Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 06:33 pm GMT

PDB ID	:	2VZ2
Title	:	Human MAO B in complex with mofegiline
Authors	:	Bonivento, D.; Mattevi, A.
Deposited on	:	2008-07-29
Resolution	:	2.30 Å(reported)

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

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

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

PERCENTILES INFOmissingINFO

1 Entry composition

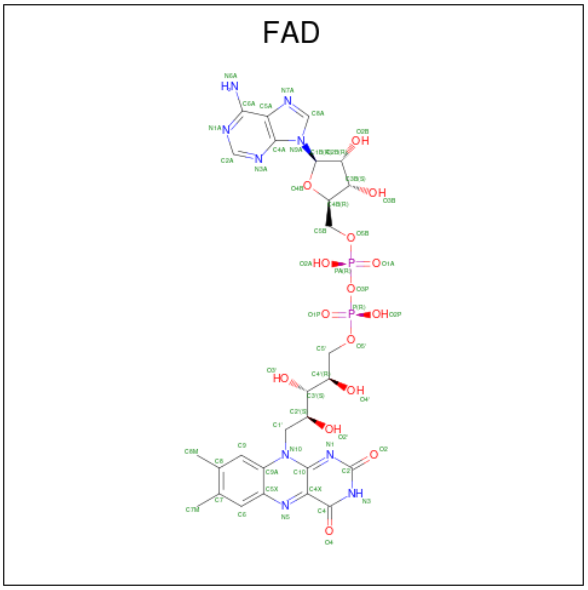
There are 5 unique types of molecules in this entry. The entry contains 8528 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AMINE OXIDASE [FLAVIN-CONTAINING] B.

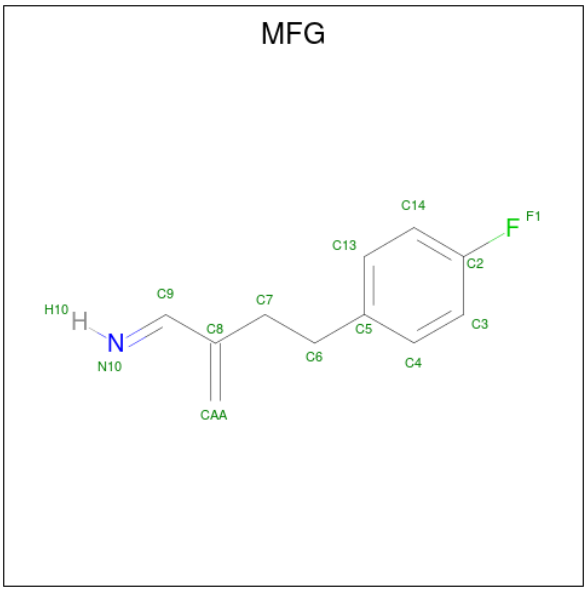
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	1	0
			3979	2545	681	728	25			
1	B	494	Total	C	N	O	S	0	0	0
			3940	2519	676	721	24			

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



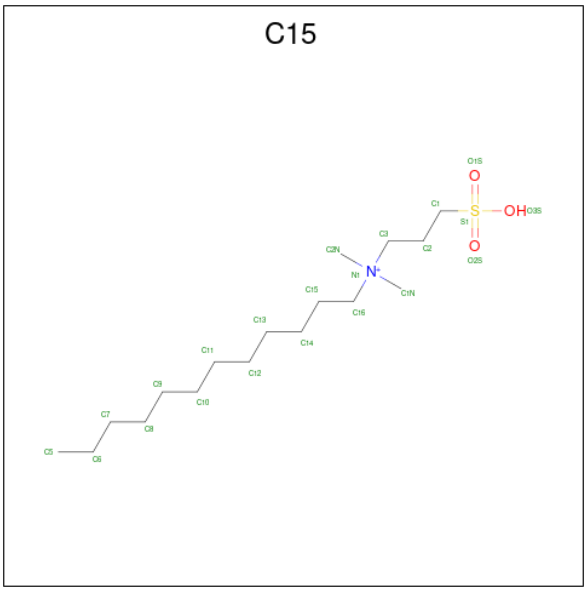
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is (1Z)-4-(4-FLUOROPHENYL)-2-METHYLIDENEBUTAN-1-IMINE (three-letter code: MFG) (formula: $C_{11}H_{12}FN$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	0	0
			13	11	1	1		
3	B	1	Total	C	F	N	0	0
			13	11	1	1		

- Molecule 4 is N-DODECYL-N,N-DIMETHYL-3-AMMONIO-1-PROPANESULFONATE (three-letter code: C15) (formula: $C_{17}H_{38}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			22	17	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			22	17	1	3	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	197	Total	O	0	0
			197	197		
5	B	236	Total	O	0	0
			236	236		

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	132.03Å 223.73Å 86.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.74 – 2.30 29.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.74-2.30) 97.6 (29.73-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.187 , 0.229 0.195 , 0.234	Depositor DCC
R_{free} test set	1449 reflections (2.59%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.007 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.015 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8528	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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.

3 Model quality

3.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MFG, FAD, C15

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	0.40	0/4073	0.52	0/5529
1	B	0.40	0/4037	0.53	0/5479
All	All	0.40	0/8110	0.52	0/11008

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

3.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3979	0	3985	28	0
1	B	3940	0	3937	30	0
2	A	53	0	29	1	0
2	B	53	0	29	3	0
3	A	13	0	10	2	0
3	B	13	0	10	2	0
4	A	22	0	38	1	0
4	B	22	0	38	0	0
5	A	197	0	0	3	0
5	B	236	0	0	2	0
All	All	8528	0	8076	55	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 3.

All (55) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ALA:HB1	1:B:280:MET:HE1	1.53	0.89
1:A:242:ARG:HE	1:A:246:LEU:HD11	1.46	0.79
1:B:117:ASN:HD22	1:B:120:ARG:HH21	1.35	0.74
1:A:323:PRO:HB3	1:A:352:LEU:HD11	1.78	0.65
1:A:353:ALA:CB	1:B:280:MET:HE1	2.28	0.63
1:A:117:ASN:HD22	1:A:120:ARG:HH21	1.46	0.63
1:A:435:TYR:CE2	3:A:1503:MFG:H9	2.38	0.59
1:B:435:TYR:CE2	3:B:1498:MFG:H9	2.38	0.58
1:A:251:ASN:HD22	1:A:251:ASN:H	1.51	0.58
1:B:308:LYS:HE2	5:B:2176:HOH:O	2.05	0.56
1:A:251:ASN:H	1:A:251:ASN:ND2	2.04	0.56
1:B:117:ASN:HD22	1:B:120:ARG:NH2	2.05	0.54
1:B:251:ASN:ND2	1:B:251:ASN:H	2.05	0.53
1:A:252:HIS:CE1	1:B:248:GLU:OE2	2.63	0.52
1:B:323:PRO:HD2	1:B:367:LEU:HD22	1.92	0.52
1:B:251:ASN:H	1:B:251:ASN:HD22	1.58	0.51
1:A:280:MET:HG3	1:B:389:CYS:HB2	1.91	0.51
1:B:71:LEU:O	1:B:75:LEU:HG	2.11	0.51
1:B:111:THR:HG22	1:B:115:HIS:CD2	2.46	0.51
1:B:387:ASN:O	1:B:390:GLU:HG2	2.11	0.51
1:B:146:MET:HB2	1:B:150:GLU:HG3	1.94	0.49
1:A:28:LEU:HD11	1:A:454:MET:CE	2.43	0.49
1:A:242:ARG:NE	1:A:246:LEU:HD11	2.23	0.48
1:B:281:MET:HB3	1:B:413:VAL:HG11	1.95	0.48
1:B:17:MET:HE3	1:B:225:LEU:HD12	1.95	0.48
1:B:117:ASN:ND2	1:B:120:ARG:HH21	2.09	0.47
1:A:126:GLY:O	1:A:190:LYS:HG3	2.15	0.47
1:A:323:PRO:CB	1:A:352:LEU:HD11	2.44	0.47
1:A:412:ARG:HD2	5:A:2162:HOH:O	2.15	0.46
1:A:280:MET:CE	1:B:353:ALA:HB1	2.45	0.46
1:B:309:LYS:N	1:B:309:LYS:HD2	2.31	0.45
1:A:252:HIS:CD2	1:B:252:HIS:HD2	2.34	0.44
1:A:280:MET:HE2	1:B:353:ALA:HB1	1.98	0.44
1:B:148:MET:O	1:B:152:LEU:HG	2.18	0.44
1:A:280:MET:HB3	1:A:280:MET:HE3	1.67	0.44
1:B:226:GLY:O	5:B:2119:HOH:O	2.21	0.43
1:A:344:ILE:HD13	1:A:352:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LYS:HA	4:A:1504:C15:H3C2	2.01	0.43
2:A:1502:FAD:C4X	3:A:1503:MFG:C9	2.96	0.43
2:B:1497:FAD:C4X	3:B:1498:MFG:C9	2.97	0.42
1:B:8:VAL:HG23	1:B:257:ALA:HB2	2.01	0.42
1:B:195:THR:O	1:B:199:ILE:HG12	2.19	0.42
1:A:403:PRO:HG2	5:A:2113:HOH:O	2.20	0.42
1:A:60:TYR:HB3	1:A:206:GLN:HA	2.01	0.42
1:A:271:LYS:HE2	5:A:2154:HOH:O	2.19	0.42
1:B:237:TYR:HB3	1:B:248:GLU:HB3	2.01	0.41
2:B:1497:FAD:N1	2:B:1497:FAD:H2'	2.35	0.41
1:A:265:PRO:HA	1:A:266:PRO:HD3	1.97	0.41
1:A:323:PRO:HB3	1:A:352:LEU:CD1	2.48	0.41
1:B:416:GLN:HA	1:B:417:PRO:HD3	1.94	0.41
1:A:23:LEU:HB2	1:A:30:VAL:HG11	2.03	0.41
1:B:454:MET:HE3	1:B:454:MET:HB2	1.77	0.41
1:B:28:LEU:HD21	1:B:456:LYS:HE3	2.03	0.41
2:B:1497:FAD:H9	2:B:1497:FAD:H1'1	1.89	0.41
1:A:322:ALA:HA	1:A:323:PRO:HD2	1.98	0.40

There are no symmetry-related clashes.

3.3 Torsion angles (i)

3.3.1 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	498/520 (96%)	489 (98%)	9 (2%)	0	100	100
1	B	492/520 (95%)	482 (98%)	10 (2%)	0	100	100
All	All	990/1040 (95%)	971 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

3.3.2 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	429/444 (97%)	421 (98%)	8 (2%)	57 73
1	B	424/444 (96%)	415 (98%)	9 (2%)	53 70
All	All	853/888 (96%)	836 (98%)	17 (2%)	55 72

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	ARG
1	A	251	ASN
1	A	280	MET
1	A	321	GLU
1	A	350	ARG
1	A	379	GLU
1	A	397	CYS
1	A	441	GLU
1	B	78	GLU
1	B	93	LYS
1	B	95	LYS
1	B	103	PHE
1	B	251	ASN
1	B	350	ARG
1	B	379	GLU
1	B	397	CYS
1	B	495	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	251	ASN
1	A	252	HIS
1	A	284	GLN
1	A	387	ASN

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Mol	Chain	Res	Type
1	A	452	HIS
1	B	117	ASN
1	B	251	ASN

3.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

3.6 Ligand geometry (i)

6 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	MFG	A	1503	2	11,13,13	0.84	0	12,16,16	1.04	0
4	C15	B	1499	-	21,21,21	1.80	1 (4%)	25,26,26	1.10	2 (8%)
2	FAD	B	1497	3,1	53,58,58	1.18	2 (3%)	68,89,89	1.41	11 (16%)
3	MFG	B	1498	2	11,13,13	0.88	0	12,16,16	0.99	0
2	FAD	A	1502	3,1	53,58,58	1.14	3 (5%)	68,89,89	1.42	12 (17%)
4	C15	A	1504	-	21,21,21	1.74	1 (4%)	25,26,26	0.98	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MFG	A	1503	2	-	3/5/7/7	0/1/1/1
4	C15	B	1499	-	-	10/21/21/21	-
2	FAD	B	1497	3,1	-	3/30/50/50	0/6/6/6
3	MFG	B	1498	2	-	2/5/7/7	0/1/1/1
2	FAD	A	1502	3,1	-	2/30/50/50	0/6/6/6
4	C15	A	1504	-	-	7/21/21/21	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1499	C15	C1-S1	-7.28	1.67	1.77
4	A	1504	C15	C1-S1	-7.07	1.67	1.77
2	B	1497	FAD	C4X-N5	6.07	1.42	1.30
2	A	1502	FAD	C4X-N5	5.95	1.42	1.30
2	A	1502	FAD	C4-N3	-2.10	1.34	1.38
2	A	1502	FAD	C10-N10	2.10	1.41	1.37
2	B	1497	FAD	C10-N10	2.01	1.41	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1497	FAD	N3A-C2A-N1A	-5.30	120.39	128.68
2	A	1502	FAD	N3A-C2A-N1A	-4.84	121.11	128.68
2	A	1502	FAD	C9A-C5X-N5	-3.66	118.45	122.43
2	B	1497	FAD	C9A-C5X-N5	-3.52	118.60	122.43
4	B	1499	C15	O3S-S1-C1	2.72	110.17	105.77
2	A	1502	FAD	C4X-C4-N3	2.66	119.95	113.19
2	A	1502	FAD	C4-N3-C2	-2.66	120.73	125.64
4	A	1504	C15	O3S-S1-C1	2.63	110.02	105.77
4	B	1499	C15	O2S-S1-C1	2.60	110.05	106.92
2	B	1497	FAD	C4-N3-C2	-2.55	120.93	125.64
2	B	1497	FAD	C9A-N10-C10	-2.54	116.81	120.77
2	B	1497	FAD	C4X-C4-N3	2.54	119.64	113.19
2	A	1502	FAD	O4-C4-C4X	-2.47	120.05	126.60
2	B	1497	FAD	O4-C4-C4X	-2.44	120.12	126.60
2	A	1502	FAD	C9A-N10-C10	-2.44	116.96	120.77
2	A	1502	FAD	C4A-C5A-N7A	-2.32	106.98	109.40
2	A	1502	FAD	C4X-C10-N1	-2.31	119.36	124.73
2	A	1502	FAD	C10-C4X-N5	-2.27	120.03	124.86
2	B	1497	FAD	C4X-C10-N1	-2.25	119.52	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1504	C15	O2S-S1-C1	2.24	109.61	106.92
2	A	1502	FAD	C5'-C4'-C3'	-2.23	107.90	112.20
2	A	1502	FAD	P-O3P-PA	-2.15	125.43	132.83
2	B	1497	FAD	C10-C4X-N5	-2.13	120.34	124.86
2	B	1497	FAD	O4B-C1B-C2B	-2.11	103.84	106.93
2	B	1497	FAD	C4A-C5A-N7A	-2.07	107.24	109.40
2	B	1497	FAD	P-O3P-PA	-2.01	125.94	132.83
2	A	1502	FAD	C4-C4X-N5	2.00	121.08	118.23

There are no chirality outliers.

All (27) torsion outliers are listed below:

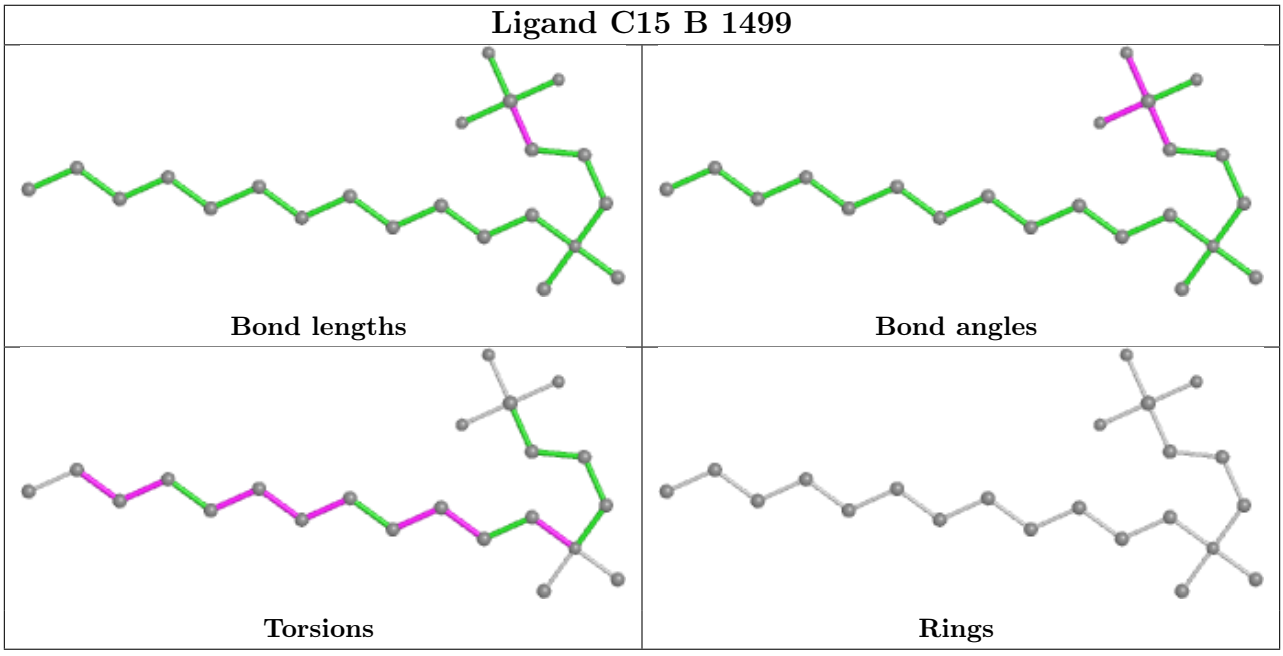
Mol	Chain	Res	Type	Atoms
2	B	1497	FAD	C2'-C1'-N10-C10
3	A	1503	MFG	C5-C6-C7-C8
3	B	1498	MFG	C5-C6-C7-C8
4	B	1499	C15	C15-C16-N1-C1N
4	B	1499	C15	C15-C16-N1-C2N
4	B	1499	C15	C15-C16-N1-C3
4	A	1504	C15	C9-C10-C11-C12
4	B	1499	C15	C11-C10-C9-C8
4	B	1499	C15	C10-C11-C12-C13
4	A	1504	C15	C11-C10-C9-C8
4	B	1499	C15	C12-C13-C14-C15
4	B	1499	C15	C13-C14-C15-C16
4	A	1504	C15	S1-C1-C2-C3
2	A	1502	FAD	C2'-C1'-N10-C10
4	B	1499	C15	C9-C10-C11-C12
4	A	1504	C15	C7-C8-C9-C10
4	A	1504	C15	C10-C11-C12-C13
4	A	1504	C15	C12-C13-C14-C15
4	B	1499	C15	C5-C6-C7-C8
3	A	1503	MFG	C6-C7-C8-C9
3	A	1503	MFG	C6-C7-C8-CAA
4	A	1504	C15	C5-C6-C7-C8
2	B	1497	FAD	PA-O3P-P-O5'
4	B	1499	C15	C6-C7-C8-C9
2	A	1502	FAD	O4B-C4B-C5B-O5B
2	B	1497	FAD	O4B-C4B-C5B-O5B
3	B	1498	MFG	C6-C7-C8-C9

There are no ring outliers.

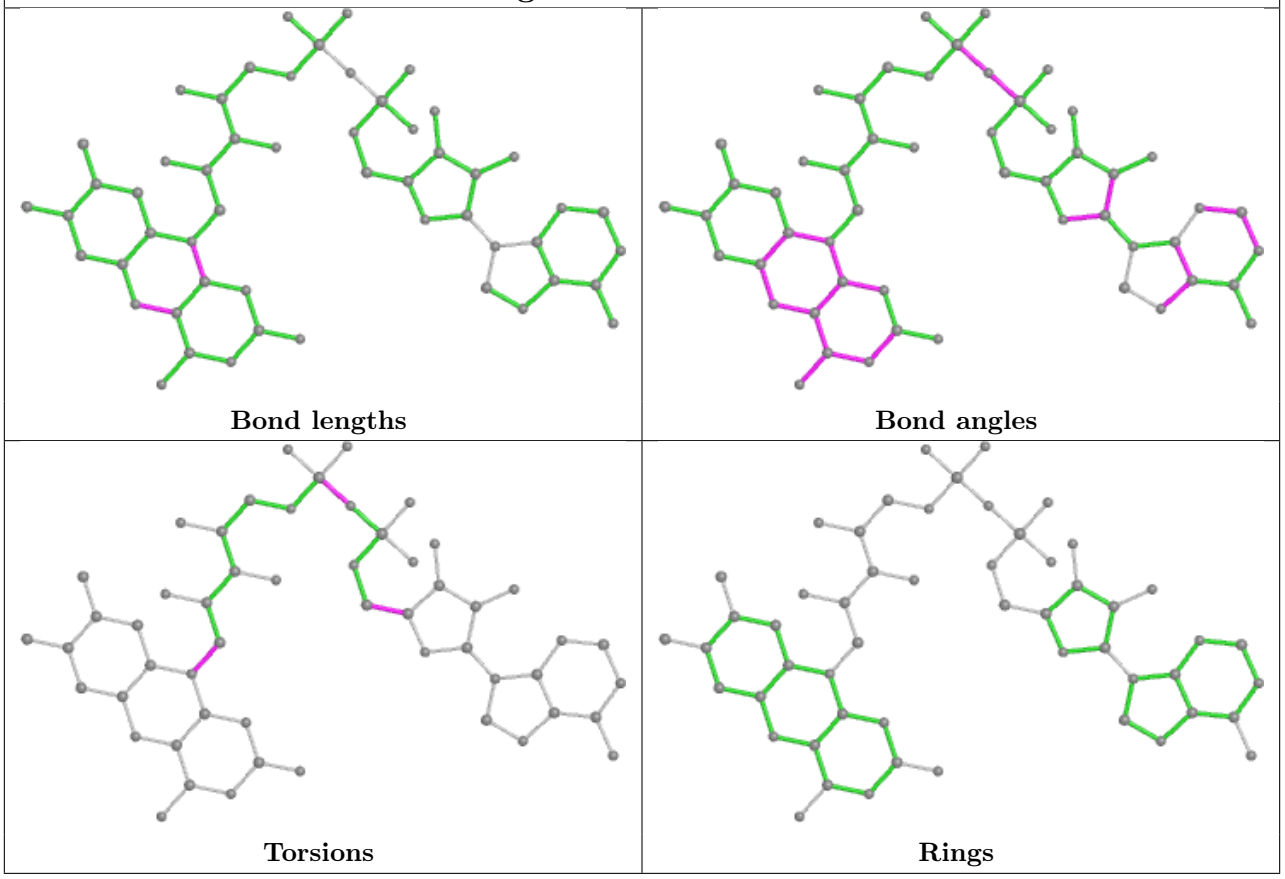
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1503	MFG	2	0
2	B	1497	FAD	3	0
3	B	1498	MFG	2	0
2	A	1502	FAD	1	0
4	A	1504	C15	1	0

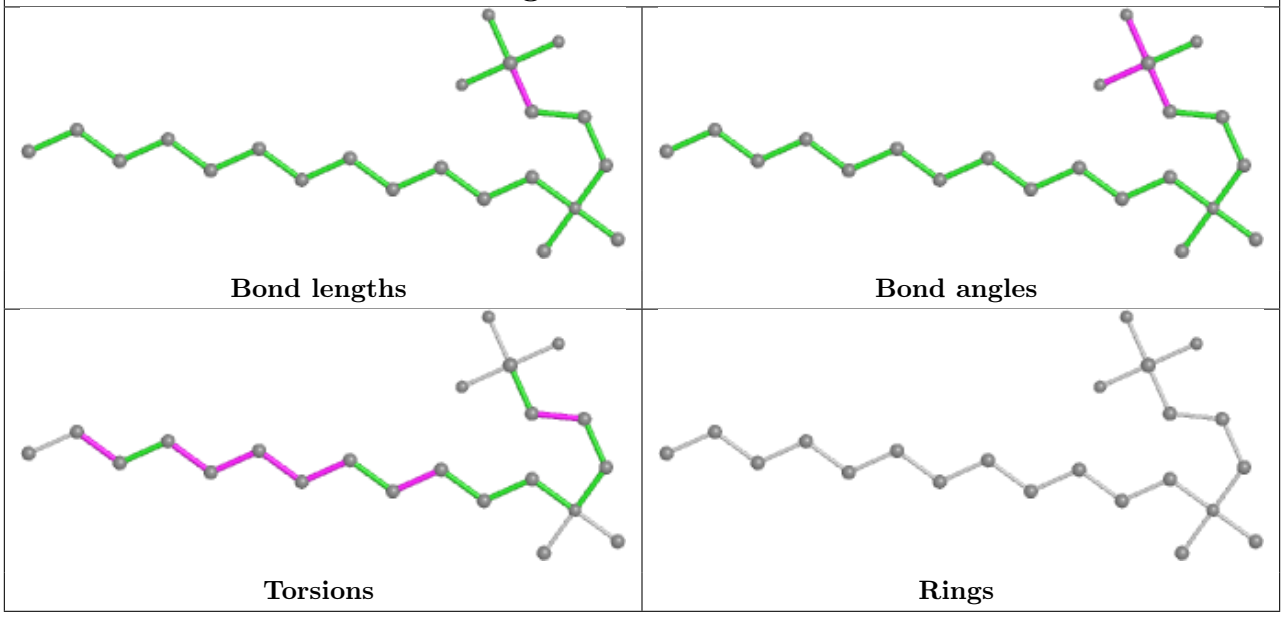
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand FAD B 1497



Ligand C15 A 1504



3.7 Other polymers (i)

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

4 Fit of model and data

4.1 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	499/520 (95%)	-0.15	15 (3%)	50	57	17, 21, 36, 56	0
1	B	494/520 (95%)	-0.10	14 (2%)	53	60	16, 21, 35, 47	0
All	All	993/1040 (95%)	-0.13	29 (2%)	51	58	16, 21, 35, 56	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	107	TRP	3.9
1	B	495	LEU	3.9
1	A	498	LEU	3.8
1	A	3	ASN	3.8
1	A	501	ILE	3.5
1	B	3	ASN	3.2
1	B	243	GLU	3.2
1	A	252	HIS	3.1
1	B	4	LYS	3.1
1	A	500	THR	3.0
1	A	4	LYS	2.8
1	A	227	ASP	2.8
1	B	496	ILE	2.7
1	B	494	ARG	2.7
1	B	242	ARG	2.5
1	A	460	ASP	2.5
1	A	243	GLU	2.4
1	A	458	PRO	2.4
1	A	107	TRP	2.3
1	B	480	THR	2.3
1	B	354	ARG	2.3
1	A	244	ASN	2.2
1	B	481	PHE	2.2
1	B	252	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	254	MET	2.2
1	B	244	ASN	2.2
1	A	494	ARG	2.2
1	A	459	GLU	2.1
1	B	254	MET	2.0

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

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

4.3 Carbohydrates (i)

There are no monosaccharides in this entry.

4.4 Ligands (i)

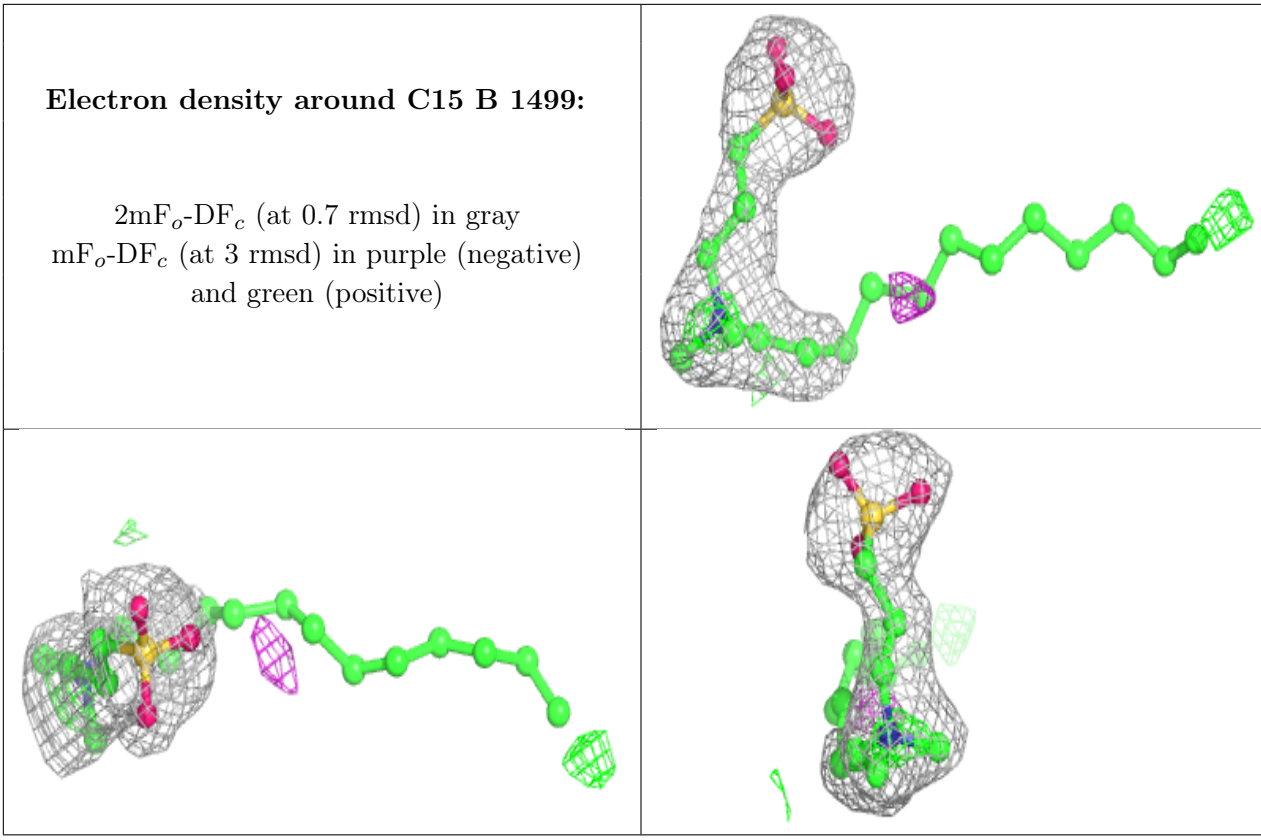
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	C15	B	1499	22/22	0.77	0.35	75,76,81,82	0
4	C15	A	1504	22/22	0.85	0.21	49,53,59,60	0
3	MFG	A	1503	13/13	0.91	0.22	26,30,31,31	0
3	MFG	B	1498	13/13	0.92	0.21	26,32,33,34	0
2	FAD	A	1502	53/53	0.96	0.15	18,20,24,24	0
2	FAD	B	1497	53/53	0.97	0.15	18,20,22,23	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.

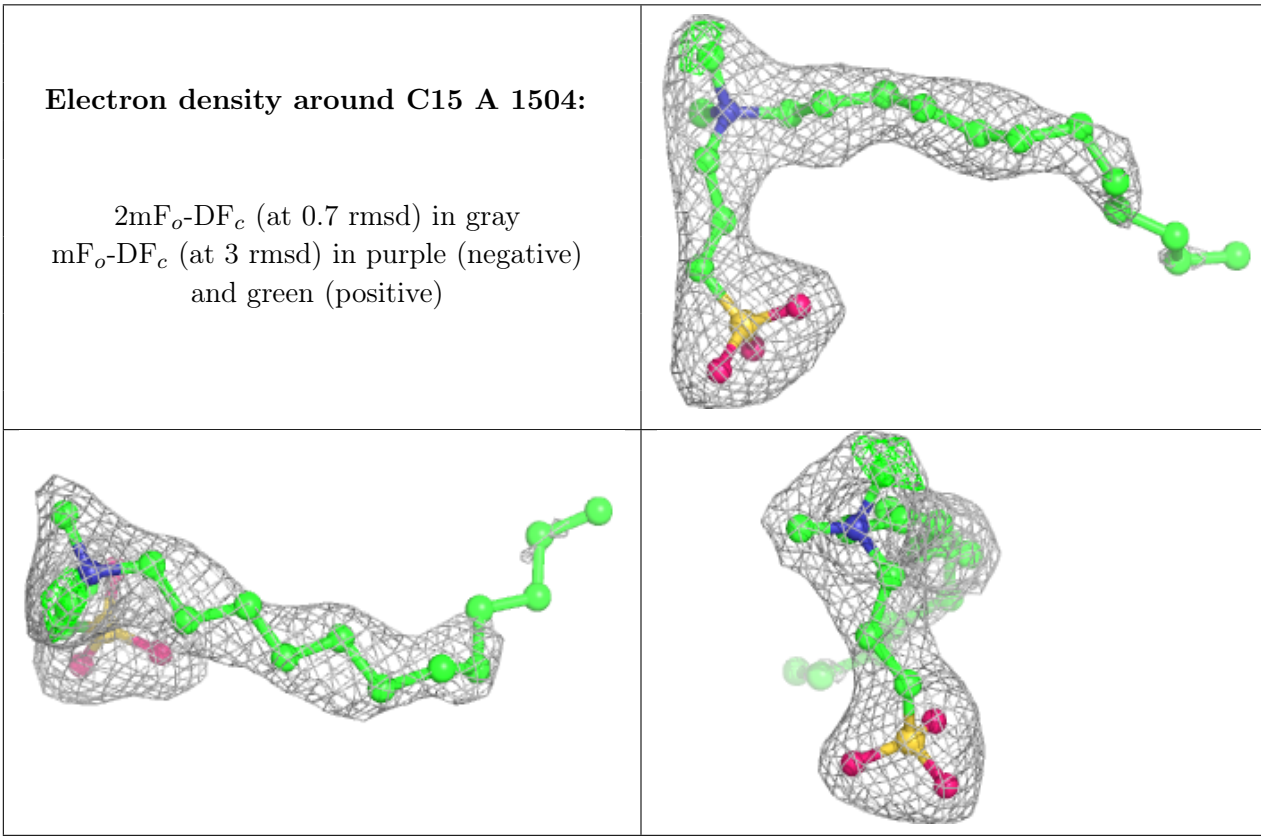
Electron density around C15 B 1499:

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



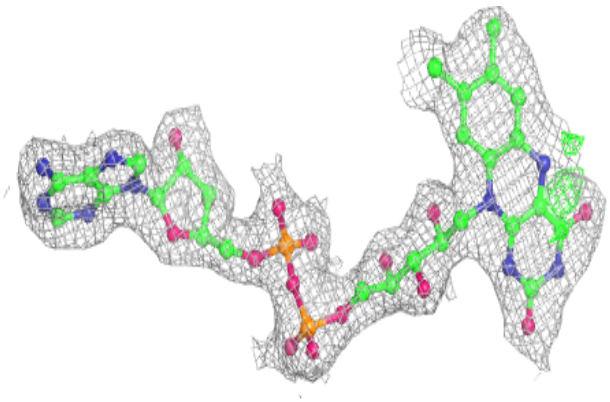
Electron density around C15 A 1504:

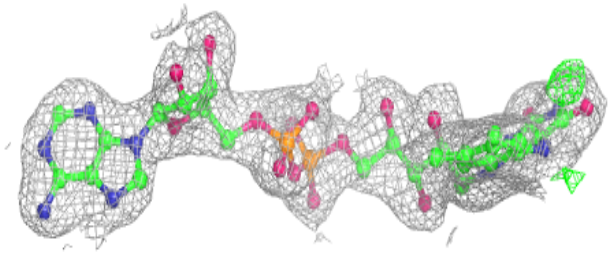
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

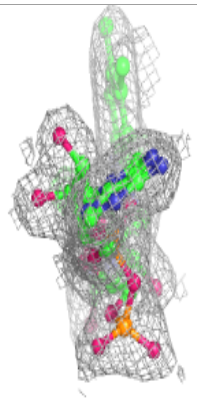


Electron density around FAD A 1502:

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

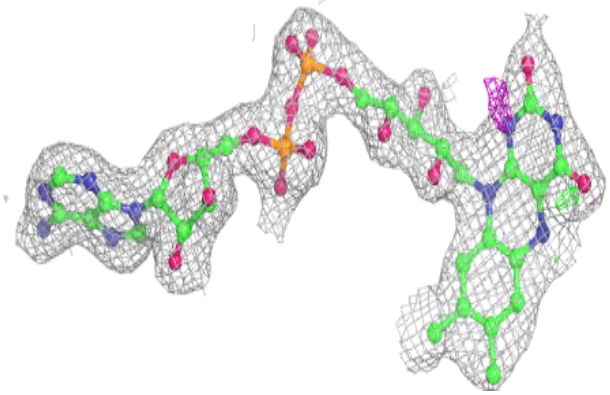


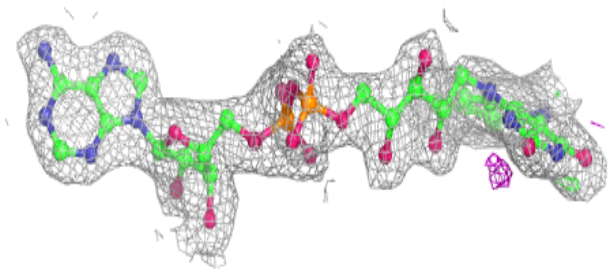


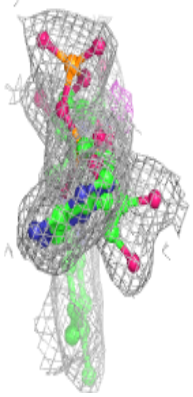


Electron density around FAD B 1497:

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







4.5 Other polymers (i)

There are no such residues in this entry.