Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 10:34 AM EDT

PDB ID	:	6ECI
Title	:	Structure of the FAD binding protein MSMEG_5243 from Mycobacterium smegmatis
Authors	:	Ahmed, F.H.; Antoney, J.; Carr, P.D.; Jackson, C.J.
Deposited on	:	2018-08-07
Resolution	:	2.69 Å(reported)

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

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

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

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

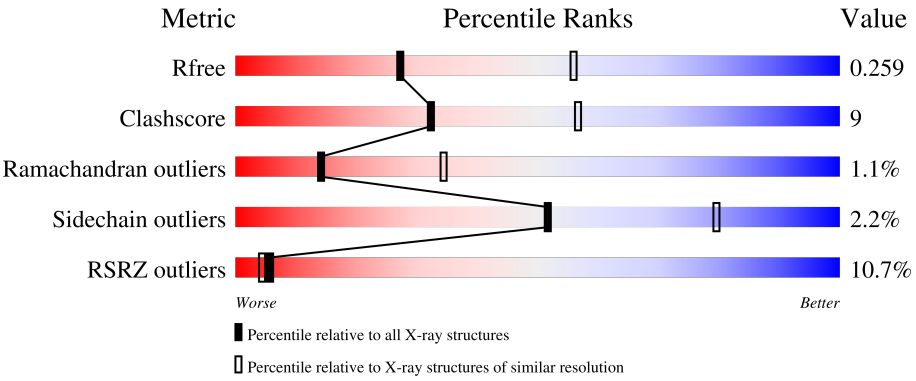
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.69 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	132	4% 78% 14% • 8%
1	B	132	6% 73% 20% • 5%
1	C	132	11% 80% 15% • •
1	D	132	9% 76% 19% • 5%
1	E	132	8% 73% 19% • 6%

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Mol	Chain	Length	Quality of chain
1	F	132	16% 81% 7% 10%
1	G	132	11% 67% 15% 18%
1	H	132	5% 67% 22% 9%
1	I	132	9% 68% 18% 13%
1	J	132	11% 80% 17%
1	K	132	8% 82% 14%
1	L	132	17% 75% 20% 5%
1	M	132	9% 73% 17% 9%
1	N	132	7% 80% 14% 5%
1	O	132	5% 70% 18% 9%
1	P	132	7% 85% 14%
1	Q	132	11% 70% 17% 12%
1	R	132	13% 64% 16% 17%
1	S	132	9% 60% 27% 11%
1	T	132	20% 64% 21% 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20506 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 Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	0	0
			966	611	177	177	1			
1	B	126	Total	C	N	O	S	0	1	0
			1005	635	183	186	1			
1	C	128	Total	C	N	O	S	0	1	0
			1019	645	185	188	1			
1	D	126	Total	C	N	O	S	0	3	0
			1008	636	186	185	1			
1	E	124	Total	C	N	O	S	0	0	0
			981	619	180	181	1			
1	F	119	Total	C	N	O	S	0	0	0
			942	592	173	176	1			
1	G	108	Total	C	N	O	S	0	0	0
			854	539	158	156	1			
1	H	120	Total	C	N	O	S	0	0	0
			957	605	176	175	1			
1	I	115	Total	C	N	O	S	0	0	0
			911	571	169	170	1			
1	J	130	Total	C	N	O	S	0	1	0
			1028	650	187	190	1			
1	K	127	Total	C	N	O	S	0	0	0
			1004	636	183	184	1			
1	L	126	Total	C	N	O	S	0	0	0
			996	630	182	183	1			
1	M	120	Total	C	N	O	S	0	0	0
			952	602	174	175	1			
1	N	125	Total	C	N	O	S	0	0	0
			988	625	180	182	1			
1	O	120	Total	C	N	O	S	0	0	0
			959	608	175	175	1			
1	P	132	Total	C	N	O	S	0	1	0
			1043	658	189	195	1			

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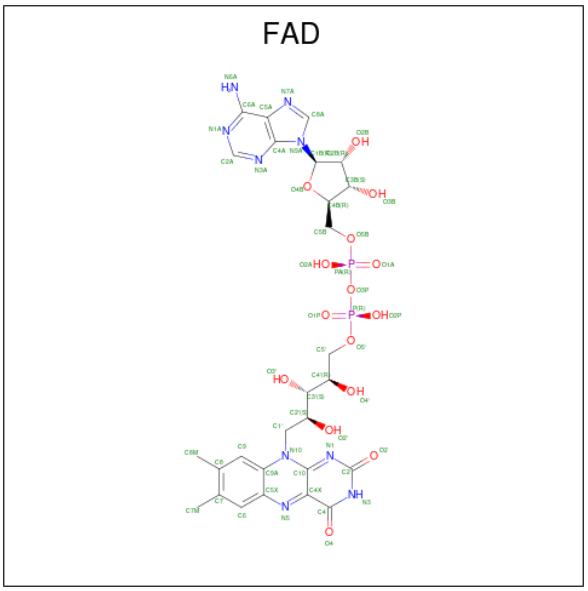
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	116	Total	C	N	O	S	0	1	0
			926	582	171	172	1			
1	R	109	Total	C	N	O	S	0	0	0
			865	548	159	157	1			
1	S	117	Total	C	N	O	S	0	1	0
			938	589	175	173	1			
1	T	113	Total	C	N	O	S	0	0	0
			902	571	167	163	1			

- 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
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	L	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	N	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	N	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	O	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	Q	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	Q	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	S	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	S	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total	O	0	0
			36	36		
4	B	35	Total	O	0	0
			35	35		
4	C	29	Total	O	0	0
			29	29		
4	D	34	Total	O	0	0
			34	34		
4	E	20	Total	O	0	0
			20	20		
4	F	5	Total	O	0	0
			5	5		

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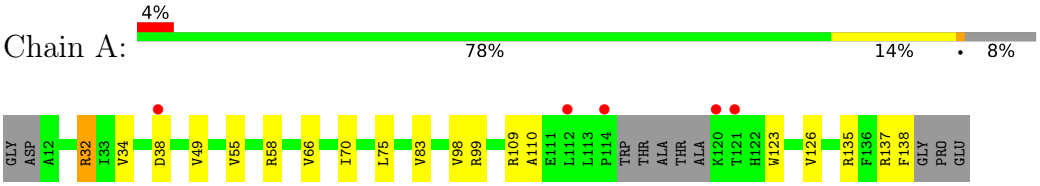
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	5	Total O 5 5	0	0
4	H	26	Total O 26 26	0	0
4	I	12	Total O 12 12	0	0
4	J	24	Total O 24 24	0	0
4	K	30	Total O 30 30	0	0
4	L	5	Total O 5 5	0	0
4	M	2	Total O 2 2	0	0
4	N	20	Total O 20 20	0	0
4	O	16	Total O 16 16	0	0
4	P	20	Total O 20 20	0	0
4	Q	7	Total O 7 7	0	0
4	R	11	Total O 11 11	0	0
4	S	14	Total O 14 14	0	0
4	T	9	Total O 9 9	0	0

3 Residue-property plots

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.

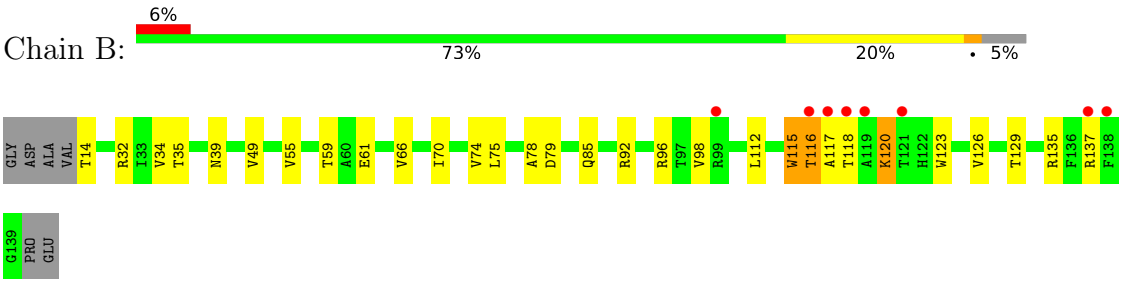
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain A:



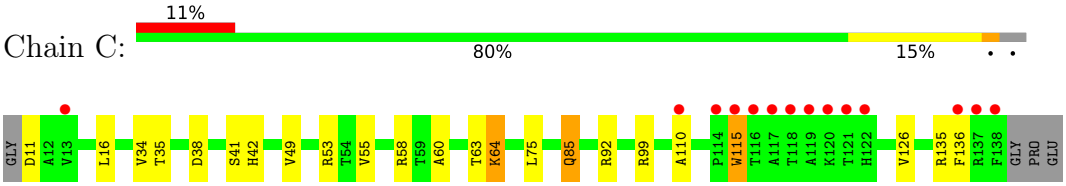
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain B:



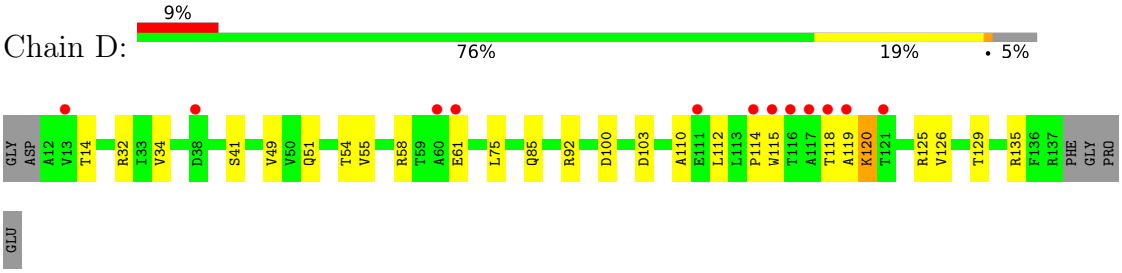
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain C:



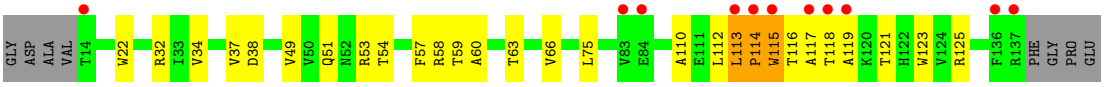
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain D:



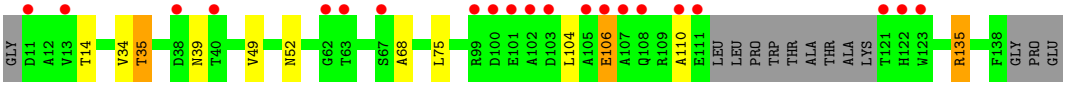
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain E:



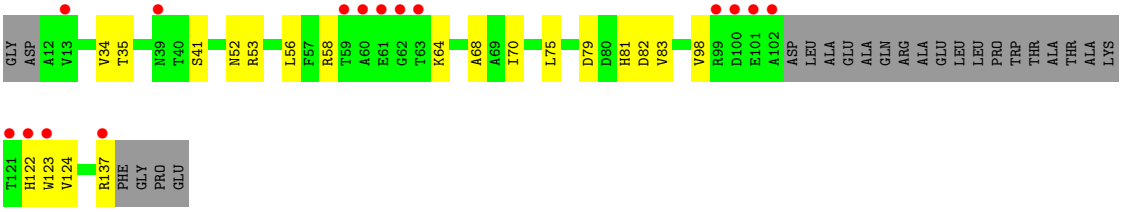
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain F:



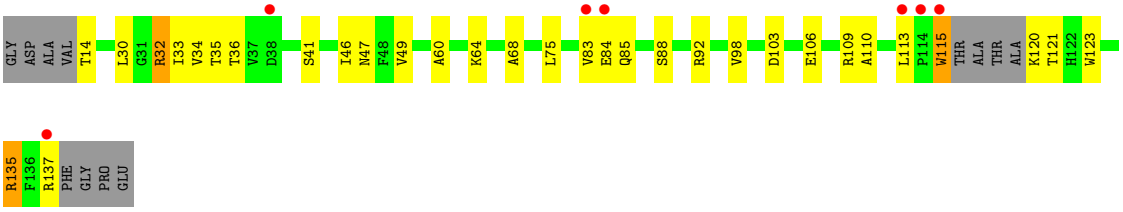
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain G:



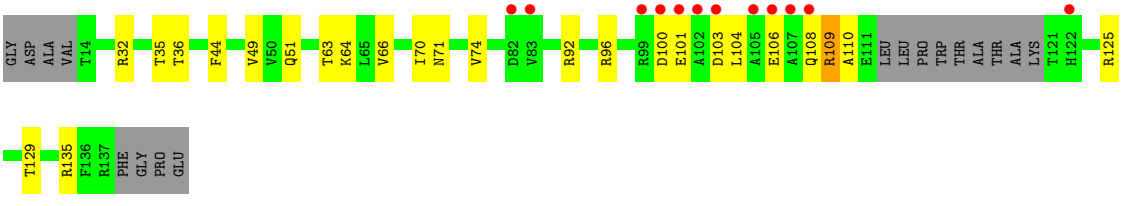
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain H:



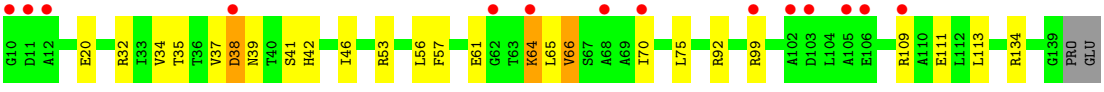
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain I:



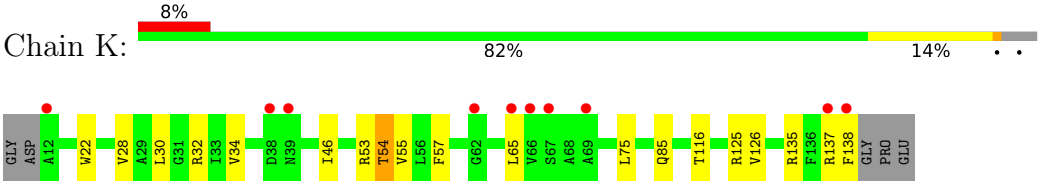
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain J:



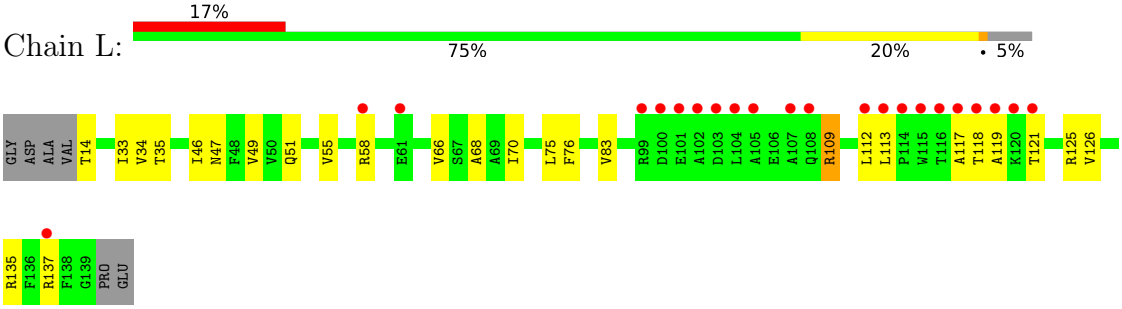
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain K:



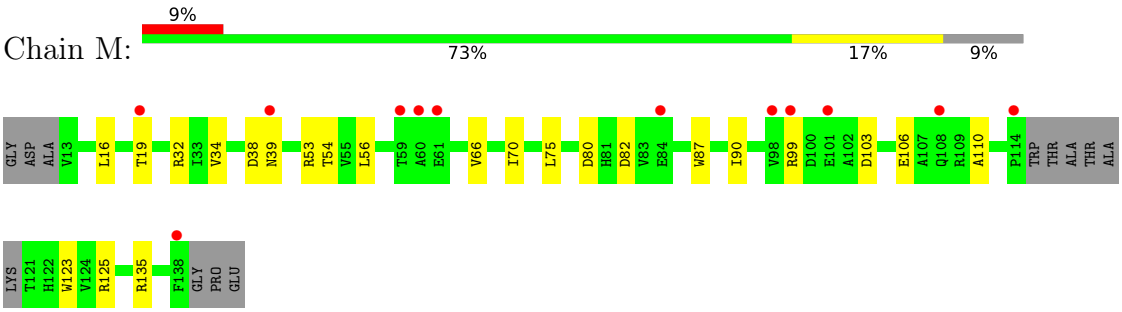
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain L:



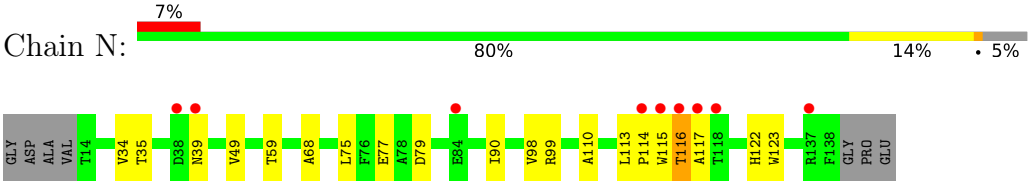
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain M:



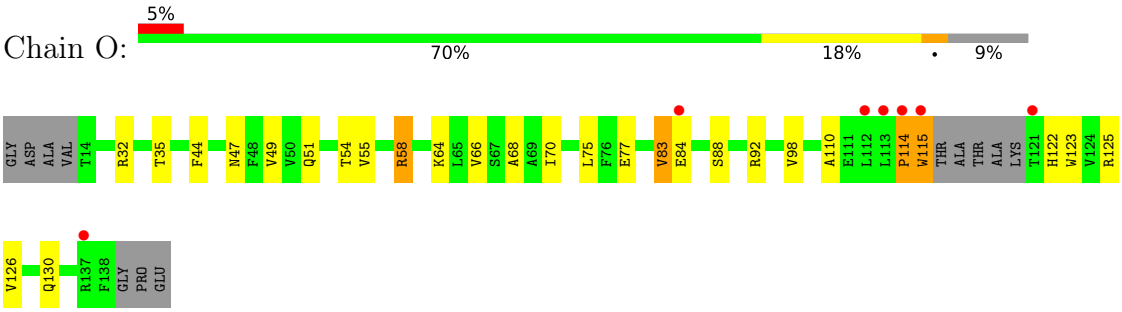
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain N:



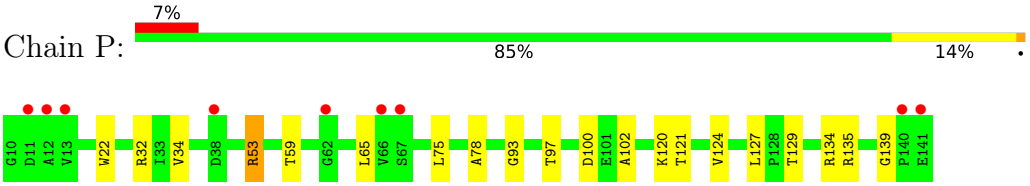
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain O:



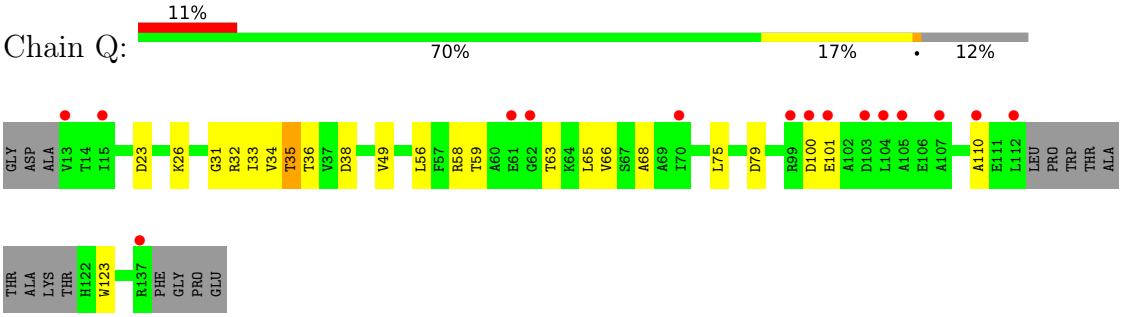
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain P:



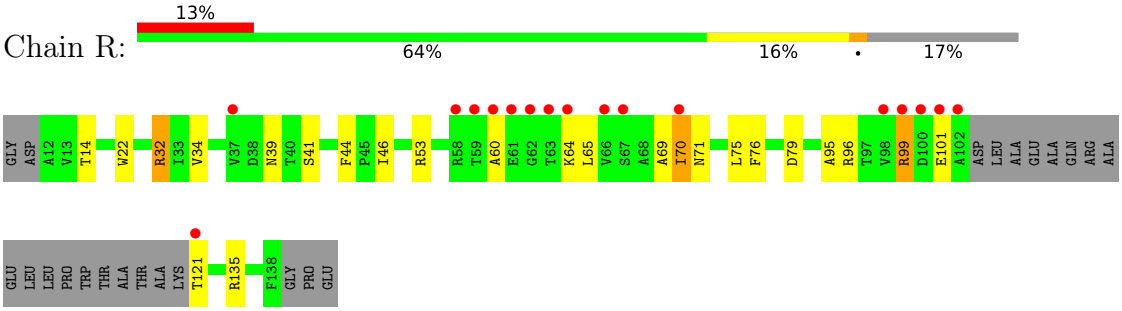
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain Q:



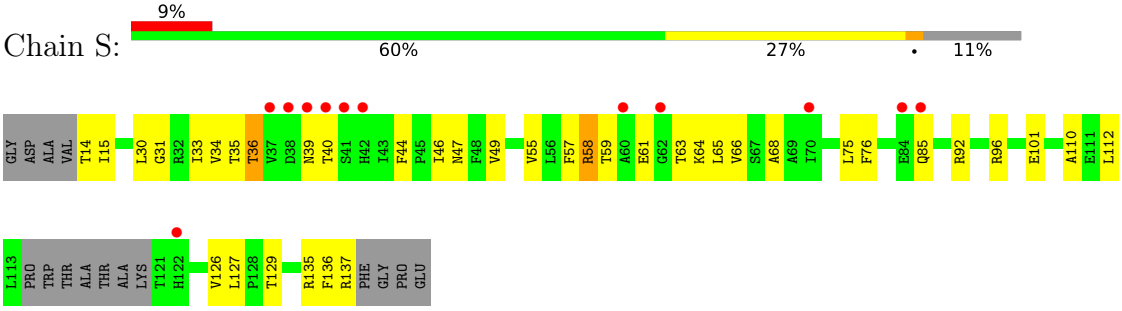
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain R:



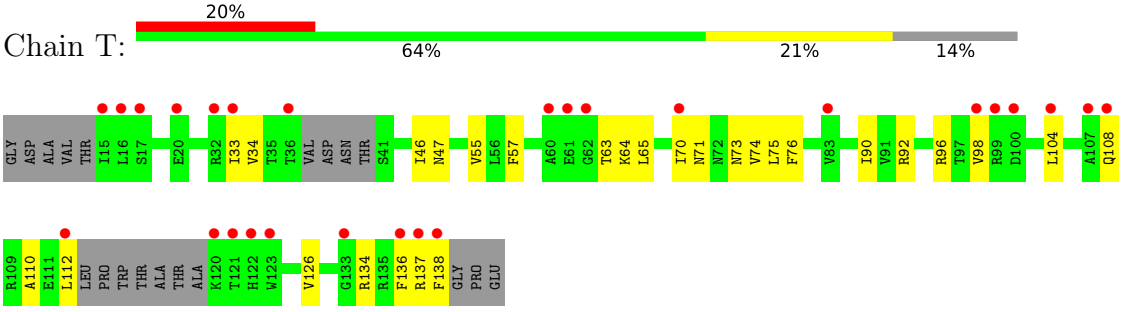
• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain S:



• Molecule 1: Pyridoxamine 5'-phosphate oxidase-related, FMN-binding protein

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.27Å 186.04Å 195.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 2.69 29.60 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.60-2.69) 99.9 (29.60-2.69)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.209 , 0.259 0.209 , 0.259	Depositor DCC
R_{free} test set	4121 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 65.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20506	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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 26.43 % 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 2.6380e-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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.25	0/982	0.46	0/1337
1	B	0.27	0/1024	0.53	0/1397
1	C	0.32	0/1038	0.52	0/1418
1	D	0.25	0/1029	0.49	0/1405
1	E	0.25	0/999	0.50	0/1364
1	F	0.26	0/957	0.48	0/1303
1	G	0.27	0/868	0.52	0/1183
1	H	0.25	0/974	0.50	0/1327
1	I	0.28	0/925	0.50	0/1259
1	J	0.26	0/1047	0.47	0/1429
1	K	0.26	0/1023	0.47	0/1397
1	L	0.25	0/1015	0.47	0/1385
1	M	0.27	0/968	0.51	0/1319
1	N	0.25	0/1007	0.47	0/1376
1	O	0.26	0/977	0.48	0/1332
1	P	0.25	0/1063	0.48	0/1452
1	Q	0.25	0/940	0.47	0/1280
1	R	0.28	0/880	0.51	0/1199
1	S	0.25	0/952	0.52	0/1295
1	T	0.27	0/916	0.54	0/1242
All	All	0.26	0/19584	0.49	0/26699

There are no bond length outliers.

There are no bond angle outliers.

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	966	0	975	12	0
1	B	1005	0	1004	18	0
1	C	1019	0	1022	18	0
1	D	1008	0	1019	29	0
1	E	981	0	987	21	0
1	F	942	0	937	8	0
1	G	854	0	861	15	0
1	H	957	0	962	25	0
1	I	911	0	910	20	0
1	J	1028	0	1030	18	0
1	K	1004	0	1010	13	0
1	L	996	0	999	21	0
1	M	952	0	957	17	0
1	N	988	0	985	14	0
1	O	959	0	958	22	0
1	P	1043	0	1039	14	0
1	Q	926	0	929	14	0
1	R	865	0	870	19	0
1	S	938	0	944	35	0
1	T	902	0	909	23	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
2	E	106	0	62	0	0
2	G	53	0	31	2	0
2	H	53	0	31	0	0
2	I	53	0	31	2	0
2	L	53	0	31	0	0
2	N	106	0	62	2	0
2	O	53	0	31	3	0
2	Q	106	0	62	1	0
2	S	106	0	62	5	0
3	A	1	0	0	0	0
4	A	36	0	0	0	0
4	B	35	0	0	1	0
4	C	29	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	34	0	0	1	0
4	E	20	0	0	1	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	26	0	0	1	0
4	I	12	0	0	0	0
4	J	24	0	0	1	0
4	K	30	0	0	2	0
4	L	5	0	0	1	0
4	M	2	0	0	0	0
4	N	20	0	0	0	0
4	O	16	0	0	1	0
4	P	20	0	0	1	0
4	Q	7	0	0	0	0
4	R	11	0	0	3	0
4	S	14	0	0	1	0
4	T	9	0	0	1	0
All	All	20506	0	19834	353	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 9.

All (353) 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:115:TRP:CD1	1:D:118:THR:HG21	1.31	1.63
1:L:49:VAL:CG2	1:L:112:LEU:HD13	1.70	1.19
1:D:115:TRP:CD1	1:D:118:THR:CG2	2.26	1.17
1:D:115:TRP:CG	1:D:118:THR:HG21	1.86	1.09
1:D:115:TRP:HD1	1:D:118:THR:CG2	1.71	0.97
1:D:115:TRP:HB2	1:D:118:THR:HG23	1.52	0.90
1:T:63:THR:HG22	1:T:65:LEU:H	1.36	0.89
2:O:201:FAD:H52A	1:P:134:ARG:HH22	1.36	0.89
1:S:14:THR:HG22	1:S:15:ILE:H	1.37	0.88
1:L:49:VAL:HG23	1:L:112:LEU:HD13	1.56	0.87
1:M:103:ASP:HB2	1:M:125:ARG:HH22	1.40	0.86
1:N:35:THR:HG21	1:N:68:ALA:HB1	1.57	0.84
1:G:52:ASN:OD1	1:G:53:ARG:N	2.10	0.84
1:D:115:TRP:HB2	1:D:118:THR:CG2	2.08	0.83
1:C:115:TRP:HA	1:C:115:TRP:CE3	2.13	0.83
1:O:75:LEU:HD21	1:O:92:ARG:HG2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:14:THR:HG22	1:R:135:ARG:HG2	1.61	0.81
1:L:35:THR:HG21	1:L:68:ALA:HB1	1.62	0.81
2:O:201:FAD:H51A	2:O:201:FAD:H8A	1.63	0.79
1:D:115:TRP:CB	1:D:118:THR:CG2	2.61	0.79
1:L:49:VAL:HG21	1:L:112:LEU:HD13	1.63	0.77
1:G:34:VAL:HB	1:G:75:LEU:HB2	1.67	0.76
1:J:99:ARG:HH21	1:J:111:GLU:HG2	1.51	0.75
1:L:49:VAL:CG2	1:L:112:LEU:CD1	2.60	0.75
1:C:41:SER:O	1:D:92:ARG:NH2	2.20	0.75
1:C:115:TRP:HA	1:C:115:TRP:HE3	1.51	0.75
1:D:115:TRP:CB	1:D:118:THR:HG23	2.16	0.74
1:K:138:PHE:HB3	1:L:113:LEU:HD13	1.69	0.74
1:N:34:VAL:HB	1:N:75:LEU:HB2	1.70	0.74
1:R:70:ILE:HG13	1:R:71:ASN:N	2.03	0.73
1:H:34:VAL:HB	1:H:75:LEU:HB2	1.70	0.73
1:O:35:THR:HG21	1:O:68:ALA:HB1	1.68	0.73
1:S:49:VAL:HG22	1:S:112:LEU:HD11	1.71	0.73
1:M:103:ASP:HB2	1:M:125:ARG:NH2	2.03	0.72
1:R:34:VAL:HB	1:R:75:LEU:HB2	1.69	0.72
1:O:66:VAL:O	1:O:70:ILE:HD12	1.89	0.72
1:L:51:GLN:HE21	1:L:125:ARG:HH12	1.37	0.72
1:Q:23:ASP:HA	1:Q:26:LYS:HE3	1.72	0.72
1:L:49:VAL:HG23	1:L:112:LEU:CD1	2.20	0.71
1:T:34:VAL:HB	1:T:75:LEU:HB2	1.71	0.71
1:S:47:ASN:O	1:S:58[B]:ARG:NH2	2.22	0.71
1:H:35:THR:HG21	1:H:68:ALA:HB1	1.73	0.71
1:S:46:ILE:HD11	1:S:57:PHE:CG	2.25	0.71
1:S:14:THR:HG22	1:S:15:ILE:N	2.05	0.70
1:G:56:LEU:HD21	1:G:123:TRP:HD1	1.56	0.70
1:G:35:THR:HG21	1:G:68:ALA:HB1	1.73	0.70
1:D:115:TRP:CG	1:D:118:THR:CG2	2.64	0.70
1:C:34:VAL:HB	1:C:75:LEU:HB2	1.72	0.69
2:O:201:FAD:H52A	1:P:134:ARG:NH2	2.06	0.69
1:J:53:ARG:NH1	4:J:201:HOH:O	2.25	0.69
1:D:54:THR:HG21	1:D:125:ARG:HD3	1.73	0.69
1:C:58:ARG:HD2	1:C:115:TRP:HE1	1.58	0.68
1:J:34:VAL:HB	1:J:75:LEU:HB2	1.75	0.68
1:E:54:THR:HG21	1:E:125:ARG:HD3	1.75	0.67
1:R:53:ARG:NH1	4:R:202:HOH:O	2.28	0.67
1:G:58:ARG:NH2	1:G:123:TRP:CH2	2.63	0.66
1:M:32:ARG:NH1	1:N:79:ASP:OD2	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:TRP:HD1	1:D:118:THR:HG21	0.88	0.66
1:S:34:VAL:HG22	1:S:75:LEU:HB2	1.77	0.66
1:K:85:GLN:HG2	1:K:137:ARG:HD2	1.76	0.66
1:E:49:VAL:HG21	1:E:110:ALA:HB1	1.77	0.66
1:F:34:VAL:HB	1:F:75:LEU:HB2	1.76	0.66
1:O:66:VAL:HG13	1:O:70:ILE:CD1	2.25	0.66
1:E:34:VAL:HB	1:E:75:LEU:HB2	1.78	0.66
1:D:49:VAL:HG23	1:D:112:LEU:HD13	1.78	0.66
1:R:99:ARG:NH1	4:R:201:HOH:O	2.28	0.66
1:L:47:ASN:OD1	1:L:58:ARG:NH2	2.29	0.65
1:S:14:THR:HB	1:S:135:ARG:HH21	1.61	0.65
1:L:109:ARG:NH2	4:L:301:HOH:O	2.29	0.64
1:L:49:VAL:HG22	1:L:112:LEU:HD13	1.77	0.64
1:M:16:LEU:HD21	1:M:135:ARG:HD3	1.78	0.64
1:E:113:LEU:HG	1:E:114:PRO:HD3	1.77	0.64
1:S:33:ILE:HG22	1:S:44:PHE:HB2	1.79	0.64
1:S:35:THR:HG21	1:S:68:ALA:HB1	1.79	0.64
1:C:92:ARG:NH2	1:D:41:SER:O	2.31	0.64
1:S:31:GLY:C	1:S:46:ILE:HG22	2.18	0.64
1:C:16:LEU:HD21	1:C:135:ARG:HG3	1.81	0.63
1:I:51:GLN:HE21	1:I:125:ARG:HH12	1.46	0.63
1:B:137:ARG:O	1:B:137:ARG:NE	2.30	0.63
1:F:49:VAL:HG21	1:F:110:ALA:HB1	1.80	0.63
1:L:34:VAL:HB	1:L:75:LEU:HB3	1.80	0.63
1:T:46:ILE:HD12	1:T:57:PHE:CG	2.34	0.62
1:N:49:VAL:HG21	1:N:110:ALA:HB1	1.81	0.62
1:P:120:LYS:HG2	1:P:121:THR:HG23	1.82	0.62
1:I:66:VAL:HA	1:I:70:ILE:HD13	1.82	0.62
1:M:34:VAL:HB	1:M:75:LEU:HB3	1.82	0.62
1:C:63:THR:O	1:C:64:LYS:HB2	1.98	0.62
1:J:61:GLU:N	1:J:61:GLU:OE1	2.33	0.62
1:G:56:LEU:HD21	1:G:123:TRP:CD1	2.34	0.62
1:B:14:THR:N	4:B:301:HOH:O	2.32	0.62
1:E:58:ARG:NH1	1:E:121:THR:OG1	2.31	0.61
1:N:39:ASN:ND2	1:N:39:ASN:O	2.33	0.61
1:A:38:ASP:O	1:B:39:ASN:N	2.25	0.61
1:D:129:THR:HG23	1:E:66:VAL:HG22	1.82	0.61
1:B:34:VAL:HB	1:B:75:LEU:HB2	1.81	0.61
1:Q:32:ARG:NH1	1:R:79:ASP:OD2	2.31	0.61
1:A:49:VAL:HG21	1:A:110:ALA:HB1	1.83	0.60
1:S:47:ASN:HB3	1:S:58[B]:ARG:HH22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:HD3	1:J:20:GLU:OE2	2.00	0.60
1:E:112:LEU:HD23	1:E:123:TRP:HZ3	1.65	0.60
1:O:47:ASN:ND2	4:O:302:HOH:O	2.33	0.60
1:D:115:TRP:CB	1:D:118:THR:HG21	2.26	0.59
1:I:101:GLU:HA	1:I:104:LEU:HB2	1.84	0.59
1:A:32:ARG:NH1	1:B:79:ASP:OD1	2.29	0.59
1:O:47:ASN:HD22	1:O:58:ARG:HH22	1.51	0.59
1:Q:35[A]:THR:HG21	1:Q:68:ALA:HB1	1.85	0.59
1:D:14:THR:HB	1:D:135:ARG:HG2	1.85	0.59
1:F:52:ASN:ND2	1:F:106:GLU:OE1	2.36	0.59
1:M:70:ILE:O	1:M:70:ILE:HD12	2.02	0.58
1:Q:49:VAL:HG21	1:Q:110:ALA:HB1	1.85	0.58
1:K:135:ARG:NH2	4:K:201:HOH:O	2.35	0.58
1:S:46:ILE:HD11	1:S:57:PHE:CD1	2.38	0.58
1:S:14:THR:CG2	1:S:15:ILE:H	2.13	0.58
1:O:44:PHE:HE2	1:O:64:LYS:HG3	1.68	0.58
1:G:41:SER:HG	1:H:36:THR:HG1	1.51	0.58
1:T:74:VAL:O	1:T:92:ARG:NH1	2.36	0.58
1:P:59[A]:THR:HG21	1:P:65:LEU:HD11	1.84	0.58
1:C:58:ARG:HD2	1:C:115:TRP:NE1	2.18	0.58
1:E:57:PHE:HA	1:E:112:LEU:HD21	1.86	0.57
1:D:119:ALA:O	1:D:120:LYS:HB2	2.04	0.57
1:A:138:PHE:HA	1:B:115:TRP:HB3	1.85	0.57
1:O:114:PRO:HG3	1:P:139:GLY:C	2.24	0.57
1:T:73:ASN:HB3	1:T:92:ARG:NH2	2.20	0.57
1:D:58[B]:ARG:HH12	1:D:114:PRO:HB3	1.70	0.56
1:H:135:ARG:HD2	1:H:137:ARG:HH22	1.70	0.56
1:I:36:THR:HG1	1:J:41:SER:HG	1.54	0.56
1:O:114:PRO:HD2	1:O:115:TRP:CD1	2.41	0.56
1:B:116:THR:OG1	1:B:117:ALA:N	2.38	0.56
1:M:19:THR:HG22	1:M:53:ARG:HH22	1.71	0.56
1:J:64:LYS:O	1:J:66:VAL:N	2.38	0.56
1:B:118:THR:OG1	1:B:120:LYS:HB3	2.06	0.55
1:E:51:GLN:O	1:E:54:THR:HB	2.06	0.55
1:P:93:GLY:HA2	1:P:129:THR:HG23	1.86	0.55
1:S:136:PHE:CE2	1:S:137:ARG:HG3	2.41	0.55
1:Q:38:ASP:O	1:R:39:ASN:ND2	2.39	0.55
1:T:73:ASN:HB3	1:T:92:ARG:HH22	1.71	0.55
1:B:49:VAL:HG13	1:B:112:LEU:HG	1.88	0.55
1:L:49:VAL:HG23	1:L:112:LEU:HD22	1.89	0.55
1:S:61:GLU:OE1	1:S:61:GLU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:HB	1:A:126:VAL:HB	1.89	0.55
1:G:82:ASP:OD1	1:G:83:VAL:N	2.38	0.55
1:I:44:PHE:CE2	1:I:64:LYS:HG3	2.42	0.55
1:K:54:THR:HG21	1:K:125:ARG:HH11	1.72	0.55
1:N:116:THR:OG1	1:N:117:ALA:N	2.39	0.55
1:B:85:GLN:HG2	1:B:137:ARG:HA	1.89	0.55
1:G:70:ILE:HD11	1:G:124:VAL:HG21	1.89	0.54
1:I:44:PHE:HE2	1:I:64:LYS:HG3	1.72	0.54
1:J:46[A]:ILE:CG2	1:J:57:PHE:HB2	2.38	0.54
1:A:32:ARG:HH11	1:B:79:ASP:CG	2.09	0.54
1:I:100:ASP:HB2	1:I:103:ASP:HB2	1.88	0.54
1:M:56:LEU:HB2	1:M:125:ARG:HD3	1.88	0.54
1:S:46:ILE:HD11	1:S:57:PHE:CD2	2.43	0.54
1:T:75:LEU:HD23	1:T:92:ARG:HD2	1.88	0.54
1:I:104:LEU:O	1:I:108:GLN:HG2	2.06	0.54
2:Q:202:FAD:O3P	2:Q:202:FAD:H8A	2.07	0.54
1:M:56:LEU:HA	1:M:125:ARG:HG2	1.88	0.54
1:H:98:VAL:HB	1:H:123:TRP:HB2	1.89	0.54
1:S:58[B]:ARG:H	1:S:58[B]:ARG:NE	2.04	0.54
1:T:76:PHE:O	1:T:90:ILE:HD12	2.07	0.54
1:E:59:THR:HG21	1:E:66:VAL:HB	1.89	0.53
1:D:61:GLU:OE1	1:D:119:ALA:O	2.26	0.53
1:J:35:THR:HG22	1:J:42:HIS:HB2	1.90	0.53
1:R:46:ILE:HD11	1:R:76:PHE:HE1	1.73	0.53
1:L:117:ALA:O	1:L:119:ALA:N	2.38	0.53
1:K:138:PHE:HB3	1:L:113:LEU:CD1	2.38	0.53
1:R:46:ILE:HD11	1:R:76:PHE:CE1	2.44	0.53
1:D:51:GLN:O	1:D:54:THR:HB	2.09	0.52
1:E:60:ALA:O	1:E:63:THR:HG22	2.08	0.52
1:J:37:VAL:O	1:J:39:ASN:N	2.42	0.52
1:D:55:VAL:HB	1:D:126:VAL:HB	1.91	0.52
1:Q:34:VAL:HB	1:Q:75:LEU:HB2	1.92	0.52
1:T:74:VAL:C	1:T:92:ARG:NH1	2.63	0.52
1:G:79:ASP:OD2	1:H:32:ARG:NH1	2.42	0.52
1:C:11:ASP:OD1	1:C:11:ASP:N	2.43	0.52
1:D:100:ASP:OD1	1:N:99:ARG:HG2	2.09	0.52
1:Q:59:THR:HG23	1:Q:65:LEU:HD23	1.92	0.52
1:S:58[B]:ARG:H	1:S:58[B]:ARG:HE	1.57	0.52
1:E:58:ARG:HD3	1:E:115:TRP:CD1	2.46	0.51
1:M:103:ASP:HA	1:M:106:GLU:HB3	1.91	0.51
1:Q:100:ASP:OD1	1:Q:101:GLU:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:14:THR:HA	1:H:135:ARG:NE	2.25	0.51
1:H:106:GLU:OE1	1:H:109:ARG:NH1	2.43	0.51
1:P:97:THR:HA	1:P:124:VAL:HA	1.93	0.51
1:S:64:LYS:NZ	2:S:201:FAD:O2A	2.31	0.51
1:R:60:ALA:O	1:R:121:THR:HA	2.11	0.51
1:C:55:VAL:HB	1:C:126:VAL:HB	1.92	0.51
1:Q:63:THR:HG22	1:Q:66:VAL:HG23	1.91	0.51
1:B:35:THR:HG22	1:B:74:VAL:HG12	1.92	0.51
1:A:98:VAL:HB	1:A:123:TRP:HB2	1.93	0.51
1:H:60:ALA:HB2	1:H:115:TRP:CH2	2.46	0.51
1:N:90:ILE:HG12	2:N:201:FAD:C2A	2.41	0.51
1:R:99:ARG:HG2	1:R:99:ARG:HH11	1.76	0.51
1:D:34:VAL:HB	1:D:75:LEU:HB2	1.94	0.50
1:I:109:ARG:HG3	1:I:109:ARG:O	2.12	0.50
1:M:54:THR:CG2	1:M:125:ARG:HD2	2.42	0.50
1:S:96:ARG:HG3	1:S:127:LEU:HD12	1.94	0.50
1:J:38:ASP:H	1:J:70:ILE:HD11	1.77	0.49
1:G:41:SER:OG	1:H:36:THR:OG1	2.24	0.49
1:G:64:LYS:HE2	2:G:201:FAD:O2A	2.13	0.49
1:O:92:ARG:HB2	1:O:130:GLN:HG2	1.93	0.49
1:E:112:LEU:HD23	1:E:123:TRP:CZ3	2.47	0.49
1:S:55:VAL:HB	1:S:126:VAL:HB	1.95	0.49
1:S:75:LEU:HD21	1:S:92:ARG:HG2	1.94	0.49
1:H:60:ALA:HB2	1:H:115:TRP:HH2	1.76	0.48
1:I:36:THR:OG1	1:J:41:SER:OG	2.30	0.48
1:I:63:THR:O	1:I:66:VAL:HG22	2.13	0.48
1:O:44:PHE:CE2	1:O:64:LYS:HG3	2.47	0.48
1:P:22:TRP:CD1	1:P:53:ARG:HG2	2.48	0.48
1:O:49:VAL:HG21	1:O:110:ALA:HB1	1.94	0.48
1:A:109:ARG:NH2	1:E:53:ARG:HD2	2.29	0.48
1:I:71:ASN:OD1	1:I:96:ARG:NH1	2.46	0.48
1:O:75:LEU:HD23	1:O:75:LEU:HA	1.57	0.48
1:M:66:VAL:O	1:M:70:ILE:HG13	2.14	0.48
1:O:98:VAL:HB	1:O:123:TRP:HB2	1.95	0.48
1:N:115:TRP:CE3	1:N:115:TRP:HA	2.49	0.47
1:B:55:VAL:HB	1:B:126:VAL:HB	1.96	0.47
1:C:49:VAL:HG21	1:C:110:ALA:HB1	1.95	0.47
1:I:35:THR:HG22	1:I:74:VAL:HG12	1.96	0.47
1:O:114:PRO:HG2	1:O:115:TRP:HD1	1.78	0.47
1:Q:31:GLY:O	1:Q:32:ARG:HG3	2.15	0.47
1:T:71:ASN:OD1	1:T:96:ARG:NH1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:49:VAL:HG23	1:L:112:LEU:CD2	2.44	0.47
1:S:14:THR:CG2	1:S:15:ILE:N	2.75	0.47
1:T:33:ILE:HG12	1:T:46:ILE:HD13	1.95	0.47
1:J:109:ARG:HG2	1:J:113:LEU:HD12	1.96	0.47
1:S:110:ALA:HB1	1:S:112:LEU:HD13	1.97	0.47
1:L:66:VAL:HA	1:L:70:ILE:HD13	1.97	0.47
1:Q:79:ASP:OD2	1:R:32:ARG:HD2	2.14	0.47
2:S:201:FAD:O5B	1:T:134:ARG:NH2	2.47	0.47
1:T:136:PHE:HD1	1:T:138:PHE:HD1	1.61	0.47
1:G:41:SER:OG	1:H:41:SER:OG	2.31	0.47
1:C:38:ASP:OD2	1:F:39:ASN:ND2	2.47	0.47
1:I:64:LYS:HE3	2:I:201:FAD:PA	2.55	0.46
1:L:33:ILE:HG12	1:L:46:ILE:HD13	1.97	0.46
1:H:49:VAL:HG21	1:H:110:ALA:HB1	1.96	0.46
2:I:201:FAD:O2A	1:J:134:ARG:NH2	2.47	0.46
1:T:104:LEU:O	1:T:108:GLN:HG3	2.16	0.46
1:B:32:ARG:HH21	1:B:78:ALA:HA	1.79	0.46
1:D:58[B]:ARG:NH1	1:D:114:PRO:HB3	2.31	0.46
1:F:14:THR:HB	1:F:135:ARG:HB2	1.98	0.46
1:M:75:LEU:HD21	1:M:90:ILE:HG23	1.97	0.46
2:S:201:FAD:C8A	1:T:134:ARG:HH12	2.29	0.46
1:C:35:THR:HG22	1:C:42:HIS:HB2	1.97	0.46
1:H:83:VAL:HG13	1:H:84:GLU:HG3	1.98	0.46
1:P:34:VAL:HB	1:P:75:LEU:HB2	1.97	0.46
1:O:54:THR:HG21	1:O:125:ARG:HD3	1.97	0.46
1:T:75:LEU:HD22	1:T:90:ILE:HD11	1.98	0.46
1:H:32:ARG:NH2	4:H:303:HOH:O	2.48	0.46
1:H:75:LEU:HD23	1:H:92:ARG:HG2	1.96	0.46
1:N:59:THR:HG22	1:N:122:HIS:HB3	1.97	0.46
1:P:32:ARG:HH21	1:P:78:ALA:HA	1.80	0.46
1:B:98:VAL:HB	1:B:123:TRP:HB2	1.97	0.45
2:D:201:FAD:H9	2:D:201:FAD:H1'1	1.83	0.45
1:I:51:GLN:NE2	1:I:125:ARG:HH22	2.15	0.45
1:P:97:THR:HG22	1:P:124:VAL:HG22	1.99	0.45
1:H:14:THR:HA	1:H:135:ARG:HE	1.82	0.45
1:N:98:VAL:HB	1:N:123:TRP:HB2	1.99	0.45
1:S:63:THR:O	1:S:66:VAL:HG22	2.16	0.45
1:T:110:ALA:O	1:T:112:LEU:N	2.50	0.45
1:R:70:ILE:HG13	1:R:71:ASN:H	1.76	0.45
1:Q:36:THR:OG1	1:R:41:SER:OG	2.27	0.45
1:E:38:ASP:O	1:F:39:ASN:ND2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14:THR:HA	1:L:135:ARG:HG2	1.98	0.45
1:I:51:GLN:CD	1:I:106:GLU:HG3	2.37	0.45
1:R:22:TRP:CD1	1:R:53:ARG:HG2	2.51	0.45
1:E:53:ARG:NH1	4:E:303:HOH:O	2.50	0.45
1:K:54:THR:HG21	1:K:125:ARG:NH1	2.32	0.45
1:O:83:VAL:HG12	1:O:84:GLU:HG3	1.99	0.45
1:I:104:LEU:HD22	1:I:108:GLN:HE21	1.82	0.44
1:S:49:VAL:CG2	1:S:112:LEU:HD11	2.45	0.44
1:T:92:ARG:HE	1:T:92:ARG:HB3	1.47	0.44
1:O:32:ARG:NH1	1:O:77:GLU:OE1	2.49	0.44
2:S:202:FAD:H5'1	1:T:64:LYS:HE3	2.00	0.44
1:B:14:THR:HB	1:B:135:ARG:HB3	2.00	0.44
1:E:37:VAL:O	1:E:38:ASP:HB2	2.17	0.44
2:G:201:FAD:N6A	1:H:88:SER:OG	2.42	0.44
1:I:49:VAL:HG21	1:I:110:ALA:HB1	2.00	0.44
1:L:55:VAL:HB	1:L:126:VAL:HB	1.98	0.44
1:S:36:THR:HG23	1:S:40:THR:O	2.18	0.44
1:G:81:HIS:HB3	1:H:30:LEU:HD22	2.00	0.44
1:K:55:VAL:HB	1:K:126:VAL:HB	2.00	0.44
1:P:135:ARG:NH1	4:P:203:HOH:O	2.50	0.44
1:R:99:ARG:NH1	1:R:99:ARG:HG2	2.32	0.44
1:R:44:PHE:CG	1:R:65:LEU:HD13	2.53	0.43
1:S:31:GLY:O	1:S:46:ILE:HG22	2.16	0.43
1:S:59:THR:HG23	1:S:65:LEU:HD23	1.99	0.43
1:S:92:ARG:O	1:S:129:THR:N	2.47	0.43
1:F:35:THR:HG21	1:F:68:ALA:HB1	1.99	0.43
1:B:75:LEU:HD21	1:B:92:ARG:NH1	2.34	0.43
1:K:22:TRP:CD1	1:K:53:ARG:HG3	2.53	0.43
1:M:38:ASP:HB3	1:M:39:ASN:H	1.63	0.43
1:O:115:TRP:HD1	1:O:115:TRP:H	1.64	0.43
1:E:113:LEU:HD12	1:E:113:LEU:HA	1.87	0.42
1:Q:56:LEU:HD11	1:Q:123:TRP:HB3	2.01	0.42
1:T:75:LEU:CD2	1:T:92:ARG:HD2	2.48	0.42
1:P:100:ASP:C	1:P:102:ALA:H	2.23	0.42
1:S:30:LEU:HD12	1:S:46:ILE:O	2.19	0.42
1:K:34:VAL:HB	1:K:75:LEU:HB2	2.01	0.42
1:N:113:LEU:O	1:N:115:TRP:N	2.52	0.42
1:R:69:ALA:O	1:R:95:ALA:HB3	2.18	0.42
1:C:85:GLN:OE1	1:C:135:ARG:NH2	2.46	0.42
1:L:46:ILE:HD11	1:L:76:PHE:CE1	2.55	0.42
1:F:104:LEU:HD23	1:F:104:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:54:THR:HG22	1:M:125:ARG:HD2	2.02	0.42
1:O:75:LEU:CD2	1:O:92:ARG:HG2	2.41	0.42
1:P:127:LEU:HD22	1:R:96:ARG:HD2	2.02	0.42
1:G:98:VAL:O	1:G:122:HIS:NE2	2.49	0.42
2:S:202:FAD:H9	2:S:202:FAD:H1'1	1.84	0.42
1:H:47:ASN:OD1	1:H:113:LEU:HB2	2.20	0.42
1:T:136:PHE:HD1	1:T:138:PHE:CD1	2.37	0.42
1:T:55:VAL:HB	1:T:126:VAL:CG2	2.49	0.41
1:H:85:GLN:HE21	1:H:137:ARG:CZ	2.33	0.41
1:I:103:ASP:OD1	1:I:125:ARG:NH2	2.53	0.41
1:K:46:ILE:HD13	1:K:57:PHE:HB2	2.02	0.41
1:S:136:PHE:CD2	1:S:137:ARG:HG3	2.55	0.41
1:A:34:VAL:HB	1:A:75:LEU:HB2	2.01	0.41
1:D:32:ARG:NH2	4:D:304:HOH:O	2.52	0.41
1:D:119:ALA:O	1:D:120:LYS:CB	2.68	0.41
1:H:120:LYS:HG3	1:H:121:THR:HG23	2.02	0.41
1:M:54:THR:HG21	1:M:125:ARG:HD2	2.03	0.41
1:I:92:ARG:O	1:I:129:THR:N	2.49	0.41
1:Q:33:ILE:HA	1:Q:75:LEU:O	2.20	0.41
2:C:201:FAD:H9	2:C:201:FAD:H1'1	1.88	0.41
1:D:85:GLN:NE2	1:D:135:ARG:HD2	2.34	0.41
1:E:116:THR:OG1	1:E:117:ALA:N	2.53	0.41
1:K:65:LEU:HG	1:K:116:THR:HG22	2.02	0.41
1:J:46[A]:ILE:HD13	1:J:46[A]:ILE:HA	1.92	0.41
1:J:75:LEU:HD23	1:J:92:ARG:HG2	2.03	0.41
1:C:60:ALA:HB3	1:C:63:THR:HG21	2.03	0.41
1:J:56:LEU:HD22	4:R:201:HOH:O	2.20	0.41
1:K:53:ARG:NH1	4:K:206:HOH:O	2.53	0.41
1:N:77:GLU:HG2	1:N:90:ILE:HD13	2.03	0.41
1:C:85:GLN:HE21	1:C:85:GLN:HB3	1.63	0.41
1:J:35:THR:CG2	1:J:42:HIS:HB2	2.51	0.41
1:C:58:ARG:HD2	1:C:115:TRP:CD1	2.56	0.41
1:H:33:ILE:HG12	1:H:46:ILE:HD13	2.02	0.41
1:H:98:VAL:HG13	1:H:103:ASP:CG	2.41	0.41
1:O:55:VAL:HB	1:O:126:VAL:HB	2.01	0.41
1:H:64:LYS:HD3	1:H:64:LYS:HA	1.92	0.41
1:K:28:VAL:HG12	1:K:30:LEU:H	1.86	0.41
1:A:66:VAL:HG13	1:A:70:ILE:HD12	2.03	0.40
1:A:99:ARG:NH2	1:N:99:ARG:O	2.54	0.40
1:B:66:VAL:HG13	1:B:70:ILE:HD12	2.03	0.40
1:E:22:TRP:NE1	1:E:53:ARG:HG2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:46:ILE:HG21	1:S:76:PHE:HE1	1.86	0.40
1:D:103:ASP:OD1	1:D:125:ARG:NE	2.37	0.40
1:E:114:PRO:O	1:E:115:TRP:HB2	2.22	0.40
1:O:51:GLN:O	1:O:54:THR:HB	2.21	0.40
1:M:80:ASP:HB3	1:M:87:TRP:NE1	2.37	0.40
2:N:202:FAD:H9	2:N:202:FAD:H1'1	1.82	0.40
1:S:85:GLN:OE1	4:S:301:HOH:O	2.21	0.40
1:T:47:ASN:HB3	4:T:201:HOH:O	2.20	0.40
1:S:101:GLU:CD	1:S:101:GLU:H	2.25	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	118/132 (89%)	117 (99%)	1 (1%)	0	100 100
1	B	125/132 (95%)	118 (94%)	6 (5%)	1 (1%)	19 43
1	C	127/132 (96%)	120 (94%)	6 (5%)	1 (1%)	19 43
1	D	126/132 (96%)	120 (95%)	5 (4%)	1 (1%)	19 43
1	E	122/132 (92%)	109 (89%)	8 (7%)	5 (4%)	3 6
1	F	115/132 (87%)	110 (96%)	5 (4%)	0	100 100
1	G	104/132 (79%)	101 (97%)	3 (3%)	0	100 100
1	H	116/132 (88%)	113 (97%)	3 (3%)	0	100 100
1	I	111/132 (84%)	104 (94%)	7 (6%)	0	100 100
1	J	129/132 (98%)	122 (95%)	3 (2%)	4 (3%)	4 9
1	K	125/132 (95%)	118 (94%)	7 (6%)	0	100 100
1	L	124/132 (94%)	114 (92%)	7 (6%)	3 (2%)	6 15
1	M	116/132 (88%)	110 (95%)	5 (4%)	1 (1%)	17 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	123/132 (93%)	112 (91%)	9 (7%)	2 (2%)	9 24
1	O	116/132 (88%)	110 (95%)	4 (3%)	2 (2%)	9 23
1	P	131/132 (99%)	124 (95%)	7 (5%)	0	100 100
1	Q	113/132 (86%)	108 (96%)	5 (4%)	0	100 100
1	R	105/132 (80%)	95 (90%)	6 (6%)	4 (4%)	3 7
1	S	114/132 (86%)	109 (96%)	4 (4%)	1 (1%)	17 40
1	T	107/132 (81%)	97 (91%)	8 (8%)	2 (2%)	8 20
All	All	2367/2640 (90%)	2231 (94%)	109 (5%)	27 (1%)	14 34

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	116	THR
1	E	114	PRO
1	J	64	LYS
1	O	114	PRO
1	S	36	THR
1	C	64	LYS
1	E	113	LEU
1	E	118	THR
1	J	38	ASP
1	J	66	VAL
1	M	110	ALA
1	R	99	ARG
1	T	70	ILE
1	D	110	ALA
1	J	65	LEU
1	L	83	VAL
1	L	118	THR
1	L	121	THR
1	N	116	THR
1	R	70	ILE
1	E	119	ALA
1	R	64	LYS
1	E	115	TRP
1	O	83	VAL
1	R	101	GLU
1	T	98	VAL
1	N	114	PRO

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	105/111 (95%)	101 (96%)	4 (4%)	33	62
1	B	108/111 (97%)	102 (94%)	6 (6%)	21	45
1	C	110/111 (99%)	105 (96%)	5 (4%)	27	55
1	D	109/111 (98%)	108 (99%)	1 (1%)	78	92
1	E	106/111 (96%)	105 (99%)	1 (1%)	78	92
1	F	102/111 (92%)	99 (97%)	3 (3%)	42	71
1	G	94/111 (85%)	93 (99%)	1 (1%)	73	90
1	H	104/111 (94%)	101 (97%)	3 (3%)	42	71
1	I	99/111 (89%)	96 (97%)	3 (3%)	41	70
1	J	110/111 (99%)	109 (99%)	1 (1%)	78	92
1	K	108/111 (97%)	106 (98%)	2 (2%)	57	82
1	L	107/111 (96%)	105 (98%)	2 (2%)	57	82
1	M	104/111 (94%)	101 (97%)	3 (3%)	42	71
1	N	106/111 (96%)	106 (100%)	0	100	100
1	O	104/111 (94%)	100 (96%)	4 (4%)	33	62
1	P	112/111 (101%)	111 (99%)	1 (1%)	78	92
1	Q	101/111 (91%)	98 (97%)	3 (3%)	41	70
1	R	95/111 (86%)	94 (99%)	1 (1%)	73	90
1	S	102/111 (92%)	99 (97%)	3 (3%)	42	71
1	T	97/111 (87%)	96 (99%)	1 (1%)	76	91
All	All	2083/2220 (94%)	2035 (98%)	48 (2%)	52	78

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	58	ARG
1	A	83	VAL

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Mol	Chain	Res	Type
1	A	137	ARG
1	B	59	THR
1	B	61	GLU
1	B	96	ARG
1	B	115	TRP
1	B	120	LYS
1	B	129	THR
1	C	53	ARG
1	C	85	GLN
1	C	99	ARG
1	C	115	TRP
1	C	136	PHE
1	D	120	LYS
1	E	32	ARG
1	F	35	THR
1	F	106	GLU
1	F	135	ARG
1	G	137	ARG
1	H	32	ARG
1	H	115	TRP
1	H	135	ARG
1	I	32	ARG
1	I	109	ARG
1	I	135	ARG
1	J	32	ARG
1	K	32	ARG
1	K	54	THR
1	L	109	ARG
1	L	137	ARG
1	M	82	ASP
1	M	99	ARG
1	M	123	TRP
1	O	58	ARG
1	O	88	SER
1	O	115	TRP
1	O	122	HIS
1	P	53	ARG
1	Q	35[A]	THR
1	Q	35[B]	THR
1	Q	58	ARG
1	R	32	ARG
1	S	39	ASN

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Mol	Chain	Res	Type
1	S	58[A]	ARG
1	S	58[B]	ARG
1	T	137	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	47	ASN
1	D	52	ASN
1	F	51	GLN
1	G	85	GLN
1	H	85	GLN
1	I	51	GLN
1	I	72	ASN
1	I	108	GLN
1	J	85	GLN
1	L	39	ASN
1	L	42	HIS
1	L	51	GLN
1	N	42	HIS
1	N	85	GLN
1	O	47	ASN
1	R	39	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	O	201	-	53,58,58	0.46	0	68,89,89	0.63	2 (2%)
2	FAD	N	202	-	53,58,58	0.46	0	68,89,89	0.53	1 (1%)
2	FAD	I	201	-	53,58,58	0.48	0	68,89,89	0.53	1 (1%)
2	FAD	D	201	-	53,58,58	0.45	0	68,89,89	0.69	3 (4%)
2	FAD	E	202	-	53,58,58	0.44	0	68,89,89	0.62	3 (4%)
2	FAD	Q	201	-	53,58,58	0.44	0	68,89,89	0.62	3 (4%)
2	FAD	Q	202	-	53,58,58	0.47	0	68,89,89	0.78	3 (4%)
2	FAD	S	201	-	53,58,58	0.45	0	68,89,89	0.65	3 (4%)
2	FAD	B	201	-	53,58,58	0.45	0	68,89,89	0.54	2 (2%)
2	FAD	C	201	-	53,58,58	0.44	0	68,89,89	0.68	3 (4%)
2	FAD	N	201	-	53,58,58	0.45	0	68,89,89	0.57	1 (1%)
2	FAD	S	202	-	53,58,58	0.45	0	68,89,89	0.66	2 (2%)
2	FAD	L	201	-	53,58,58	0.45	0	68,89,89	0.69	3 (4%)
2	FAD	G	201	-	53,58,58	0.45	0	68,89,89	0.59	2 (2%)
2	FAD	A	201	-	53,58,58	0.46	0	68,89,89	0.54	1 (1%)
2	FAD	H	201	-	53,58,58	0.45	0	68,89,89	0.57	2 (2%)
2	FAD	E	201	-	53,58,58	0.46	0	68,89,89	0.55	2 (2%)

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	O	201	-	-	7/30/50/50	0/6/6/6
2	FAD	N	202	-	-	9/30/50/50	0/6/6/6
2	FAD	I	201	-	-	4/30/50/50	0/6/6/6
2	FAD	D	201	-	-	10/30/50/50	0/6/6/6
2	FAD	E	202	-	-	10/30/50/50	0/6/6/6
2	FAD	Q	201	-	-	6/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	Q	202	-	-	3/30/50/50	0/6/6/6
2	FAD	S	201	-	-	11/30/50/50	0/6/6/6
2	FAD	B	201	-	-	4/30/50/50	0/6/6/6
2	FAD	C	201	-	-	5/30/50/50	0/6/6/6
2	FAD	N	201	-	-	10/30/50/50	0/6/6/6
2	FAD	S	202	-	-	5/30/50/50	0/6/6/6
2	FAD	L	201	-	-	12/30/50/50	0/6/6/6
2	FAD	G	201	-	-	10/30/50/50	0/6/6/6
2	FAD	A	201	-	-	11/30/50/50	0/6/6/6
2	FAD	H	201	-	-	3/30/50/50	0/6/6/6
2	FAD	E	201	-	-	7/30/50/50	0/6/6/6

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	202	FAD	P-O3P-PA	-3.74	119.98	132.83
2	D	201	FAD	P-O3P-PA	-3.38	121.24	132.83
2	L	201	FAD	P-O3P-PA	-3.18	121.90	132.83
2	C	201	FAD	P-O3P-PA	-3.01	122.50	132.83
2	G	201	FAD	P-O3P-PA	-2.94	122.74	132.83
2	Q	202	FAD	C3B-C2B-C1B	2.85	105.27	100.98
2	S	201	FAD	P-O3P-PA	-2.76	123.35	132.83
2	S	202	FAD	C3B-C2B-C1B	2.71	105.06	100.98
2	C	201	FAD	C3B-C2B-C1B	2.70	105.04	100.98
2	L	201	FAD	C3B-C2B-C1B	2.61	104.91	100.98
2	S	201	FAD	C3B-C2B-C1B	2.61	104.91	100.98
2	E	202	FAD	C3B-C2B-C1B	2.59	104.88	100.98
2	B	201	FAD	C5A-C6A-N6A	2.58	124.27	120.35
2	E	201	FAD	P-O3P-PA	-2.58	123.98	132.83
2	Q	201	FAD	P-O3P-PA	-2.54	124.11	132.83
2	A	201	FAD	C5A-C6A-N6A	2.49	124.14	120.35
2	N	202	FAD	C5A-C6A-N6A	2.40	124.00	120.35
2	E	202	FAD	C5A-C6A-N6A	2.38	123.97	120.35
2	O	201	FAD	C5A-C6A-N6A	2.38	123.97	120.35
2	O	201	FAD	C3B-C2B-C1B	2.36	104.54	100.98
2	H	201	FAD	P-O3P-PA	-2.36	124.73	132.83
2	I	201	FAD	C5A-C6A-N6A	2.32	123.88	120.35
2	E	201	FAD	C5A-C6A-N6A	2.30	123.85	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	201	FAD	C5A-C6A-N6A	2.30	123.85	120.35
2	G	201	FAD	C5A-C6A-N6A	2.30	123.85	120.35
2	N	201	FAD	C5A-C6A-N6A	2.29	123.83	120.35
2	L	201	FAD	C5A-C6A-N6A	2.28	123.82	120.35
2	H	201	FAD	C5A-C6A-N6A	2.28	123.82	120.35
2	S	202	FAD	C5A-C6A-N6A	2.27	123.80	120.35
2	Q	201	FAD	C5A-C6A-N6A	2.27	123.80	120.35
2	Q	202	FAD	C5A-C6A-N6A	2.26	123.79	120.35
2	B	201	FAD	P-O3P-PA	-2.26	125.08	132.83
2	C	201	FAD	C5A-C6A-N6A	2.22	123.72	120.35
2	S	201	FAD	C5A-C6A-N6A	2.21	123.71	120.35
2	Q	201	FAD	C3B-C2B-C1B	2.08	104.12	100.98
2	E	202	FAD	P-O3P-PA	-2.05	125.80	132.83
2	D	201	FAD	C3B-C2B-C1B	2.04	104.05	100.98

There are no chirality outliers.

All (127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	FAD	C1'-C2'-C3'-O3'
2	A	201	FAD	C1'-C2'-C3'-C4'
2	A	201	FAD	O2'-C2'-C3'-O3'
2	A	201	FAD	O2'-C2'-C3'-C4'
2	A	201	FAD	C5'-O5'-P-O3P
2	C	201	FAD	C5B-O5B-PA-O1A
2	C	201	FAD	C5B-O5B-PA-O3P
2	C	201	FAD	C5'-O5'-P-O1P
2	D	201	FAD	N10-C1'-C2'-O2'
2	D	201	FAD	N10-C1'-C2'-C3'
2	D	201	FAD	C1'-C2'-C3'-O3'
2	D	201	FAD	C1'-C2'-C3'-C4'
2	D	201	FAD	C3'-C4'-C5'-O5'
2	D	201	FAD	O4'-C4'-C5'-O5'
2	D	201	FAD	C5'-O5'-P-O1P
2	E	201	FAD	C5B-O5B-PA-O3P
2	E	202	FAD	C5B-O5B-PA-O1A
2	E	202	FAD	C5B-O5B-PA-O3P
2	E	202	FAD	C1'-C2'-C3'-O3'
2	E	202	FAD	C1'-C2'-C3'-C4'
2	E	202	FAD	O2'-C2'-C3'-O3'
2	E	202	FAD	O2'-C2'-C3'-C4'
2	E	202	FAD	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
2	G	201	FAD	O4B-C4B-C5B-O5B
2	G	201	FAD	C1'-C2'-C3'-C4'
2	G	201	FAD	C5'-O5'-P-O3P
2	H	201	FAD	C5'-O5'-P-O3P
2	I	201	FAD	C5B-O5B-PA-O1A
2	L	201	FAD	C1'-C2'-C3'-C4'
2	L	201	FAD	C5'-O5'-P-O1P
2	N	201	FAD	C5B-O5B-PA-O3P
2	N	201	FAD	C1'-C2'-C3'-C4'
2	N	201	FAD	C5'-O5'-P-O1P
2	N	201	FAD	C5'-O5'-P-O2P
2	N	202	FAD	C1'-C2'-C3'-O3'
2	N	202	FAD	C1'-C2'-C3'-C4'
2	O	201	FAD	C5B-O5B-PA-O3P
2	O	201	FAD	C1'-C2'-C3'-C4'
2	Q	201	FAD	C5B-O5B-PA-O1A
2	Q	201	FAD	C1'-C2'-C3'-C4'
2	Q	202	FAD	O4B-C4B-C5B-O5B
2	Q	202	FAD	C3B-C4B-C5B-O5B
2	S	201	FAD	C5B-O5B-PA-O1A
2	S	201	FAD	C1'-C2'-C3'-O3'
2	S	201	FAD	C1'-C2'-C3'-C4'
2	S	201	FAD	C3'-C4'-C5'-O5'
2	S	201	FAD	O4'-C4'-C5'-O5'
2	S	201	FAD	C5'-O5'-P-O1P
2	S	201	FAD	C5'-O5'-P-O2P
2	S	201	FAD	C5'-O5'-P-O3P
2	S	202	FAD	C5'-O5'-P-O1P
2	S	202	FAD	C5'-O5'-P-O3P
2	N	202	FAD	O3'-C3'-C4'-O4'
2	G	201	FAD	C3B-C4B-C5B-O5B
2	D	201	FAD	O2'-C2'-C3'-C4'
2	N	202	FAD	C2'-C3'-C4'-O4'
2	N	202	FAD	C2'-C3'-C4'-C5'
2	E	201	FAD	O3'-C3'-C4'-C5'
2	N	202	FAD	O3'-C3'-C4'-C5'
2	D	201	FAD	O2'-C2'-C3'-O3'
2	E	201	FAD	O3'-C3'-C4'-O4'
2	N	202	FAD	O2'-C2'-C3'-O3'
2	S	201	FAD	O2'-C2'-C3'-O3'
2	E	201	FAD	C2'-C3'-C4'-O4'
2	L	201	FAD	C2'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
2	S	201	FAD	O2'-C2'-C3'-C4'
2	L	201	FAD	C2'-C3'-C4'-C5'
2	Q	201	FAD	O2'-C2'-C3'-O3'
2	G	201	FAD	O2'-C2'-C3'-C4'
2	L	201	FAD	O2'-C2'-C3'-C4'
2	Q	201	FAD	O2'-C2'-C3'-C4'
2	G	201	FAD	O2'-C2'-C3'-O3'
2	L	201	FAD	O3'-C3'-C4'-O4'
2	L	201	FAD	O3'-C3'-C4'-C5'
2	N	201	FAD	O2'-C2'-C3'-C4'
2	N	202	FAD	O2'-C2'-C3'-C4'
2	O	201	FAD	O2'-C2'-C3'-C4'
2	I	201	FAD	O2'-C2'-C3'-C4'
2	E	201	FAD	C2'-C3'-C4'-C5'
2	N	201	FAD	O2'-C2'-C3'-O3'
2	O	201	FAD	O2'-C2'-C3'-O3'
2	S	202	FAD	C2'-C3'-C4'-O4'
2	B	201	FAD	C5'-O5'-P-O3P
2	C	201	FAD	C5'-O5'-P-O3P
2	L	201	FAD	C5'-O5'-P-O3P
2	O	201	FAD	C5'-O5'-P-O3P
2	O	201	FAD	O4B-C4B-C5B-O5B
2	Q	202	FAD	PA-O3P-P-O1P
2	A	201	FAD	C5'-O5'-P-O1P
2	A	201	FAD	C5'-O5'-P-O2P
2	E	201	FAD	C5B-O5B-PA-O2A
2	E	202	FAD	C5'-O5'-P-O1P
2	E	202	FAD	C5'-O5'-P-O2P
2	G	201	FAD	C5'-O5'-P-O1P
2	G	201	FAD	C5'-O5'-P-O2P
2	H	201	FAD	C5'-O5'-P-O1P
2	H	201	FAD	C5'-O5'-P-O2P
2	L	201	FAD	C5B-O5B-PA-O2A
2	N	201	FAD	C5B-O5B-PA-O1A
2	L	201	FAD	O2'-C2'-C3'-O3'
2	C	201	FAD	PA-O3P-P-O2P
2	G	201	FAD	PA-O3P-P-O2P
2	B	201	FAD	O2'-C2'-C3'-C4'
2	N	201	FAD	C2'-C3'-C4'-O4'
2	I	201	FAD	O2'-C2'-C3'-O3'
2	E	202	FAD	O3'-C3'-C4'-C5'
2	A	201	FAD	C5B-O5B-PA-O3P

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Mol	Chain	Res	Type	Atoms
2	D	201	FAD	C5'-O5'-P-O3P
2	I	201	FAD	C5B-O5B-PA-O3P
2	L	201	FAD	C5B-O5B-PA-O3P
2	N	201	FAD	C5'-O5'-P-O3P
2	Q	201	FAD	C5B-O5B-PA-O3P
2	E	201	FAD	O2'-C2'-C3'-C4'
2	A	201	FAD	O3'-C3'-C4'-C5'
2	S	201	FAD	O4B-C4B-C5B-O5B
2	S	202	FAD	O3'-C3'-C4'-O4'
2	A	201	FAD	C5B-O5B-PA-O2A
2	B	201	FAD	C5'-O5'-P-O1P
2	N	202	FAD	C5B-O5B-PA-O1A
2	S	202	FAD	C5'-O5'-P-O2P
2	G	201	FAD	C1'-C2'-C3'-O3'
2	L	201	FAD	C1'-C2'-C3'-O3'
2	N	201	FAD	C1'-C2'-C3'-O3'
2	O	201	FAD	C1'-C2'-C3'-O3'
2	Q	201	FAD	C1'-C2'-C3'-O3'
2	B	201	FAD	O2'-C2'-C3'-O3'
2	A	201	FAD	N10-C1'-C2'-O2'

There are no ring outliers.

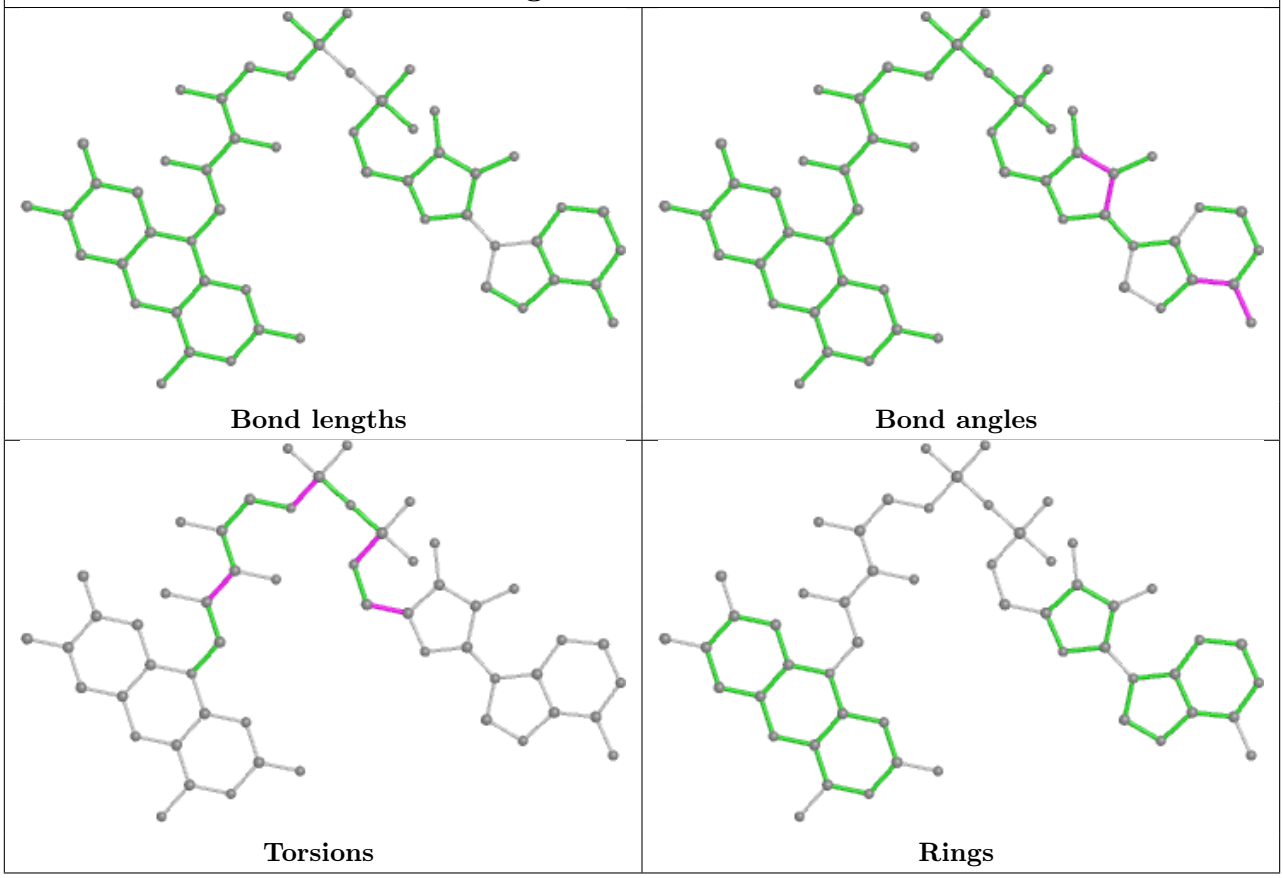
10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	201	FAD	3	0
2	N	202	FAD	1	0
2	I	201	FAD	2	0
2	D	201	FAD	1	0
2	Q	202	FAD	1	0
2	S	201	FAD	3	0
2	C	201	FAD	1	0
2	N	201	FAD	1	0
2	S	202	FAD	2	0
2	G	201	FAD	2	0

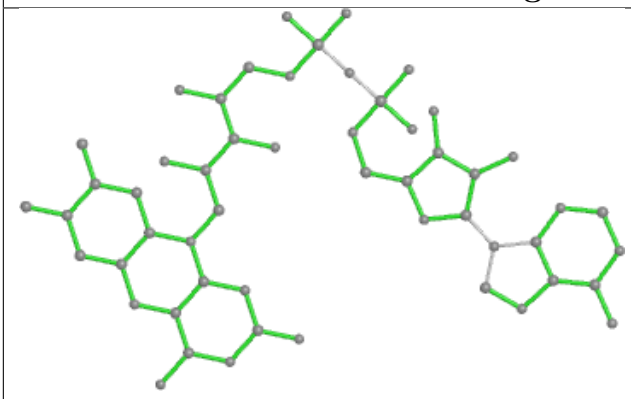
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

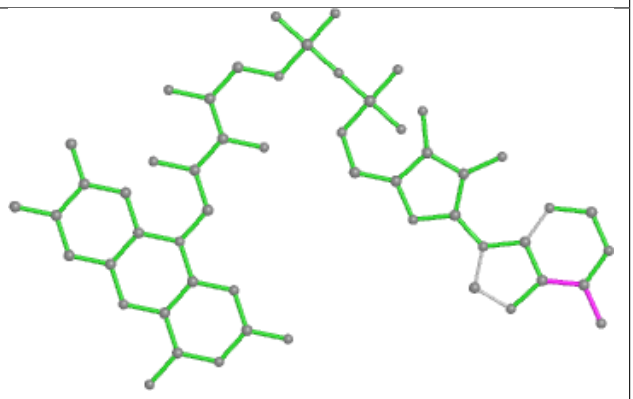
Ligand FAD O 201



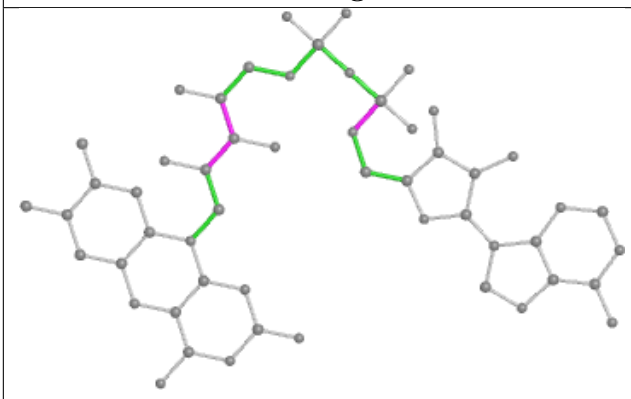
Ligand FAD N 202



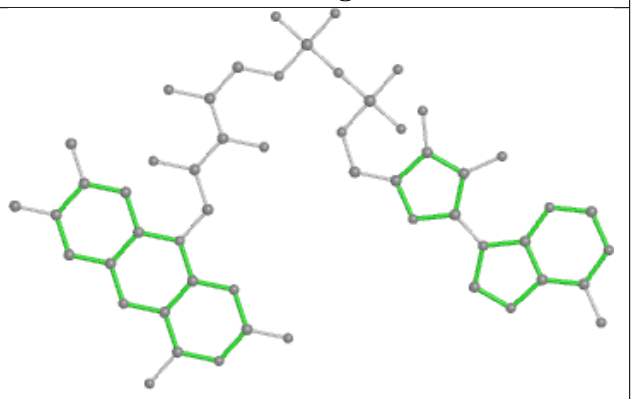
Bond lengths



Bond angles

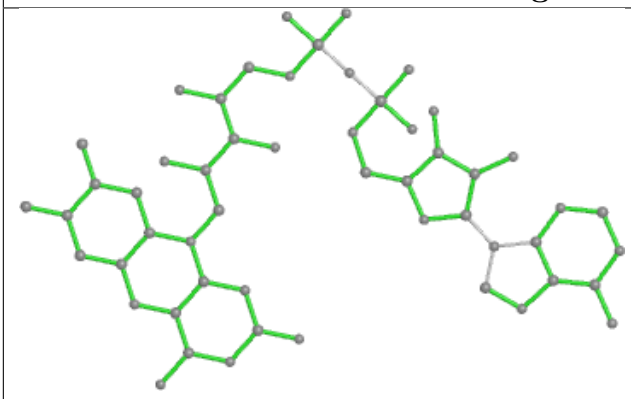


Torsions

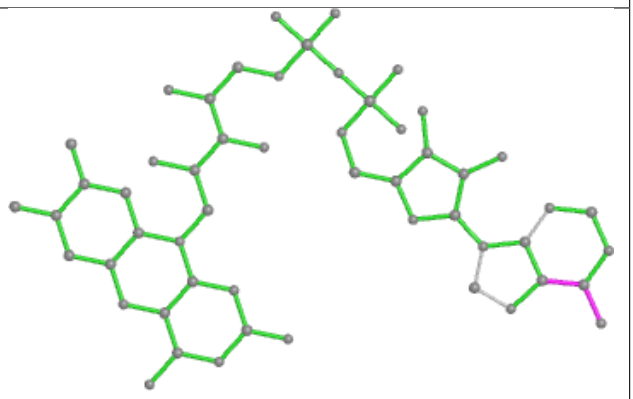


Rings

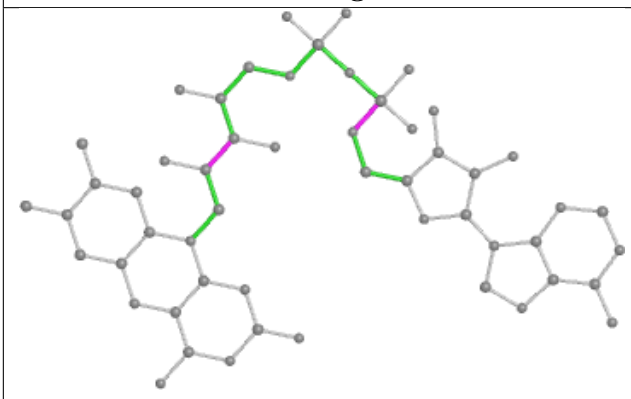
Ligand FAD I 201



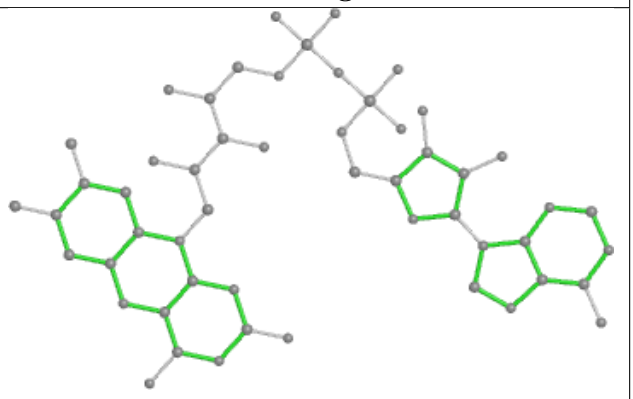
Bond lengths



Bond angles

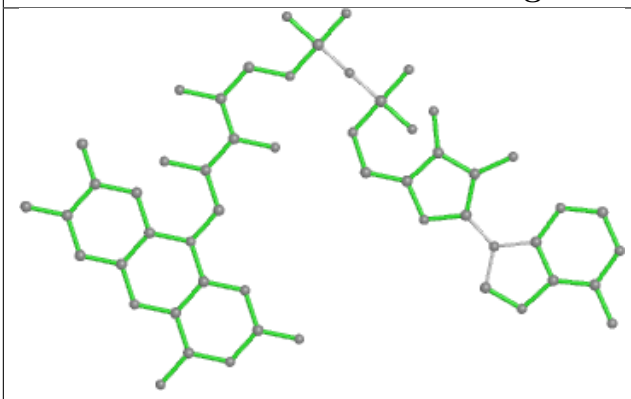


Torsions

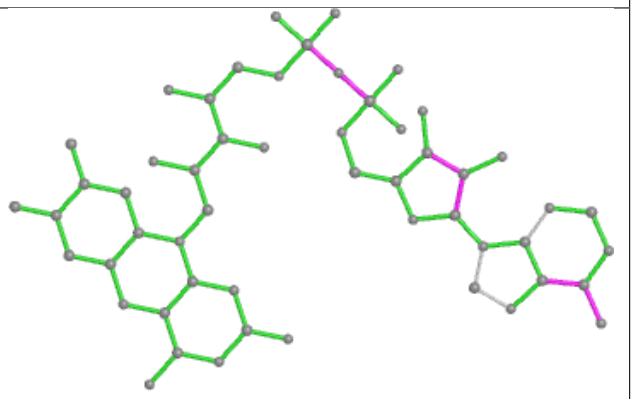


Rings

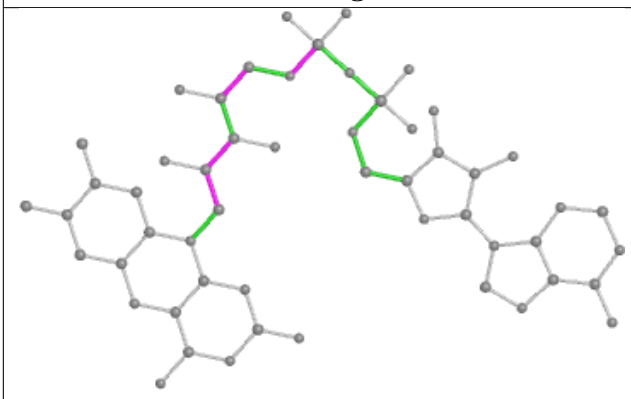
Ligand FAD D 201



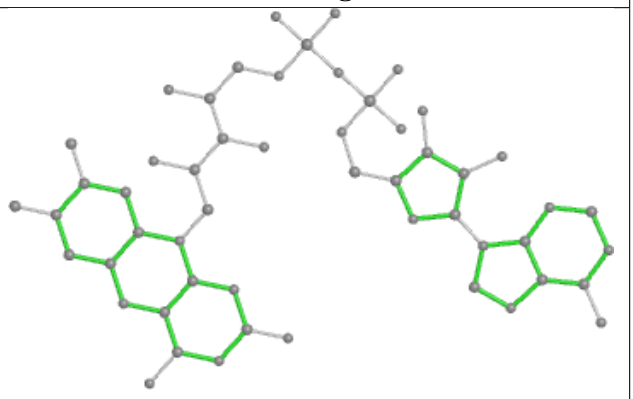
Bond lengths



Bond angles

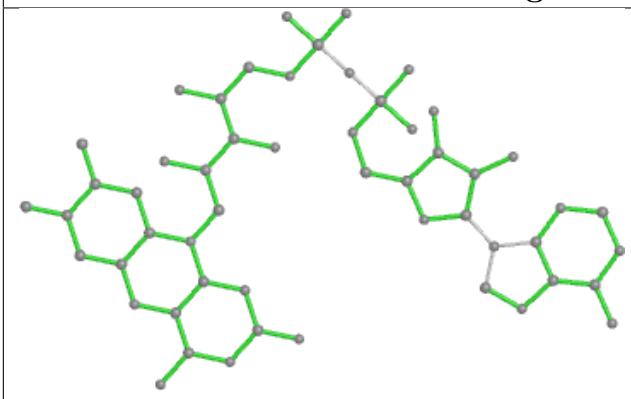


Torsions

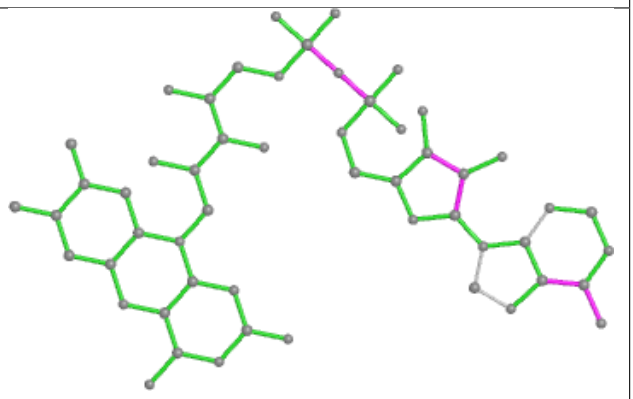


Rings

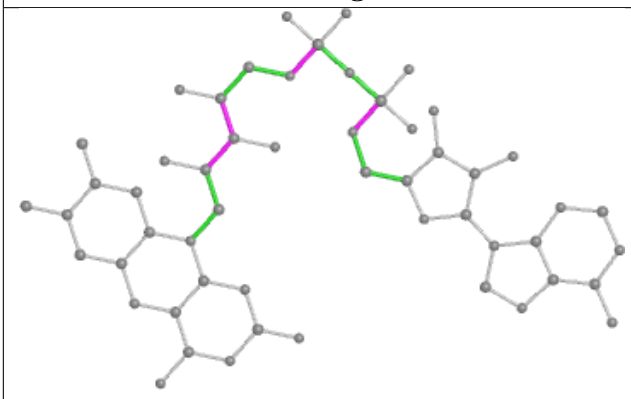
Ligand FAD E 202



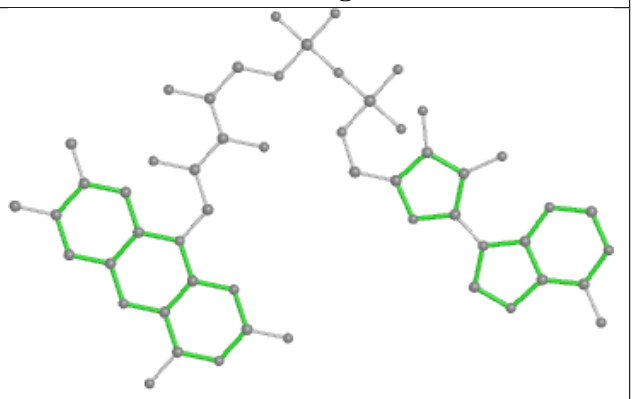
Bond lengths



Bond angles

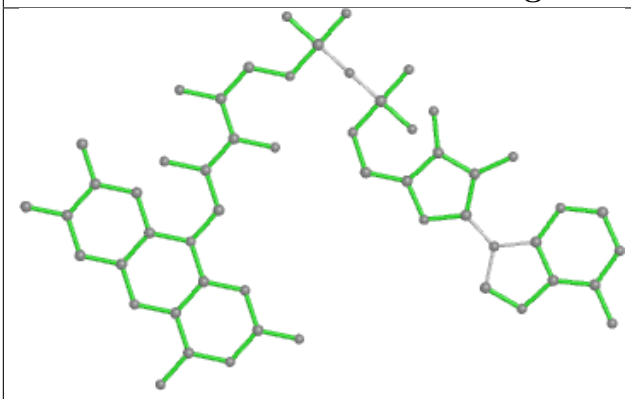


Torsions

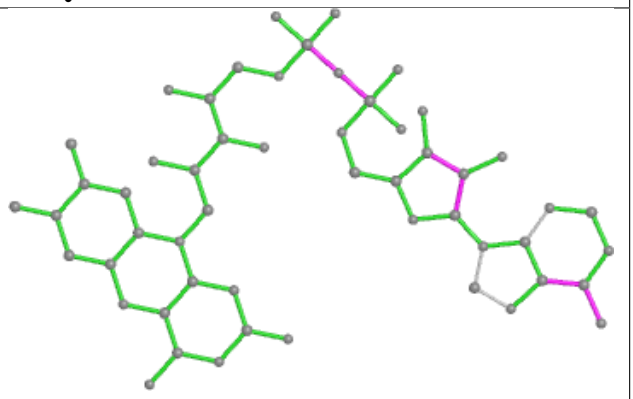


Rings

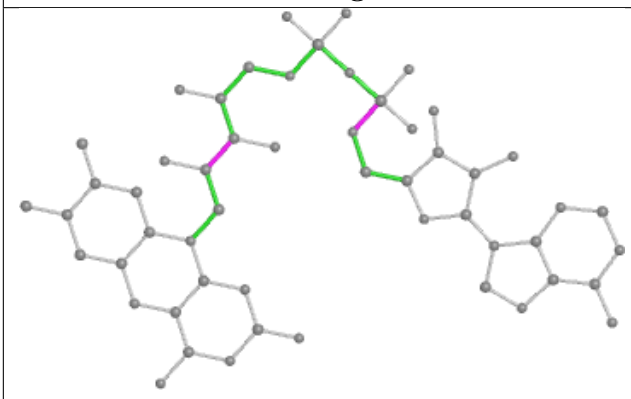
Ligand FAD Q 201



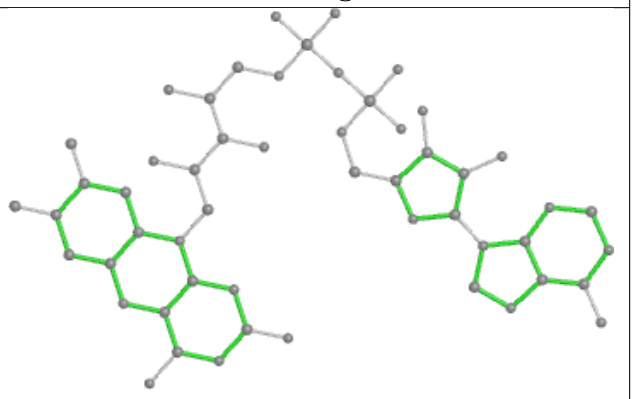
Bond lengths



Bond angles

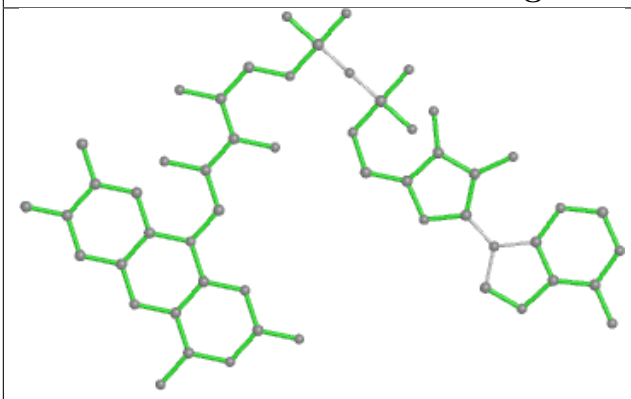


Torsions

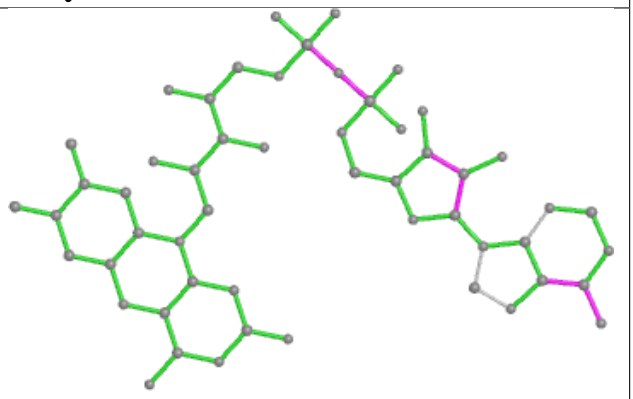


Rings

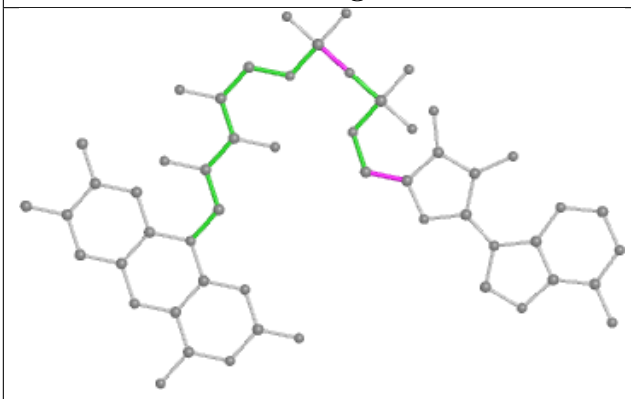
Ligand FAD Q 202



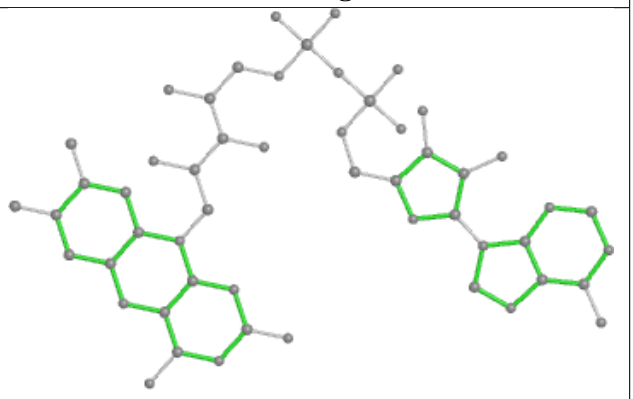
Bond lengths



Bond angles

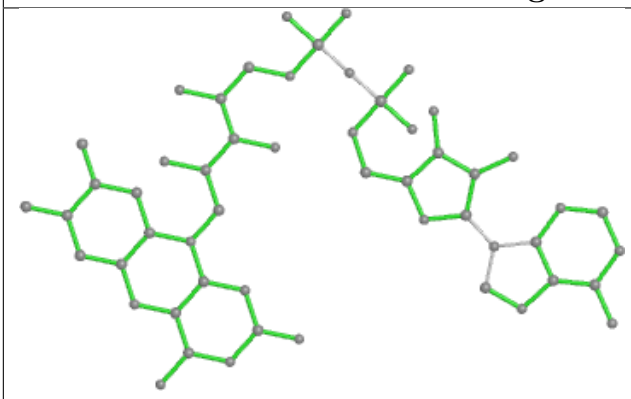


Torsions

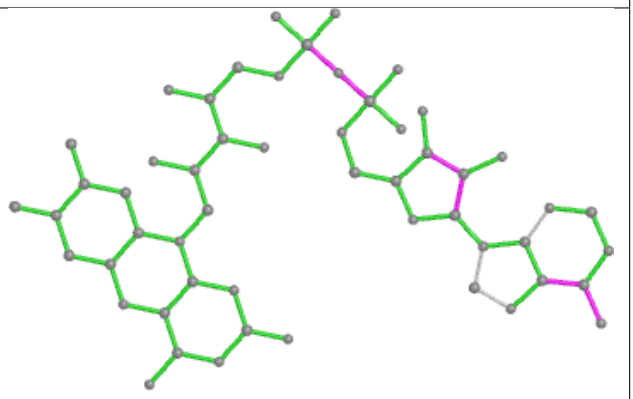


Rings

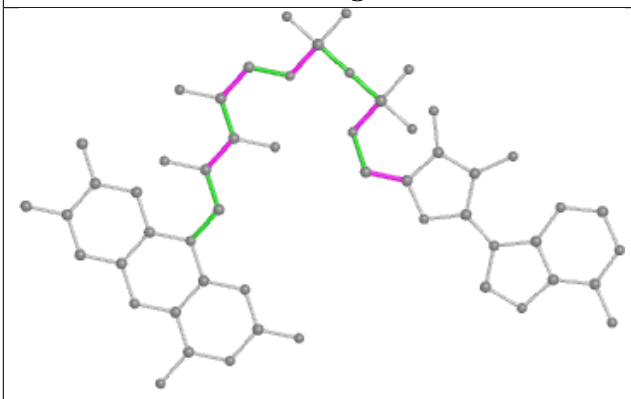
Ligand FAD S 201



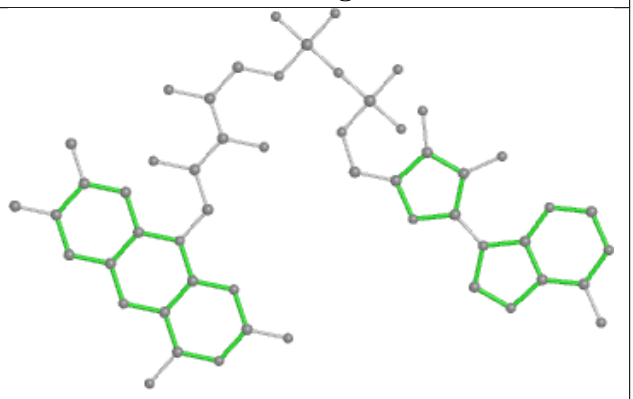
Bond lengths



Bond angles

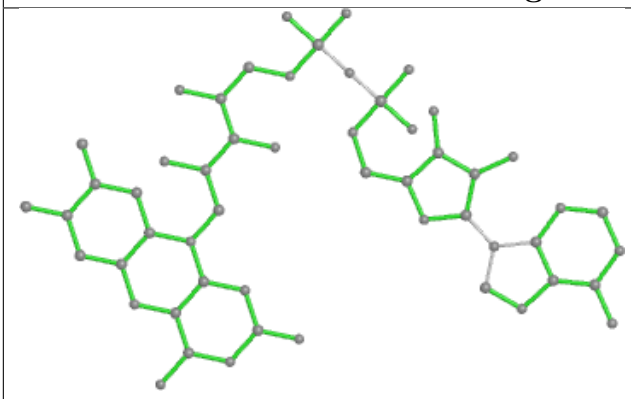


Torsions

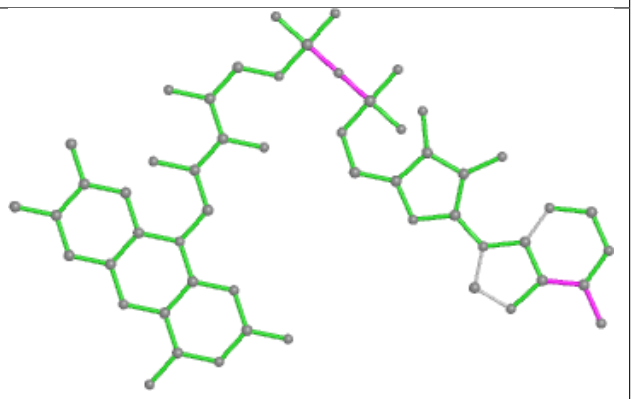


Rings

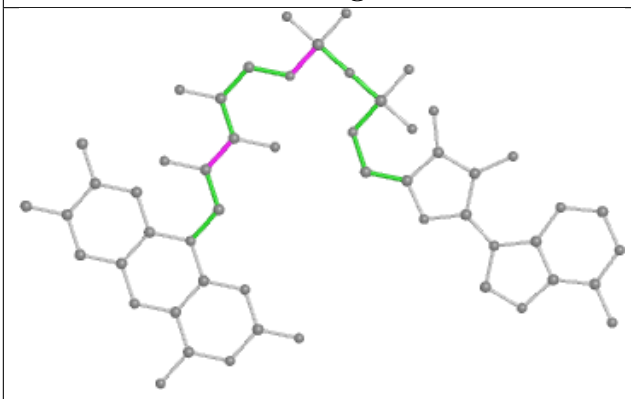
Ligand FAD B 201



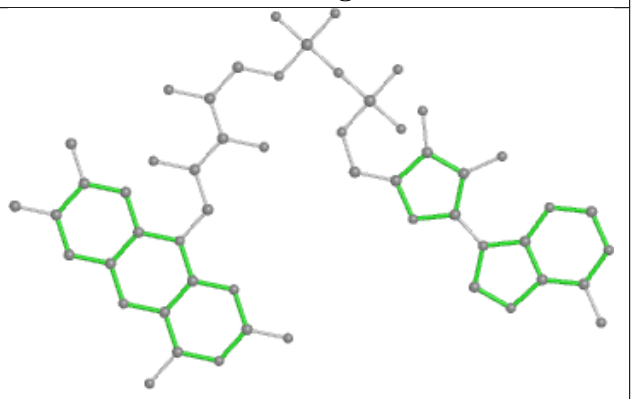
Bond lengths



Bond angles

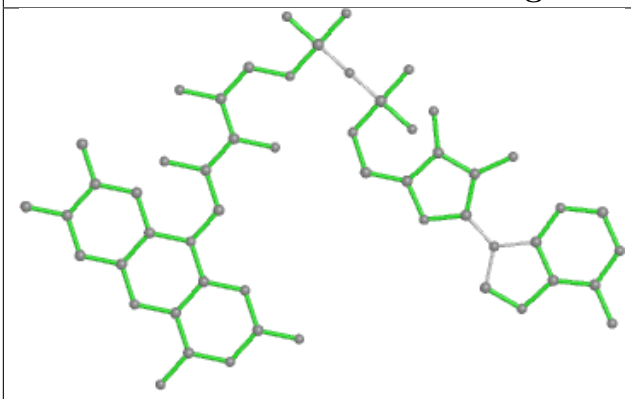


Torsions

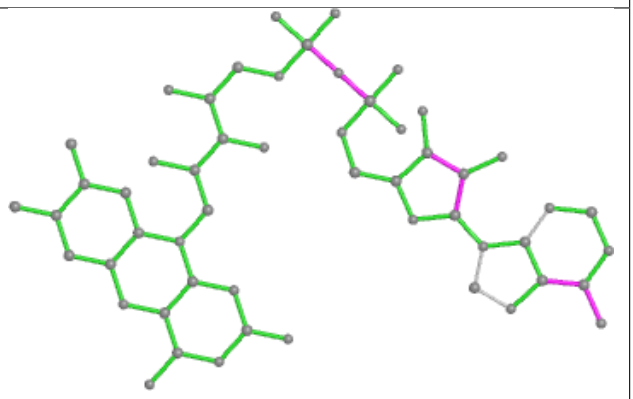


Rings

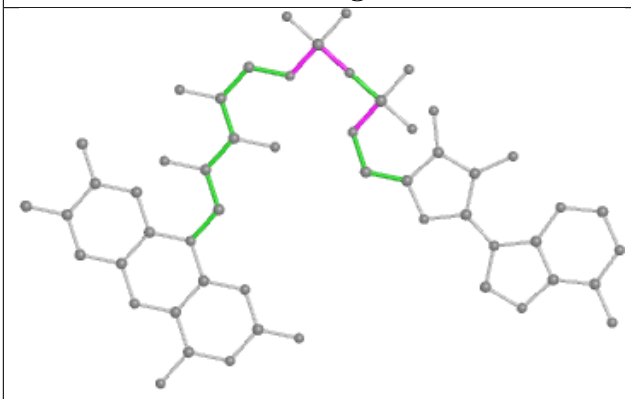
Ligand FAD C 201



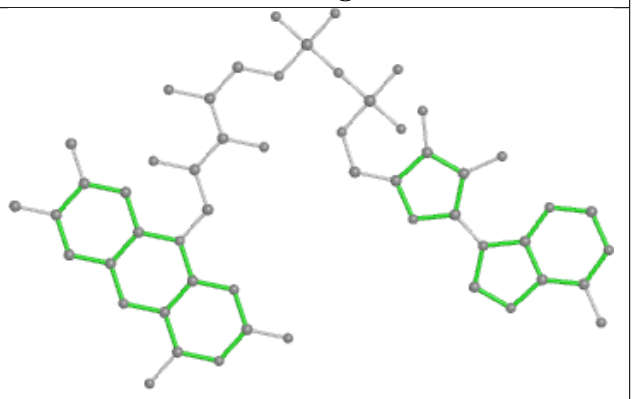
Bond lengths



Bond angles

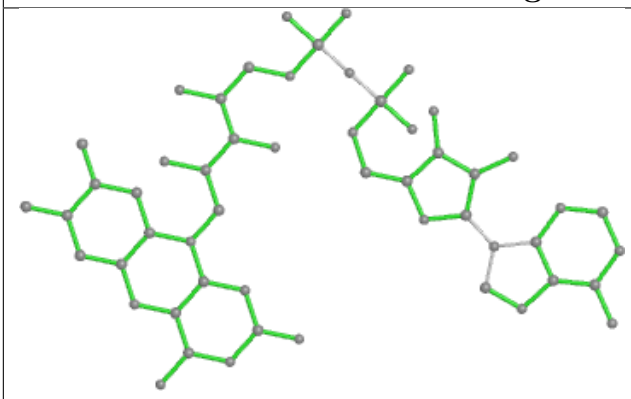


Torsions

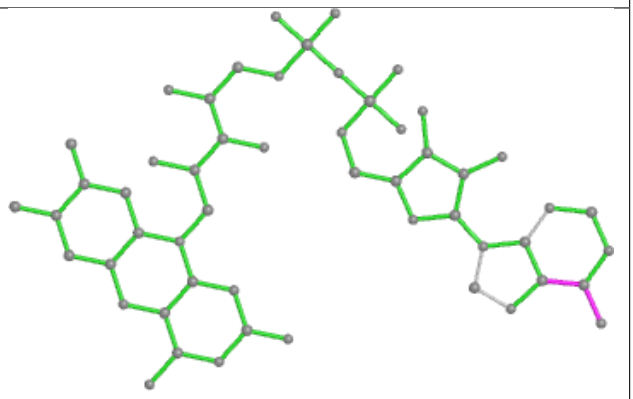


Rings

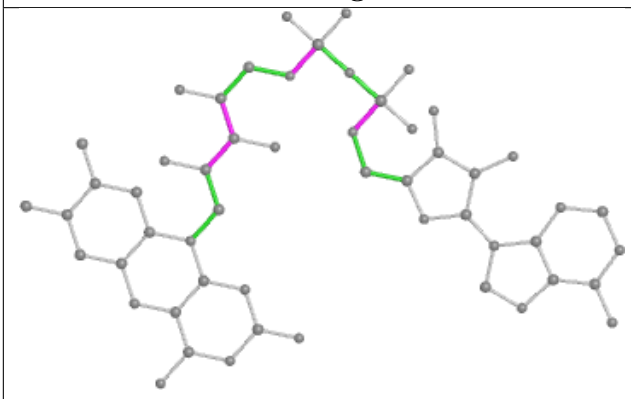
Ligand FAD N 201



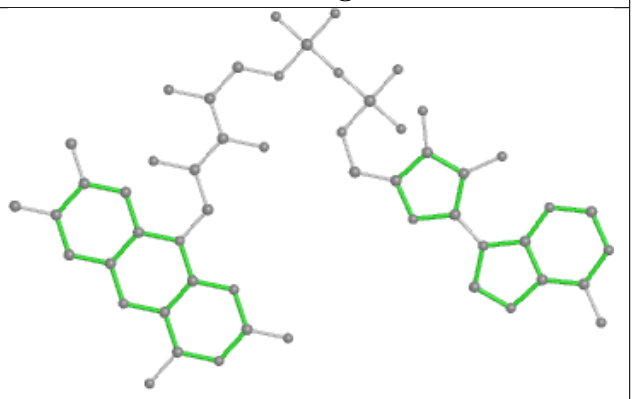
Bond lengths



Bond angles

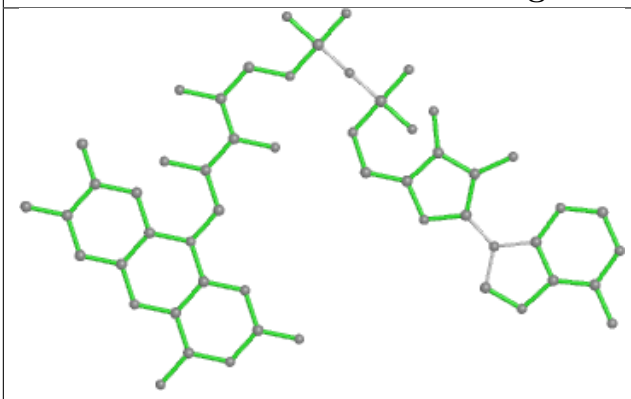


Torsions

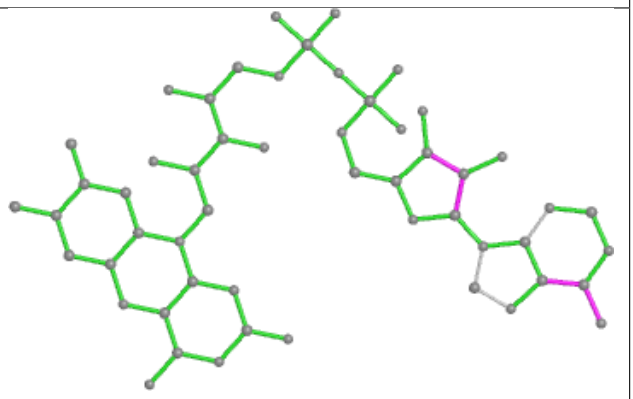


Rings

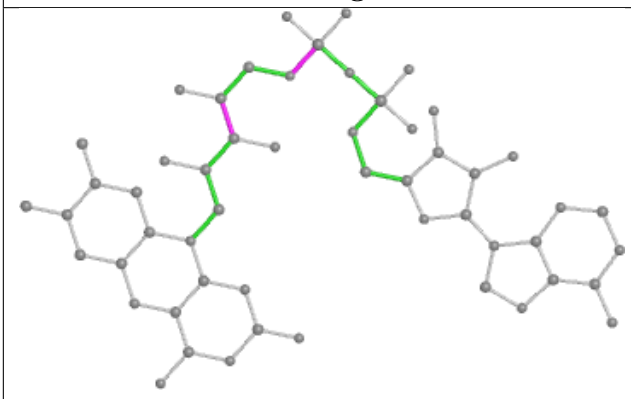
Ligand FAD S 202



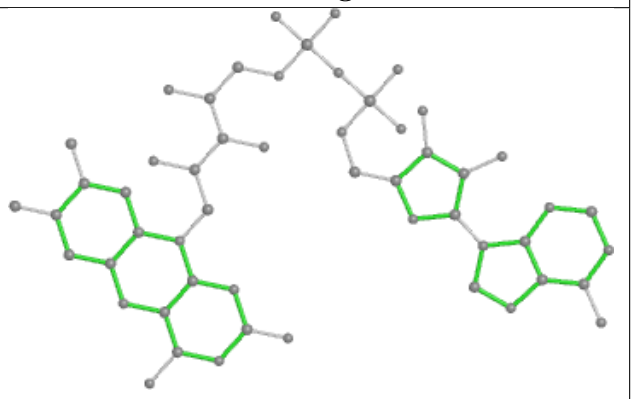
Bond lengths



Bond angles

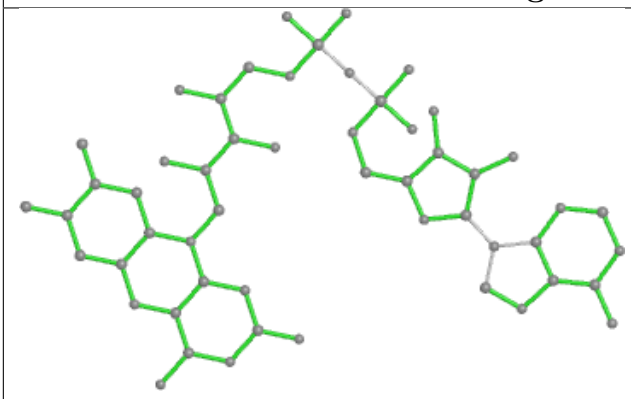


Torsions

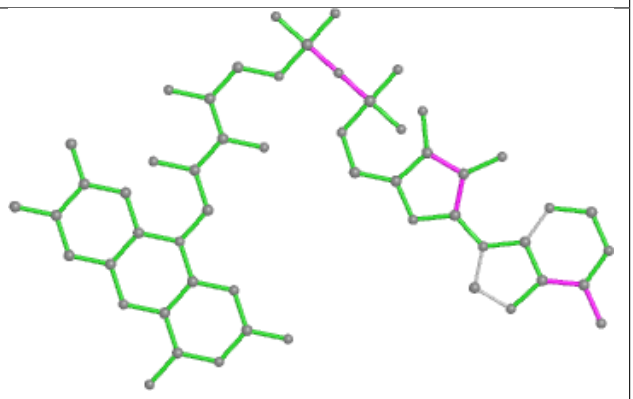


Rings

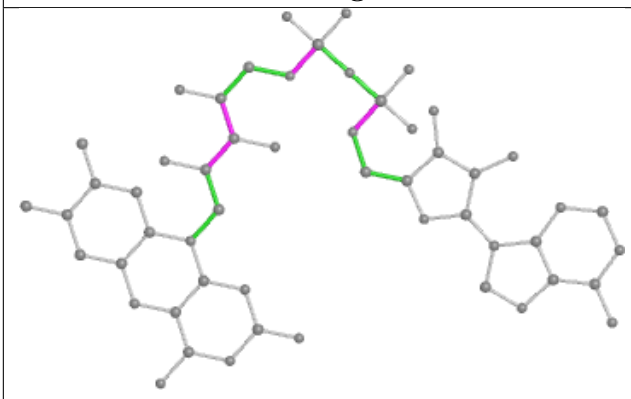
Ligand FAD L 201



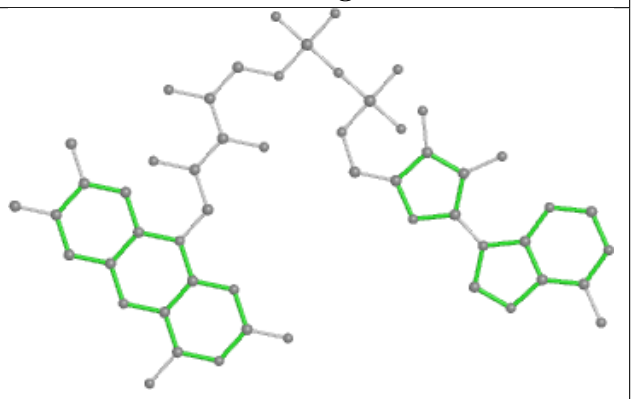
Bond lengths



Bond angles

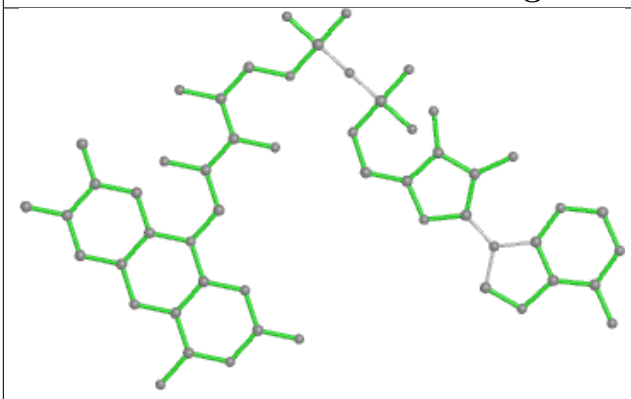


Torsions

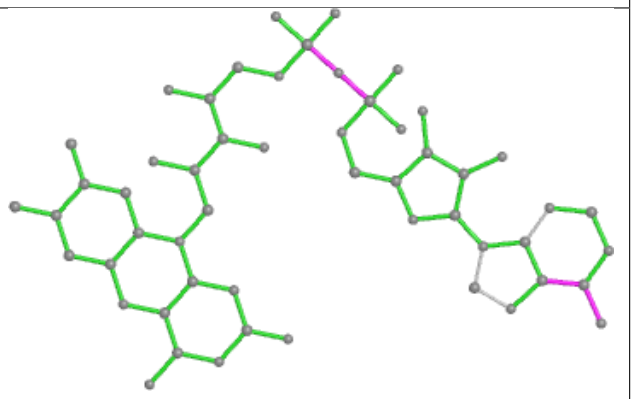


Rings

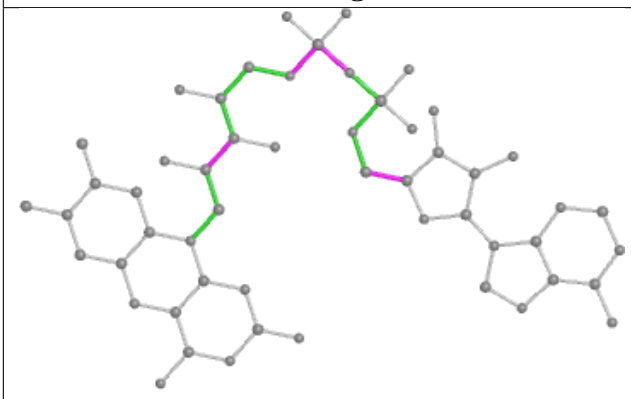
Ligand FAD G 201



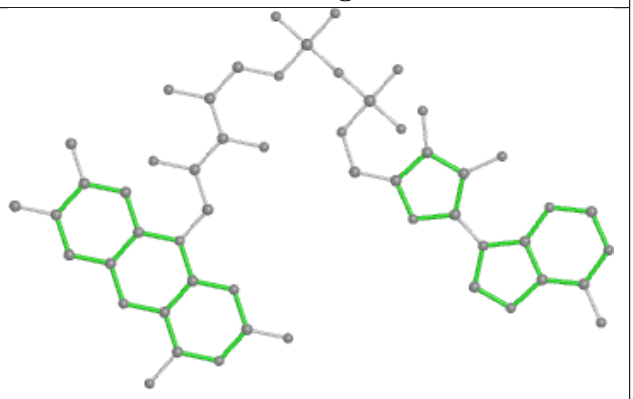
Bond lengths



Bond angles

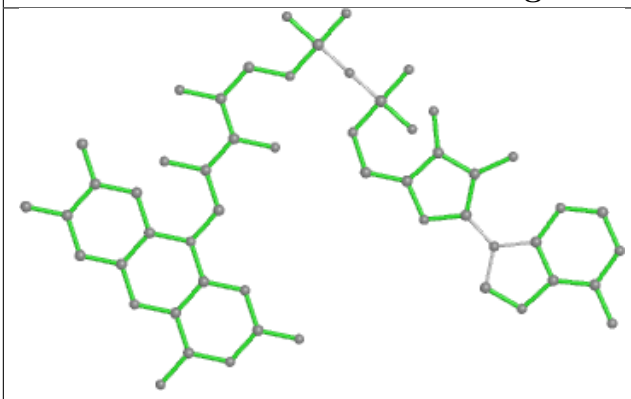


Torsions

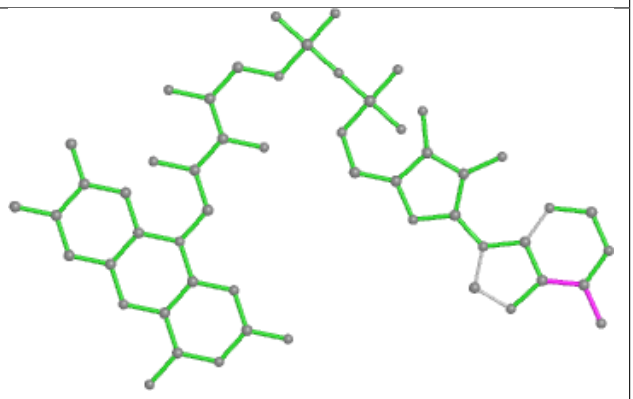


Rings

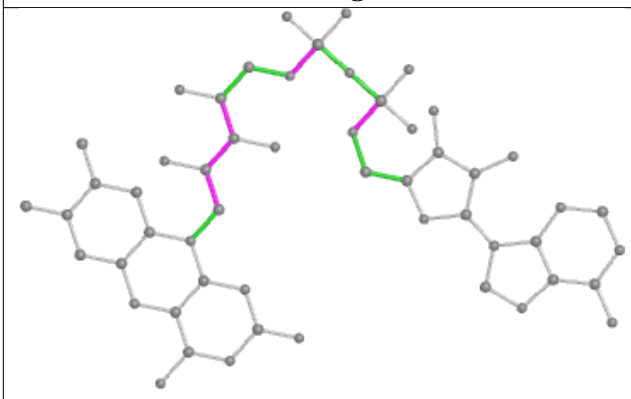
Ligand FAD A 201



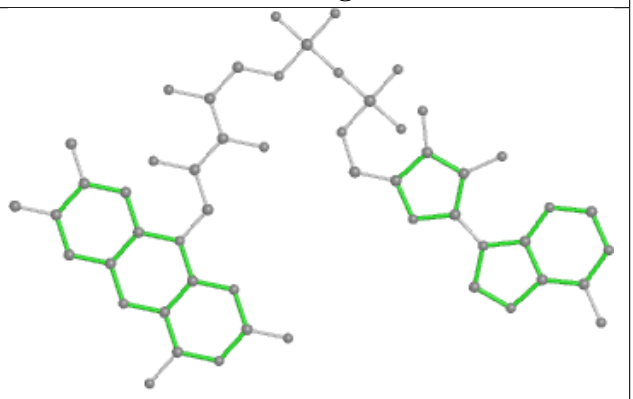
Bond lengths



Bond angles

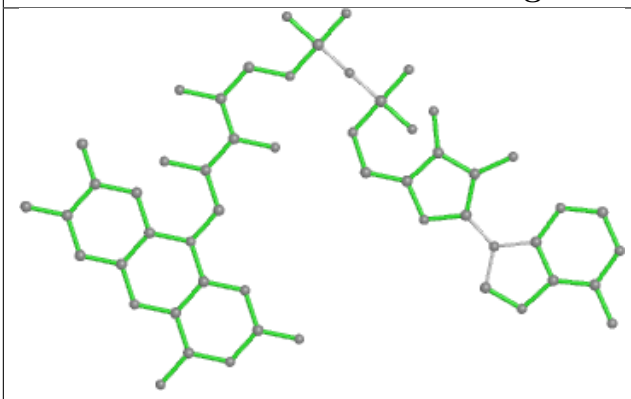


Torsions

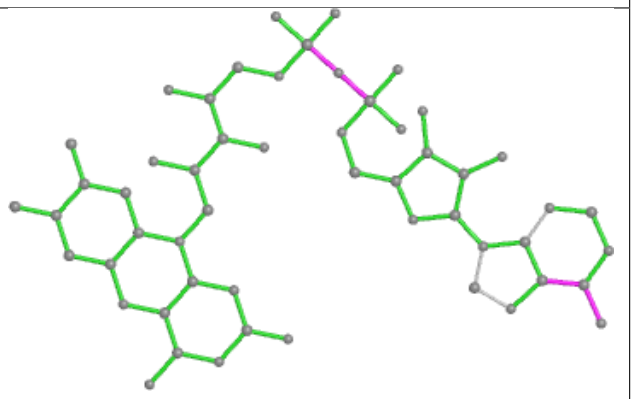


Rings

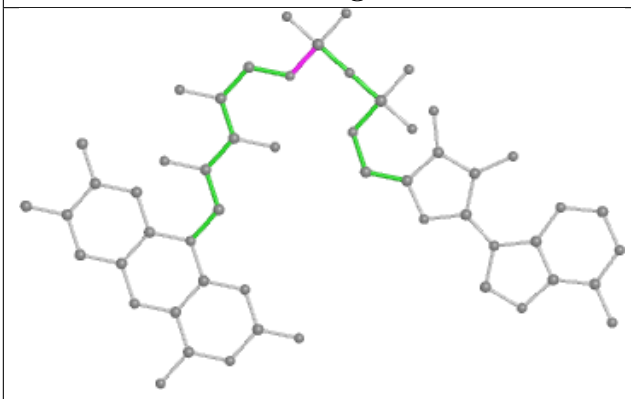
Ligand FAD H 201



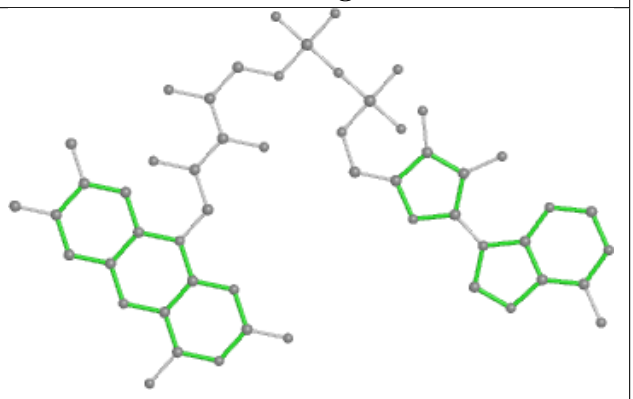
Bond lengths



Bond angles

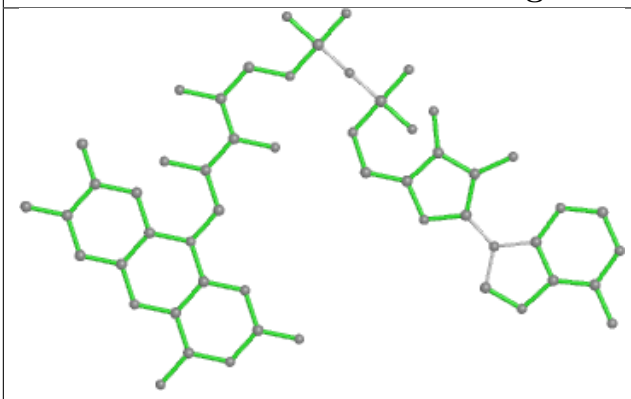


Torsions

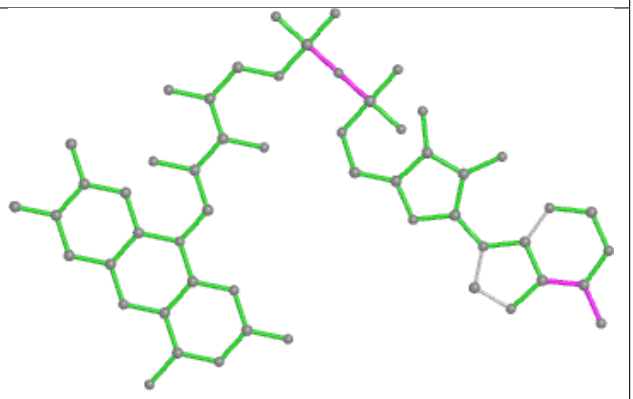


Rings

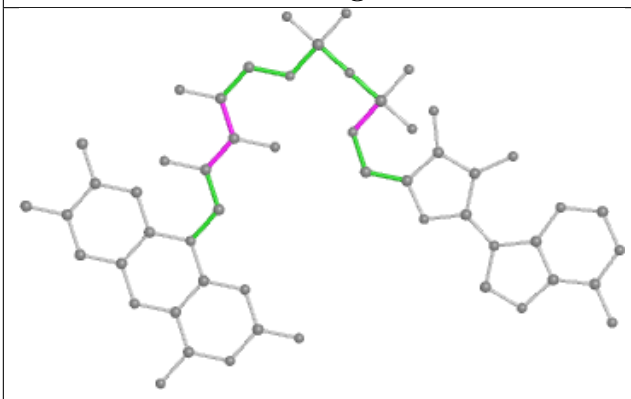
Ligand FAD E 201



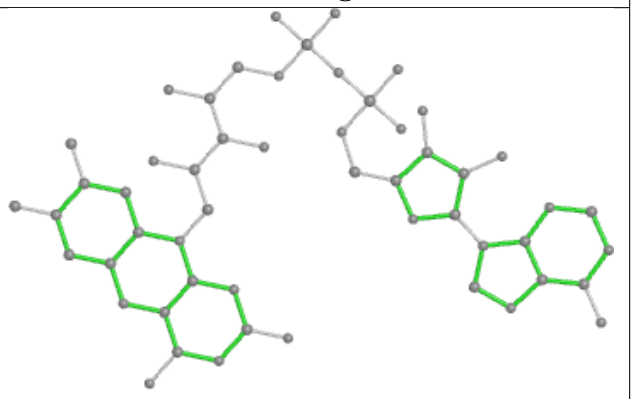
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	122/132 (92%)	-0.18	5 (4%) 37 36	11, 23, 59, 96	0
1	B	126/132 (95%)	0.10	8 (6%) 20 19	16, 30, 69, 115	0
1	C	128/132 (96%)	0.21	14 (10%) 5 4	14, 25, 83, 127	0
1	D	126/132 (95%)	0.25	12 (9%) 8 6	14, 26, 82, 125	0
1	E	124/132 (93%)	0.16	11 (8%) 9 7	16, 29, 84, 120	0
1	F	119/132 (90%)	0.73	21 (17%) 1 1	25, 47, 107, 119	0
1	G	108/132 (81%)	0.64	15 (13%) 2 2	25, 49, 96, 105	0
1	H	120/132 (90%)	0.02	7 (5%) 23 22	20, 31, 72, 93	0
1	I	115/132 (87%)	0.35	12 (10%) 6 4	19, 42, 103, 122	0
1	J	130/132 (98%)	0.35	14 (10%) 5 4	16, 34, 81, 87	0
1	K	127/132 (96%)	0.05	10 (7%) 12 10	20, 32, 69, 85	0
1	L	126/132 (95%)	0.73	22 (17%) 1 1	24, 53, 111, 146	0
1	M	120/132 (90%)	0.58	12 (10%) 7 5	28, 56, 82, 106	0
1	N	125/132 (94%)	0.17	9 (7%) 15 13	17, 36, 86, 125	0
1	O	120/132 (90%)	0.32	7 (5%) 23 22	24, 45, 77, 101	0
1	P	132/132 (100%)	0.13	9 (6%) 17 15	20, 36, 77, 92	0
1	Q	116/132 (87%)	0.57	15 (12%) 3 2	23, 52, 90, 95	0
1	R	109/132 (82%)	0.50	17 (15%) 2 1	22, 37, 101, 126	0
1	S	117/132 (88%)	0.50	12 (10%) 6 5	26, 49, 90, 105	0
1	T	113/132 (85%)	1.20	27 (23%) 0 0	39, 71, 99, 116	0
All	All	2423/2640 (91%)	0.36	259 (10%) 6 4	11, 40, 93, 146	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	118	THR	9.0
1	N	117	ALA	8.6
1	C	118	THR	8.4
1	E	118	THR	8.2
1	R	60	ALA	7.3
1	L	115	TRP	7.1
1	E	117	ALA	6.7
1	G	102	ALA	6.7
1	D	115	TRP	6.5
1	L	116	THR	6.5
1	T	99	ARG	6.4
1	L	118	THR	6.3
1	H	115	TRP	6.1
1	I	102	ALA	5.9
1	B	118	THR	5.9
1	L	119	ALA	5.8
1	D	114	PRO	5.6
1	E	114	PRO	5.6
1	N	118	THR	5.6
1	F	111	GLU	5.5
1	D	119	ALA	5.3
1	I	100	ASP	5.3
1	O	115	TRP	5.2
1	D	117	ALA	5.2
1	O	113	LEU	5.1
1	B	117	ALA	4.9
1	G	122	HIS	4.9
1	I	101	GLU	4.9
1	F	122	HIS	4.9
1	C	117	ALA	4.8
1	R	101	GLU	4.7
1	M	84	GLU	4.6
1	C	116	THR	4.5
1	B	119	ALA	4.5
1	O	114	PRO	4.5
1	L	107	ALA	4.5
1	T	112	LEU	4.5
1	L	120	LYS	4.5
1	G	121	THR	4.4
1	C	119	ALA	4.4
1	H	113	LEU	4.3
1	L	117	ALA	4.3
1	T	138	PHE	4.3

Continued on next page...

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Mol	Chain	Res	Type	RSRZ
1	J	62	GLY	4.3
1	B	116	THR	4.3
1	G	123	TRP	4.2
1	I	99	ARG	4.2
1	L	114	PRO	4.2
1	C	120	LYS	4.2
1	R	59	THR	4.1
1	L	99	ARG	4.1
1	G	99	ARG	4.0
1	G	63	THR	4.0
1	S	40	THR	4.0
1	H	114	PRO	4.0
1	R	61	GLU	4.0
1	H	137	ARG	4.0
1	P	66	VAL	4.0
1	K	62	GLY	3.9
1	P	140	PRO	3.9
1	L	61	GLU	3.9
1	F	107	ALA	3.9
1	T	121	THR	3.9
1	T	70	ILE	3.9
1	R	63	THR	3.8
1	M	99	ARG	3.8
1	L	103	ASP	3.8
1	E	14	THR	3.8
1	R	100	ASP	3.7
1	S	60	ALA	3.7
1	S	42	HIS	3.7
1	F	99	ARG	3.7
1	K	12	ALA	3.6
1	T	107	ALA	3.6
1	I	108	GLN	3.6
1	A	121	THR	3.6
1	S	39	ASN	3.6
1	Q	62	GLY	3.6
1	F	105	ALA	3.5
1	B	137	ARG	3.5
1	J	105	ALA	3.5
1	H	84	GLU	3.5
1	O	121	THR	3.5
1	L	137	ARG	3.5
1	F	103	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	61	GLU	3.4
1	T	122	HIS	3.4
1	I	107	ALA	3.4
1	C	137	ARG	3.4
1	T	16	LEU	3.4
1	F	13	VAL	3.4
1	C	115	TRP	3.4
1	R	121	THR	3.3
1	F	100	ASP	3.3
1	F	123	TRP	3.3
1	P	12	ALA	3.3
1	L	101	GLU	3.3
1	Q	137	ARG	3.3
1	T	108	GLN	3.3
1	T	120	LYS	3.2
1	J	11	ASP	3.2
1	D	13	VAL	3.2
1	N	116	THR	3.2
1	F	108	GLN	3.2
1	I	106	GLU	3.2
1	T	15	ILE	3.2
1	E	115	TRP	3.2
1	G	100	ASP	3.2
1	M	114	PRO	3.1
1	R	66	VAL	3.1
1	Q	15	ILE	3.1
1	N	38	ASP	3.1
1	P	38	ASP	3.1
1	F	121	THR	3.1
1	I	105	ALA	3.1
1	F	101	GLU	3.1
1	F	62	GLY	3.0
1	D	116	THR	3.0
1	E	83	VAL	3.0
1	J	10	GLY	3.0
1	I	83	VAL	3.0
1	L	113	LEU	3.0
1	O	112	LEU	3.0
1	G	61	GLU	3.0
1	P	141	GLU	3.0
1	R	58	ARG	3.0
1	C	136	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	R	37	VAL	3.0
1	N	115	TRP	2.9
1	C	122	HIS	2.9
1	G	60	ALA	2.9
1	J	70	ILE	2.9
1	J	109	ARG	2.9
1	T	62	GLY	2.9
1	E	84	GLU	2.9
1	B	121	THR	2.9
1	G	137	ARG	2.9
1	Q	107	ALA	2.9
1	M	108	GLN	2.9
1	F	67	SER	2.9
1	H	83	VAL	2.9
1	G	62	GLY	2.8
1	T	137	ARG	2.8
1	A	120	LYS	2.8
1	J	106	GLU	2.8
1	F	63	THR	2.8
1	Q	13	VAL	2.8
1	T	98	VAL	2.8
1	F	11	ASP	2.8
1	Q	70	ILE	2.8
1	A	114	PRO	2.8
1	N	114	PRO	2.7
1	J	12	ALA	2.7
1	T	60	ALA	2.7
1	O	84	GLU	2.7
1	R	70	ILE	2.7
1	Q	110	ALA	2.7
1	Q	99	ARG	2.7
1	C	114	PRO	2.7
1	K	137	ARG	2.7
1	E	136	PHE	2.6
1	S	62	GLY	2.6
1	M	19	THR	2.6
1	F	40	THR	2.6
1	F	102	ALA	2.6
1	A	112	LEU	2.6
1	R	102	ALA	2.6
1	T	133	GLY	2.6
1	J	38	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	T	100	ASP	2.6
1	E	113	LEU	2.5
1	Q	61	GLU	2.5
1	M	39	ASN	2.5
1	T	104	LEU	2.5
1	J	103	ASP	2.5
1	J	102	ALA	2.5
1	L	108	GLN	2.5
1	L	104	LEU	2.5
1	P	67	SER	2.5
1	I	103	ASP	2.5
1	F	110	ALA	2.4
1	L	105	ALA	2.4
1	S	38	ASP	2.4
1	E	119	ALA	2.4
1	M	59	THR	2.4
1	E	137	ARG	2.4
1	F	106	GLU	2.4
1	M	101	GLU	2.4
1	J	64	LYS	2.4
1	L	58	ARG	2.4
1	T	61	GLU	2.4
1	O	137	ARG	2.4
1	P	13	VAL	2.4
1	D	60	ALA	2.3
1	F	38	ASP	2.3
1	Q	100	ASP	2.3
1	S	85	GLN	2.3
1	B	99	ARG	2.3
1	S	70	ILE	2.3
1	C	138	PHE	2.3
1	K	39	ASN	2.3
1	S	84	GLU	2.3
1	K	38	ASP	2.3
1	Q	112	LEU	2.3
1	R	98	VAL	2.3
1	T	83	VAL	2.3
1	R	67	SER	2.2
1	D	61	GLU	2.2
1	N	84	GLU	2.2
1	H	38	ASP	2.2
1	K	65	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	121	THR	2.2
1	L	100	ASP	2.2
1	R	62	GLY	2.2
1	L	121	THR	2.2
1	T	33	ILE	2.2
1	Q	103	ASP	2.2
1	T	36	THR	2.2
1	D	111	GLU	2.2
1	R	99	ARG	2.2
1	S	37	VAL	2.2
1	L	102	ALA	2.2
1	I	122	HIS	2.1
1	Q	104	LEU	2.1
1	G	59	THR	2.1
1	J	99	ARG	2.1
1	M	138	PHE	2.1
1	M	60	ALA	2.1
1	Q	105	ALA	2.1
1	T	20	GLU	2.1
1	K	138	PHE	2.1
1	D	38	ASP	2.1
1	K	69	ALA	2.1
1	S	122	HIS	2.1
1	Q	101	GLU	2.1
1	T	123	TRP	2.1
1	L	112	LEU	2.1
1	P	62	GLY	2.1
1	C	110	ALA	2.1
1	J	68	ALA	2.1
1	G	39	ASN	2.1
1	K	67	SER	2.1
1	I	82	ASP	2.1
1	P	11	ASP	2.1
1	A	38	ASP	2.1
1	G	101	GLU	2.1
1	C	13	VAL	2.1
1	R	64	LYS	2.1
1	T	136	PHE	2.1
1	C	121	THR	2.0
1	B	138	PHE	2.0
1	T	32	ARG	2.0
1	N	39	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	S	41	SER	2.0
1	K	66	VAL	2.0
1	M	98	VAL	2.0
1	T	17	SER	2.0
1	N	137	ARG	2.0
1	G	13	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	Q	202	53/53	0.68	0.38	33,61,91,97	53
2	FAD	E	202	53/53	0.81	0.27	27,49,69,75	53
2	FAD	S	202	53/53	0.81	0.26	44,66,89,96	53
2	FAD	S	201	53/53	0.82	0.22	53,69,89,95	53
2	FAD	G	201	53/53	0.84	0.24	37,57,91,106	53
2	FAD	N	201	53/53	0.91	0.17	33,48,83,88	0
2	FAD	Q	201	53/53	0.93	0.17	18,43,68,77	0
2	FAD	N	202	53/53	0.93	0.15	28,45,65,73	0
2	FAD	A	201	53/53	0.94	0.15	19,27,42,50	0
2	FAD	D	201	53/53	0.94	0.15	20,31,47,67	0
2	FAD	L	201	53/53	0.94	0.16	30,46,68,78	0
2	FAD	C	201	53/53	0.95	0.13	16,29,53,68	0
2	FAD	O	201	53/53	0.95	0.13	19,32,54,59	0
2	FAD	I	201	53/53	0.95	0.14	18,28,53,71	0
2	FAD	B	201	53/53	0.96	0.13	20,29,41,45	0
2	FAD	E	201	53/53	0.96	0.12	24,39,52,57	0
2	FAD	H	201	53/53	0.96	0.13	27,39,49,51	0

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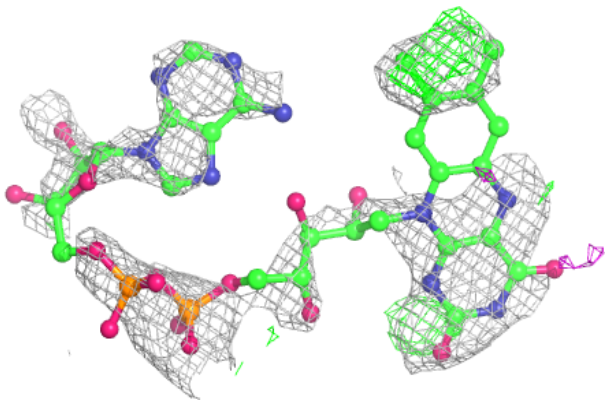
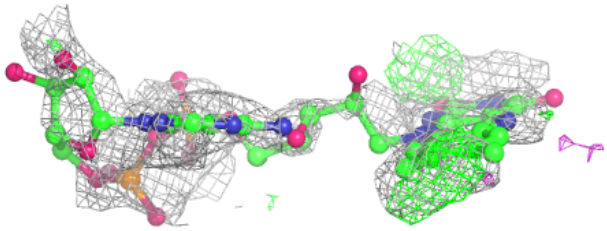
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	A	202	1/1	0.98	0.10	25,25,25,25	0

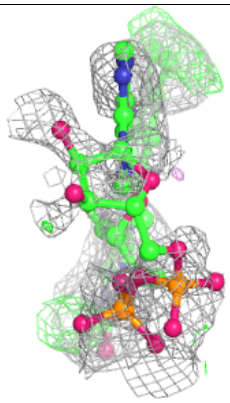
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD Q 202:

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

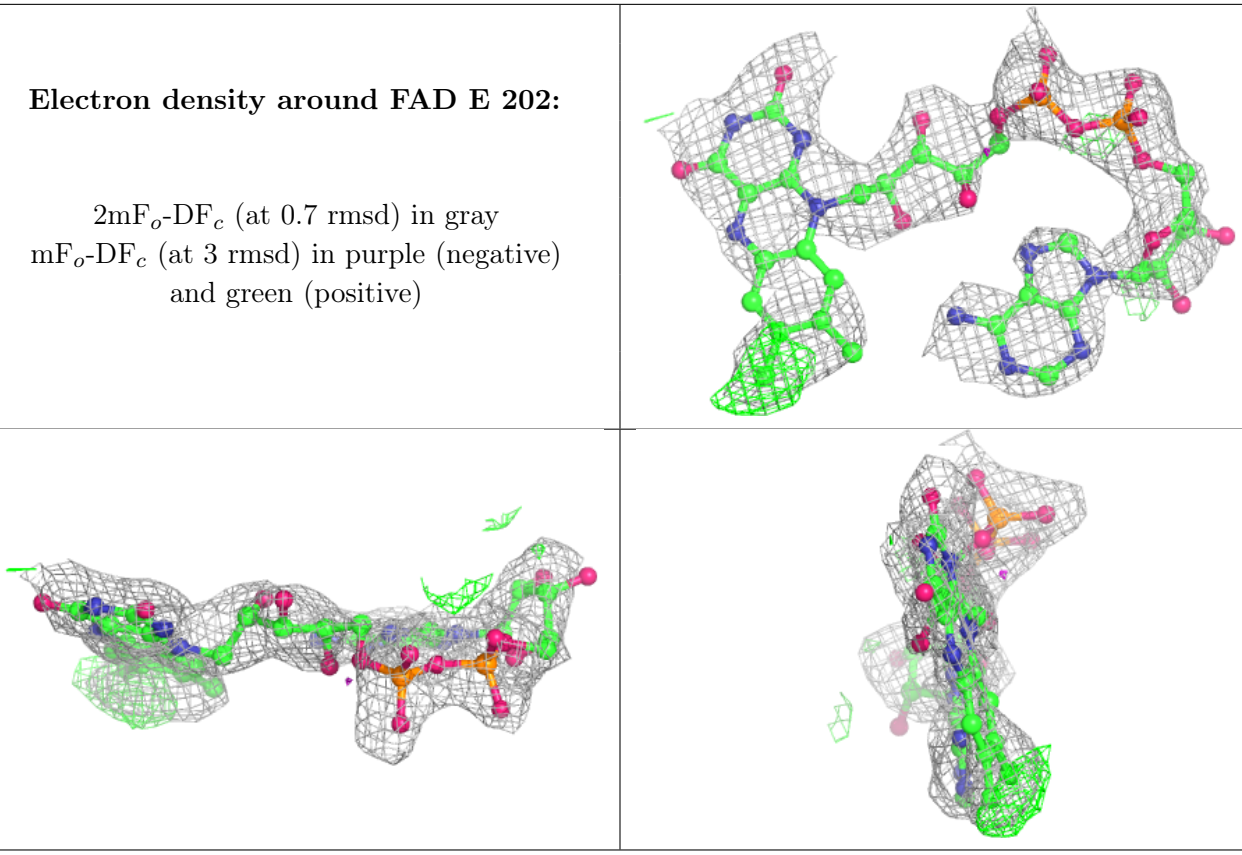






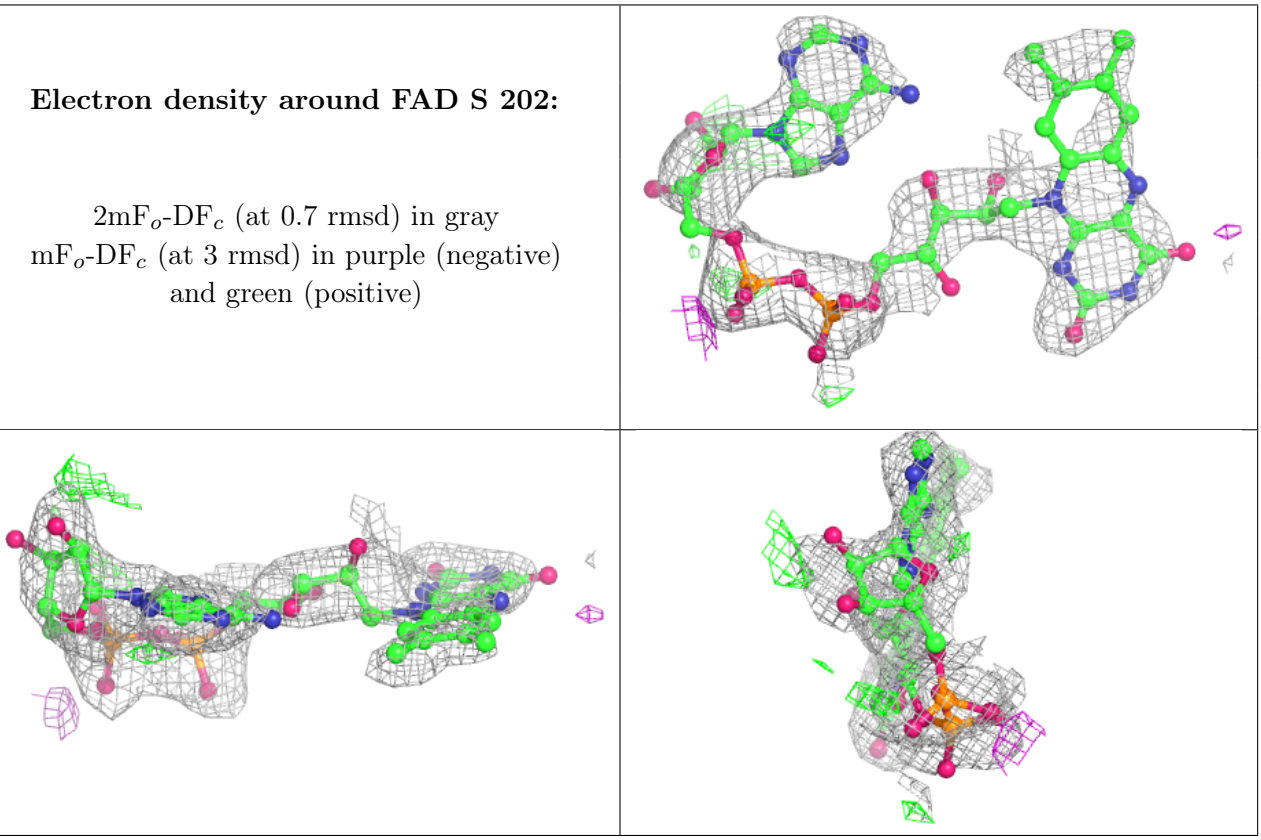
Electron density around FAD E 202:

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



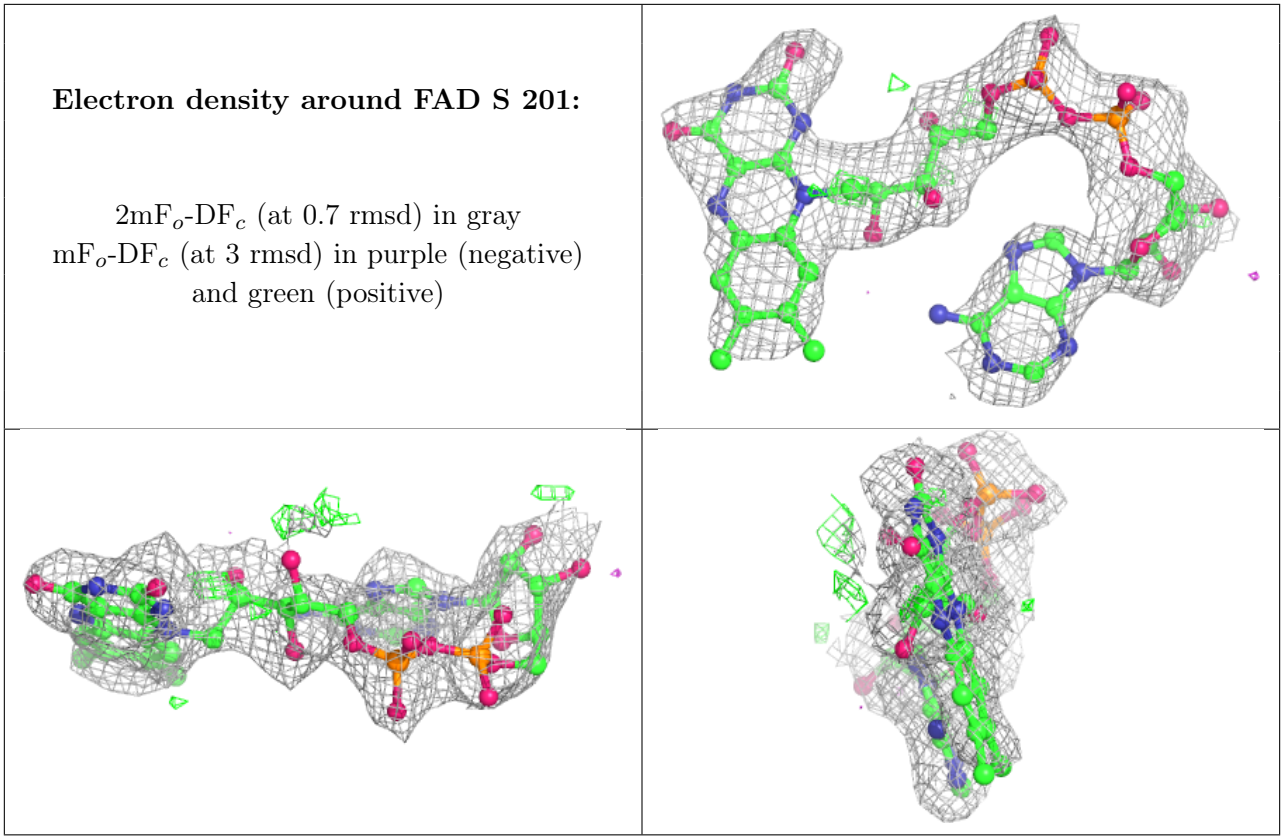
Electron density around FAD S 202:

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



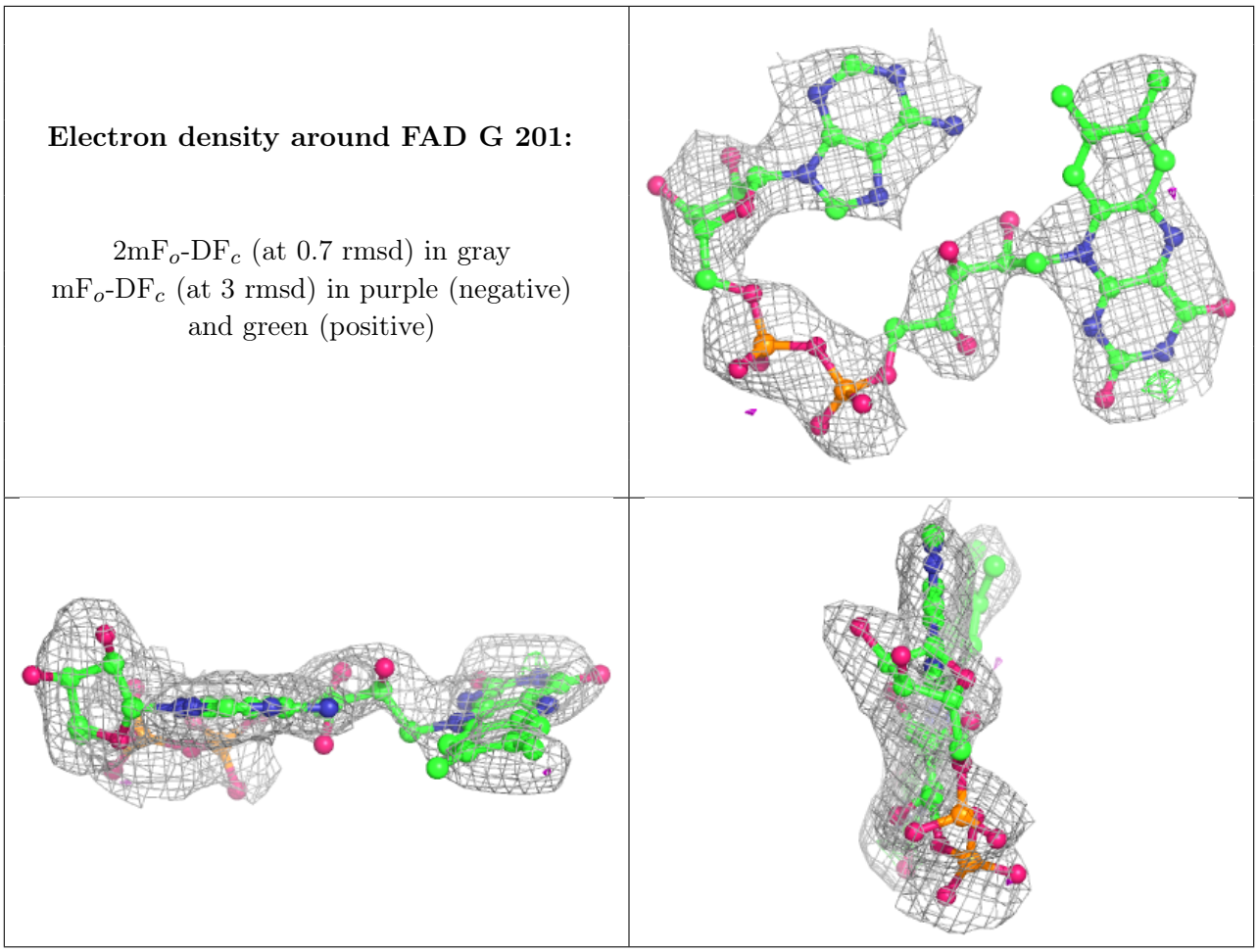
Electron density around FAD S 201:

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



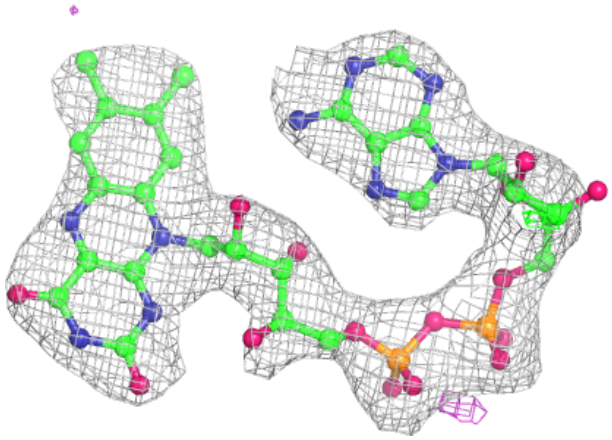
Electron density around FAD G 201:

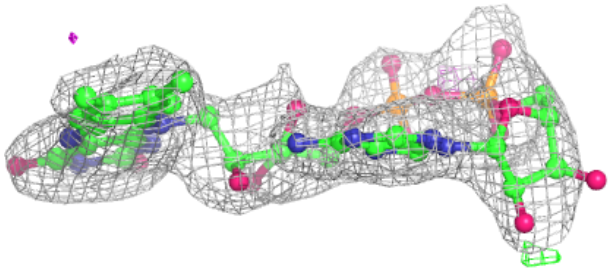
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

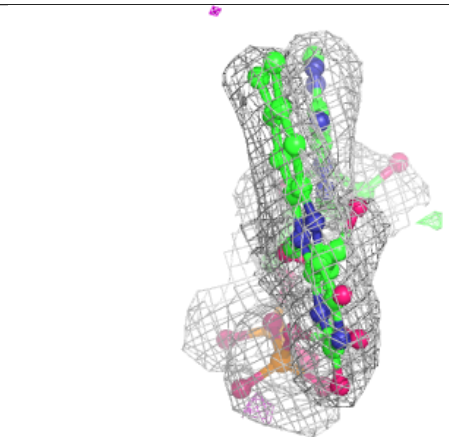


Electron density around FAD N 201:

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

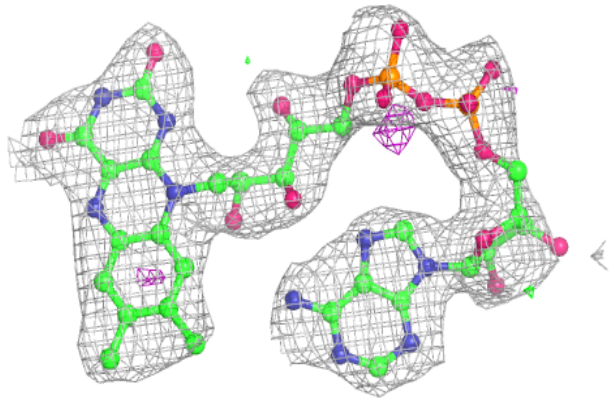


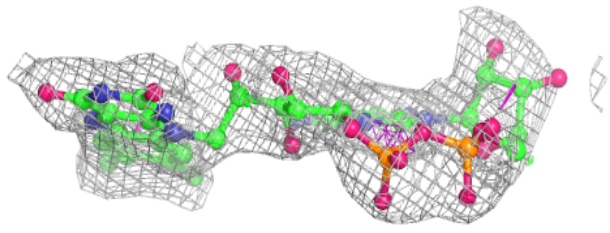


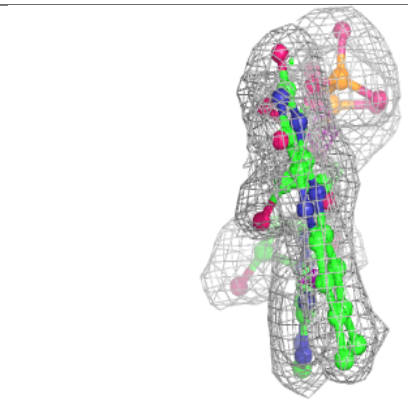


Electron density around FAD Q 201:

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

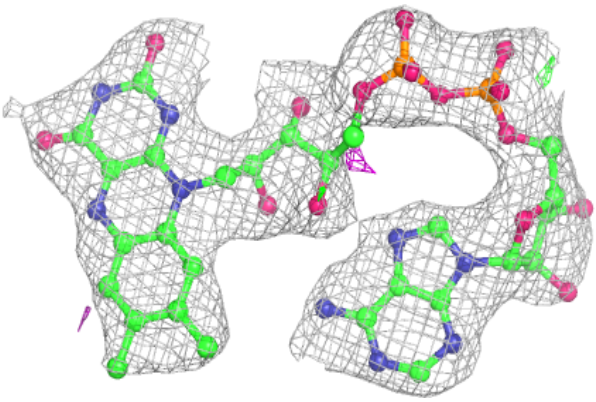


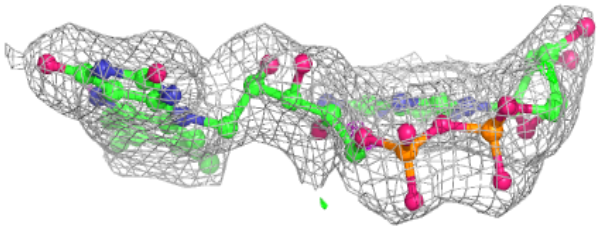


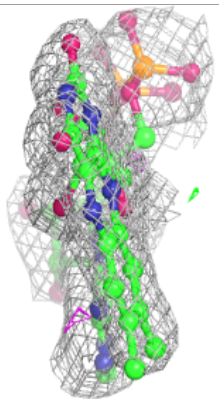


Electron density around FAD N 202:

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

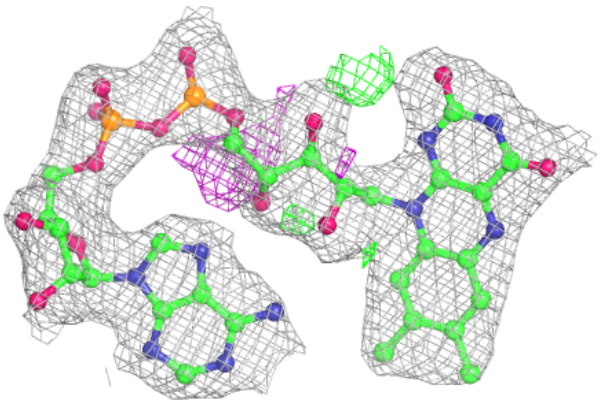


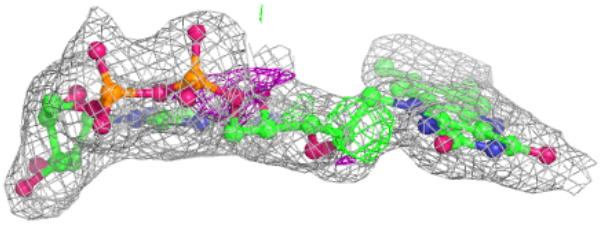


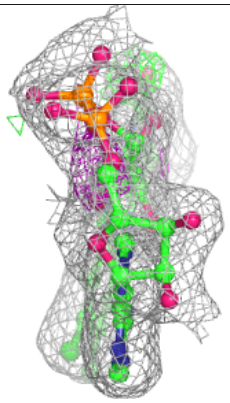


Electron density around FAD A 201:

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

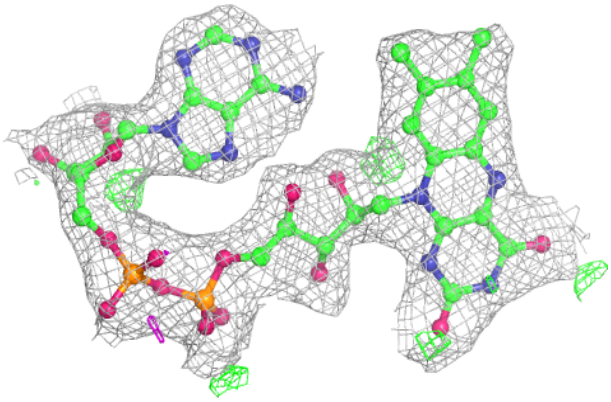


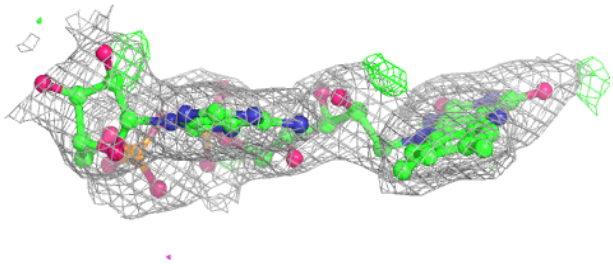


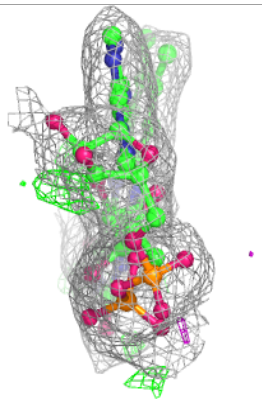


Electron density around FAD D 201:

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

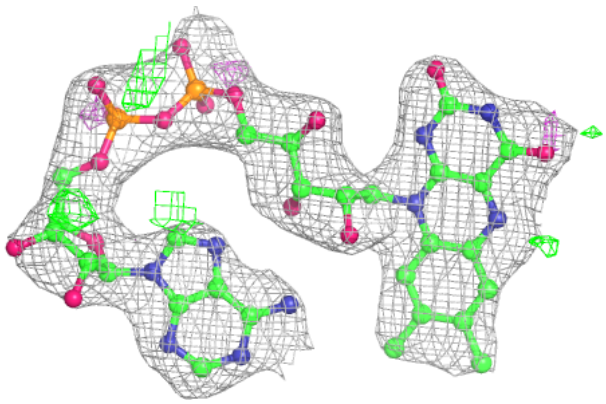


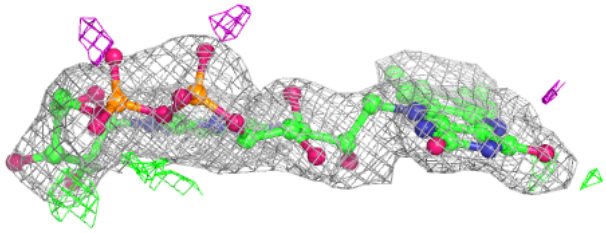


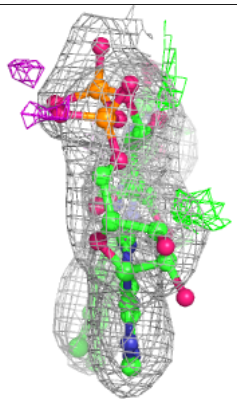


Electron density around FAD L 201:

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

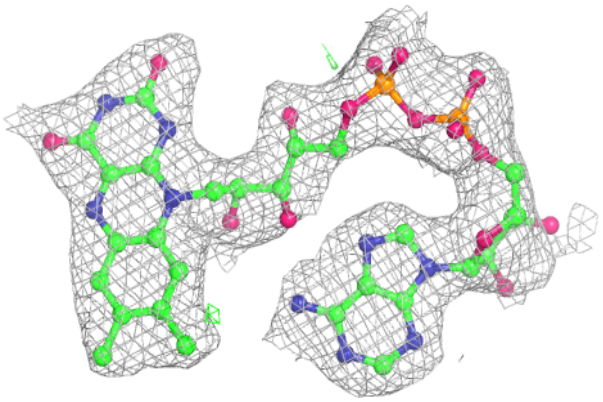


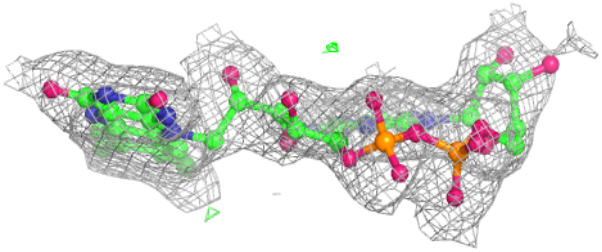


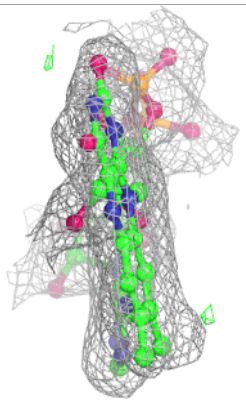


Electron density around FAD C 201:

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

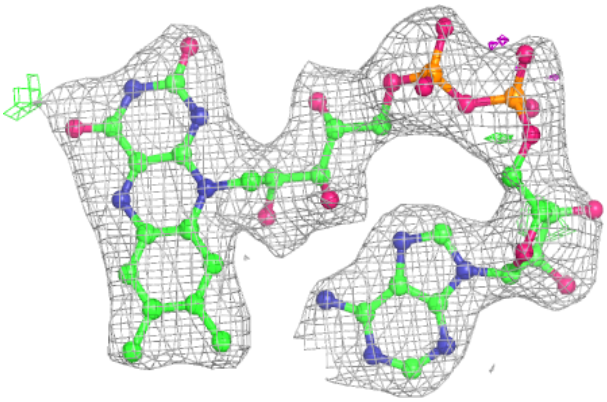


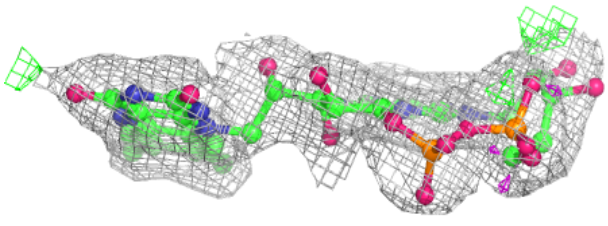


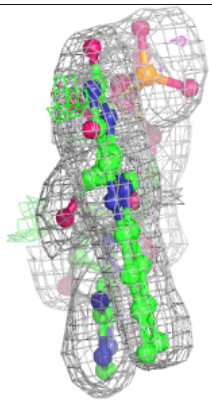


Electron density around FAD O 201:

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

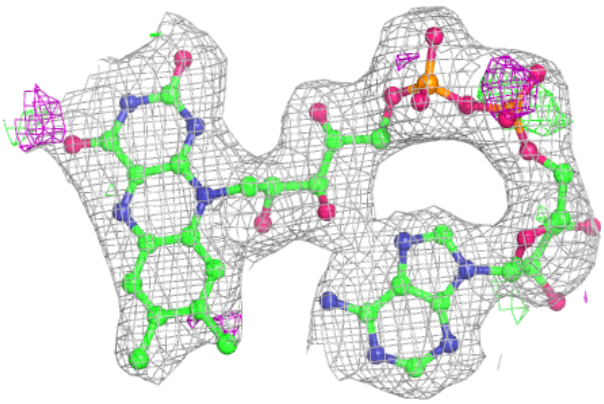


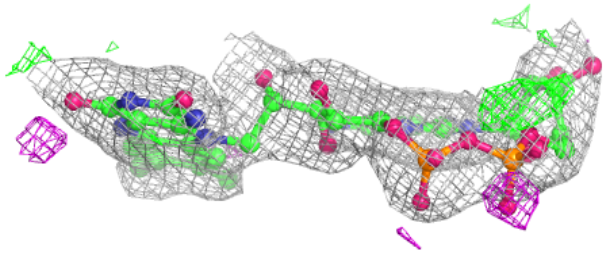


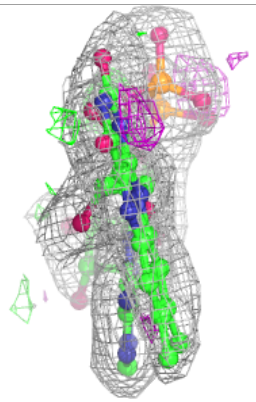


Electron density around FAD I 201:

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

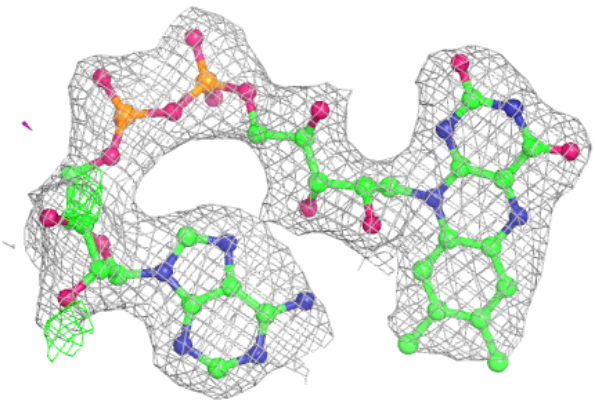


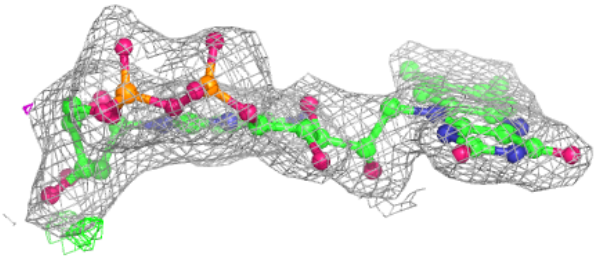


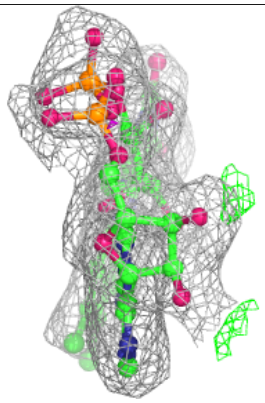


Electron density around FAD B 201:

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

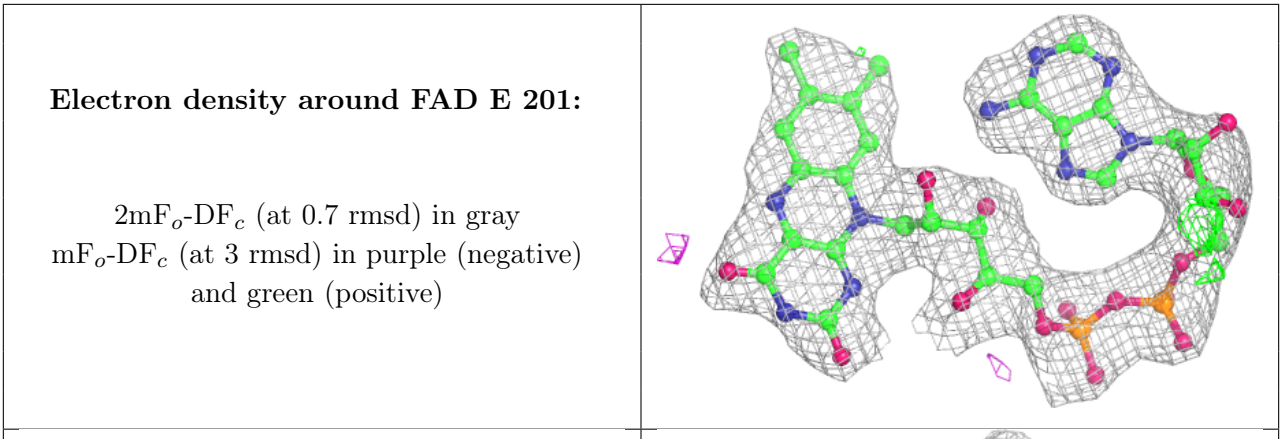






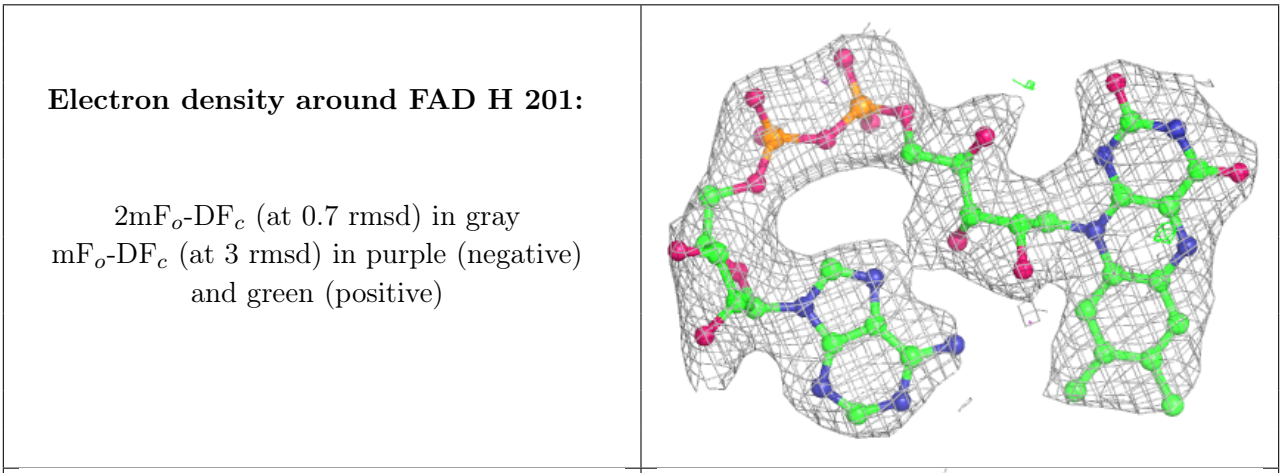
Electron density around FAD E 201:

$2mF_o$-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 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)



6.5 Other polymers (i)

There are no such residues in this entry.