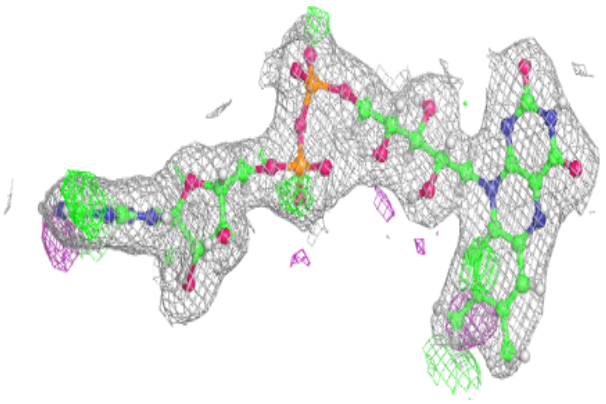


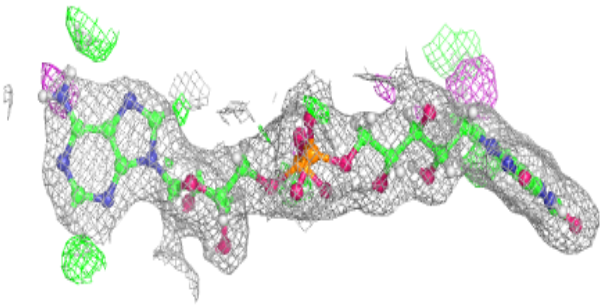


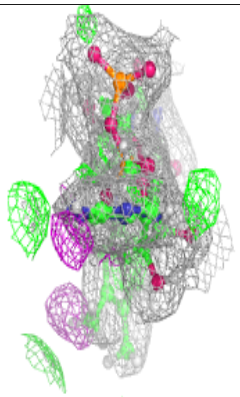


Electron density around FAD C 501:

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

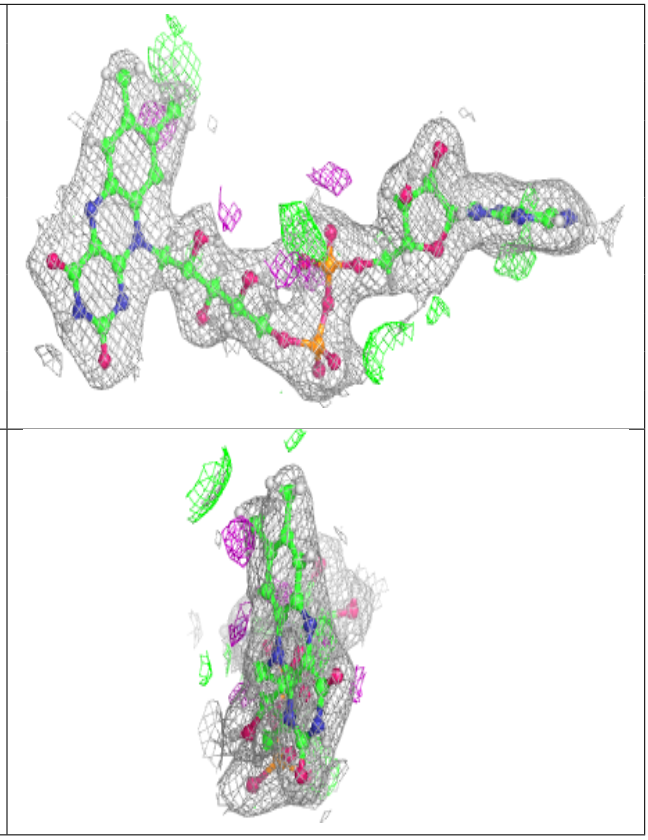






Electron density around FAD A 501:

$2mF_o$-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.