



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:51 pm BST

PDB ID : 2V60  
Title : Structure of human MAO B in complex with the selective inhibitor 7-(3- chlorobenzyloxy)-4-carboxaldehyde-coumarin  
Authors : Binda, C.; Wang, J.; Pisani, L.; Caccia, C.; Carotti, A.; Salvati, P.; Edmondson, D.E.; Mattevi, A.  
Deposited on : 2007-07-12  
Resolution : 2.00 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](mailto: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.

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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 : 2.11  
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) : 2.11

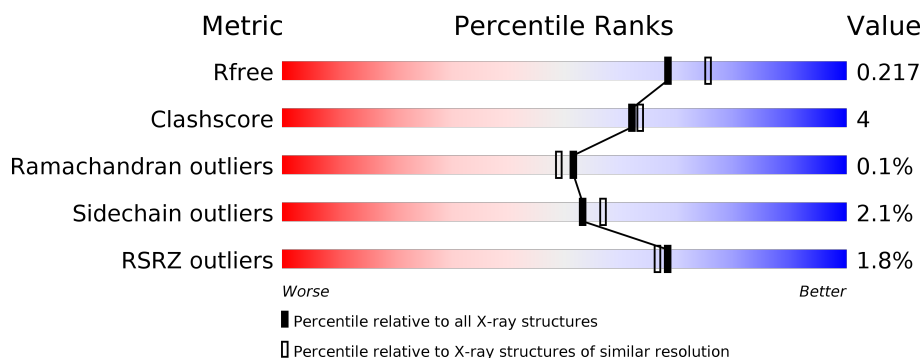
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	520	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>• •</div> </div> </div>
1	B	520	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>• 5%</div> </div> </div>

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8817 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.

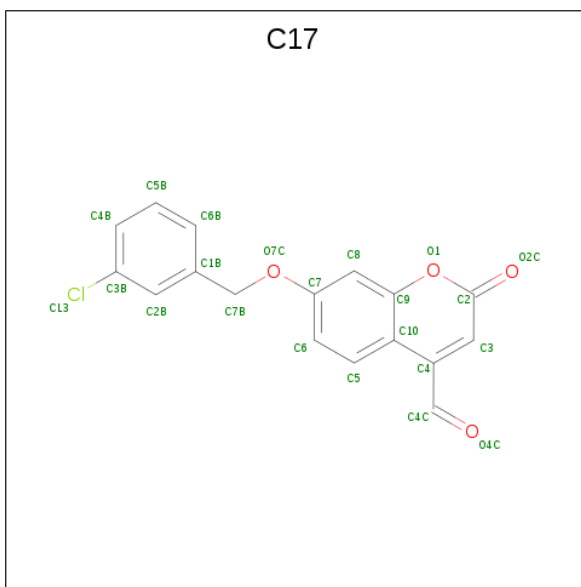
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3971	2538	681	728	24			
1	B	494	Total	C	N	O	S	0	0	0
			3940	2519	676	721	24			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



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 7-[(3-CHLOROBENZYL)OXY]-2-OXO-2H-CHROMENE-4-CARBALDEHYDE (three-letter code: C17) (formula: C<sub>17</sub>H<sub>11</sub>ClO<sub>4</sub>).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	352	Total	O	0	0
			352	352		
4	B	404	Total	O	0	0
			404	404		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.69Å 224.41Å 86.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.23 – 2.00 47.12 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (113.23-2.00) 99.0 (47.12-2.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.172 , 0.221 0.172 , 0.217	Depositor DCC
$R_{free}$ test set	2206 reflections (2.58%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8817	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: C17, 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	0.81	0/4068	0.74	4/5522 (0.1%)
1	B	0.82	0/4037	0.75	3/5479 (0.1%)
All	All	0.81	0/8105	0.75	7/11001 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	448	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	B	448	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	448	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	B	318	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	448	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	42	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	127	ARG	NE-CZ-NH2	-5.17	117.71	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3971	0	3967	37	0
1	B	3940	0	3937	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	29	1	0
2	B	53	0	29	1	0
3	A	22	0	11	4	0
3	B	22	0	11	4	0
4	A	352	0	0	8	1
4	B	404	0	0	5	0
All	All	8817	0	7984	71	1

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

All (71) 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	1.41	1.03
1:A:353:ALA:CB	1:B:280:MET:HE1	2.01	0.91
1:A:117:ASN:HD22	1:A:120:ARG:HH21	1.29	0.81
1:B:251:ASN:H	1:B:251:ASN:HD22	1.34	0.76
3:B:1498:C17:H3	4:B:1401:HOH:O	1.87	0.73
3:A:1503:C17:H3	4:A:1351:HOH:O	1.90	0.70
3:B:1498:C17:O4C	3:B:1498:C17:H5	1.92	0.69
1:B:28:LEU:HD11	1:B:454:MET:CE	2.22	0.69
1:A:28:LEU:HD11	1:A:454:MET:CE	2.25	0.67
1:A:251:ASN:H	1:A:251:ASN:HD22	1.43	0.66
1:B:246:LEU:HD22	1:B:254:MET:HE1	1.77	0.66
1:A:412:ARG:HD2	4:A:1288:HOH:O	1.96	0.64
1:A:265:PRO:HD2	1:A:268:LEU:HD12	1.81	0.62
1:B:451:LEU:HA	1:B:454:MET:HE2	1.82	0.62
1:B:412:ARG:HD2	4:B:1338:HOH:O	1.99	0.61
3:A:1503:C17:H5	3:A:1503:C17:O4C	2.00	0.60
1:B:28:LEU:HD11	1:B:454:MET:HE1	1.83	0.59
1:B:246:LEU:HD22	1:B:254:MET:CE	2.33	0.59
1:B:117:ASN:HD22	1:B:120:ARG:HH21	1.51	0.59
1:A:117:ASN:HD22	1:A:120:ARG:NH2	1.99	0.58
1:A:3:ASN:N	4:A:1001:HOH:O	2.35	0.58
1:A:321:GLU:CD	1:A:321:GLU:H	2.06	0.58
1:B:387:ASN:O	1:B:390:GLU:HG2	2.04	0.58
1:A:280:MET:HE1	1:B:353:ALA:HB1	1.87	0.57
1:A:28:LEU:HD21	1:A:456:LYS:HE3	1.87	0.56
3:A:1503:C17:H4'	4:A:1351:HOH:O	2.06	0.55
1:A:246:LEU:HB3	1:A:254:MET:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD11	1:A:454:MET:HE1	1.88	0.55
1:A:353:ALA:HB1	1:B:280:MET:CE	2.27	0.53
1:A:362:LYS:HE3	1:A:366:GLU:OE2	2.09	0.53
1:B:321:GLU:CD	1:B:321:GLU:H	2.10	0.53
1:B:451:LEU:HD23	1:B:454:MET:CE	2.38	0.52
1:A:28:LEU:HD11	1:A:454:MET:HE3	1.91	0.52
1:A:451:LEU:HD23	1:A:454:MET:CE	2.40	0.52
1:A:117:ASN:ND2	1:A:120:ARG:HH21	2.03	0.50
1:B:246:LEU:HB3	1:B:254:MET:HE1	1.94	0.49
1:B:80:TYR:CG	1:B:333:PRO:HG3	2.48	0.49
1:A:23:LEU:HD22	1:A:28:LEU:HD12	1.95	0.48
1:A:376:GLU:HG3	4:A:1260:HOH:O	2.12	0.48
1:A:58:GLY:HA2	2:A:1502:FAD:C4X	2.45	0.47
1:A:110:ILE:HG12	4:A:1094:HOH:O	2.14	0.47
1:A:280:MET:HG3	1:B:389:CYS:HB3	1.98	0.46
1:A:389:CYS:CB	1:B:280:MET:HG3	2.45	0.46
1:A:60:TYR:CE2	1:A:209:LYS:HD2	2.51	0.46
1:A:80:TYR:OH	1:A:209:LYS:HE3	2.17	0.45
1:A:163:GLN:HB3	1:A:318:ASP:OD2	2.16	0.45
1:A:95:LYS:HD3	4:A:1085:HOH:O	2.17	0.45
3:A:1503:C17:C5	3:A:1503:C17:O4C	2.65	0.44
1:A:451:LEU:HA	1:A:454:MET:HE2	1.99	0.44
1:B:28:LEU:HD11	1:B:454:MET:HE3	1.97	0.43
1:A:60:TYR:HB3	1:A:206:GLN:HA	1.99	0.43
1:B:143:TRP:HA	1:B:146:MET:HE3	1.99	0.43
1:B:17:MET:HE2	1:B:222:MET:HB2	2.00	0.43
1:A:127:ARG:NH2	4:A:1110:HOH:O	2.36	0.43
1:A:173:VAL:HG11	1:A:184:TRP:CH2	2.54	0.43
1:A:233:ARG:HG3	1:A:251:ASN:HD21	1.84	0.43
1:B:17:MET:CE	1:B:222:MET:N	2.82	0.42
1:B:226:GLY:O	4:B:1220:HOH:O	2.22	0.42
1:B:403:PRO:HG2	4:B:1246:HOH:O	2.19	0.42
1:B:17:MET:HE3	1:B:221:ILE:HB	2.02	0.42
1:B:251:ASN:N	1:B:251:ASN:HD22	2.09	0.41
1:B:52:LYS:HG2	1:B:53:TYR:HD2	1.86	0.41
1:A:389:CYS:HB2	1:B:280:MET:HG3	2.02	0.41
1:B:148:MET:O	1:B:152:LEU:HG	2.20	0.41
3:B:1498:C17:H4'	4:B:1401:HOH:O	2.20	0.41
2:B:1497:FAD:H2'	2:B:1497:FAD:N1	2.35	0.41
3:B:1498:C17:C5	3:B:1498:C17:O4C	2.61	0.41
1:A:290:PRO:HG2	1:A:401:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:MET:HG2	1:A:150:GLU:HB2	2.03	0.40
1:B:227:ASP:O	1:B:230:LYS:NZ	2.44	0.40
1:B:254:MET:HE2	1:B:254:MET:HB3	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1037:HOH:O	4:A:1037:HOH:O[3_655]	1.45	0.75

## 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	497/520 (96%)	483 (97%)	14 (3%)	0	100	100
1	B	492/520 (95%)	480 (98%)	11 (2%)	1 (0%)	47	44
All	All	989/1040 (95%)	963 (97%)	25 (2%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	52	LYS

### 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	427/444 (96%)	416 (97%)	11 (3%)	46	48
1	B	424/444 (96%)	417 (98%)	7 (2%)	60	65
All	All	851/888 (96%)	833 (98%)	18 (2%)	53	57

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	4	LYS
1	A	93	LYS
1	A	190	LYS
1	A	251	ASN
1	A	280	MET
1	A	321	GLU
1	A	350	ARG
1	A	397	CYS
1	A	412	ARG
1	A	498	LEU
1	B	3	ASN
1	B	92	VAL
1	B	251	ASN
1	B	280	MET
1	B	350	ARG
1	B	379	GLU
1	B	412	ARG

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

Mol	Chain	Res	Type
1	A	116	ASN
1	A	117	ASN
1	A	251	ASN
1	A	452	HIS
1	A	485	HIS
1	B	117	ASN
1	B	251	ASN
1	B	452	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 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
2	FAD	B	1497	1	51,58,58	1.55	7 (13%)	60,89,89	1.89	12 (20%)
3	C17	A	1503	-	22,24,24	3.00	4 (18%)	29,33,33	1.49	4 (13%)
2	FAD	A	1502	1	51,58,58	1.45	5 (9%)	60,89,89	1.82	12 (20%)
3	C17	B	1498	-	22,24,24	3.01	5 (22%)	29,33,33	1.44	4 (13%)

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	B	1497	1	-	2/30/50/50	0/6/6/6
3	C17	A	1503	-	-	0/7/7/7	0/3/3/3
2	FAD	A	1502	1	-	2/30/50/50	0/6/6/6
3	C17	B	1498	-	-	0/7/7/7	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1503	C17	C3B-CL3	-11.15	1.50	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1498	C17	C3B-CL3	-11.11	1.50	1.74
2	A	1502	FAD	C10-N1	5.93	1.40	1.33
2	B	1497	FAD	C4X-N5	5.14	1.40	1.33
3	A	1503	C17	C8-C9	5.05	1.47	1.37
3	B	1498	C17	C8-C9	4.84	1.47	1.37
2	A	1502	FAD	C4X-N5	4.64	1.40	1.33
2	B	1497	FAD	C10-N1	4.63	1.39	1.33
3	B	1498	C17	O7C-C7	4.47	1.48	1.37
3	A	1503	C17	O7C-C7	4.37	1.47	1.37
3	A	1503	C17	C5-C10	3.44	1.49	1.42
2	B	1497	FAD	C4-N3	3.27	1.38	1.33
3	B	1498	C17	C5-C10	3.20	1.48	1.42
2	A	1502	FAD	C2A-N3A	3.09	1.37	1.32
2	B	1497	FAD	C9A-N10	3.08	1.42	1.38
2	B	1497	FAD	C2A-N3A	2.86	1.36	1.32
2	A	1502	FAD	C4-N3	2.38	1.37	1.33
3	B	1498	C17	C10-C9	-2.16	1.38	1.41
2	B	1497	FAD	C1'-N10	2.11	1.50	1.48
2	B	1497	FAD	C2A-N1A	2.08	1.37	1.33
2	A	1502	FAD	C2A-N1A	2.05	1.37	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1502	FAD	C4-N3-C2	6.44	120.58	115.14
2	B	1497	FAD	N3A-C2A-N1A	-6.33	118.78	128.68
2	A	1502	FAD	N3A-C2A-N1A	-5.41	120.22	128.68
2	B	1497	FAD	C4-N3-C2	5.27	119.60	115.14
2	B	1497	FAD	C4X-N5-C5X	4.43	121.19	116.77
3	B	1498	C17	C8-C9-C10	-4.16	118.44	123.05
2	A	1502	FAD	C1'-N10-C9A	4.00	121.44	118.29
3	A	1503	C17	C8-C9-C10	-3.93	118.69	123.05
2	B	1497	FAD	C9A-C5X-N5	-3.75	116.49	122.36
2	B	1497	FAD	C9A-N10-C10	-3.53	117.28	121.91
3	B	1498	C17	O1-C9-C8	3.51	120.19	116.03
2	A	1502	FAD	C4X-N5-C5X	3.43	120.20	116.77
2	B	1497	FAD	C2A-N1A-C6A	3.42	124.60	118.75
3	B	1498	C17	C7B-O7C-C7	3.37	125.98	117.65
2	A	1502	FAD	C9A-C5X-N5	-3.30	117.20	122.36
2	B	1497	FAD	C5A-C6A-N6A	3.22	125.25	120.35
2	A	1502	FAD	C8M-C8-C7	3.11	127.11	120.74
2	B	1497	FAD	C4X-C10-N10	-3.08	117.14	120.30

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1503	C17	O1-C9-C8	3.04	119.64	116.03
2	A	1502	FAD	C9A-N10-C10	-2.97	118.02	121.91
2	A	1502	FAD	C4X-C10-N10	-2.74	117.49	120.30
2	B	1497	FAD	C4-C4X-N5	2.72	121.70	118.60
2	B	1497	FAD	C5'-C4'-C3'	-2.67	107.04	112.20
2	B	1497	FAD	C4-C4X-C10	-2.51	118.29	119.95
2	A	1502	FAD	C1B-N9A-C4A	-2.50	122.25	126.64
3	A	1503	C17	C7B-O7C-C7	2.47	123.74	117.65
2	A	1502	FAD	C4X-C4-N3	-2.29	120.30	123.43
2	A	1502	FAD	C7M-C7-C6	-2.26	114.94	120.34
3	B	1498	C17	C5-C6-C7	2.22	123.16	120.17
2	B	1497	FAD	O2B-C2B-C3B	2.17	118.83	111.82
3	A	1503	C17	C4B-C3B-CL3	2.15	122.72	119.35
2	A	1502	FAD	C8M-C8-C9	-2.08	115.38	120.34

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1497	FAD	C2'-C1'-N10-C10
2	A	1502	FAD	PA-O3P-P-O5'
2	B	1497	FAD	O4B-C4B-C5B-O5B
2	A	1502	FAD	O4B-C4B-C5B-O5B

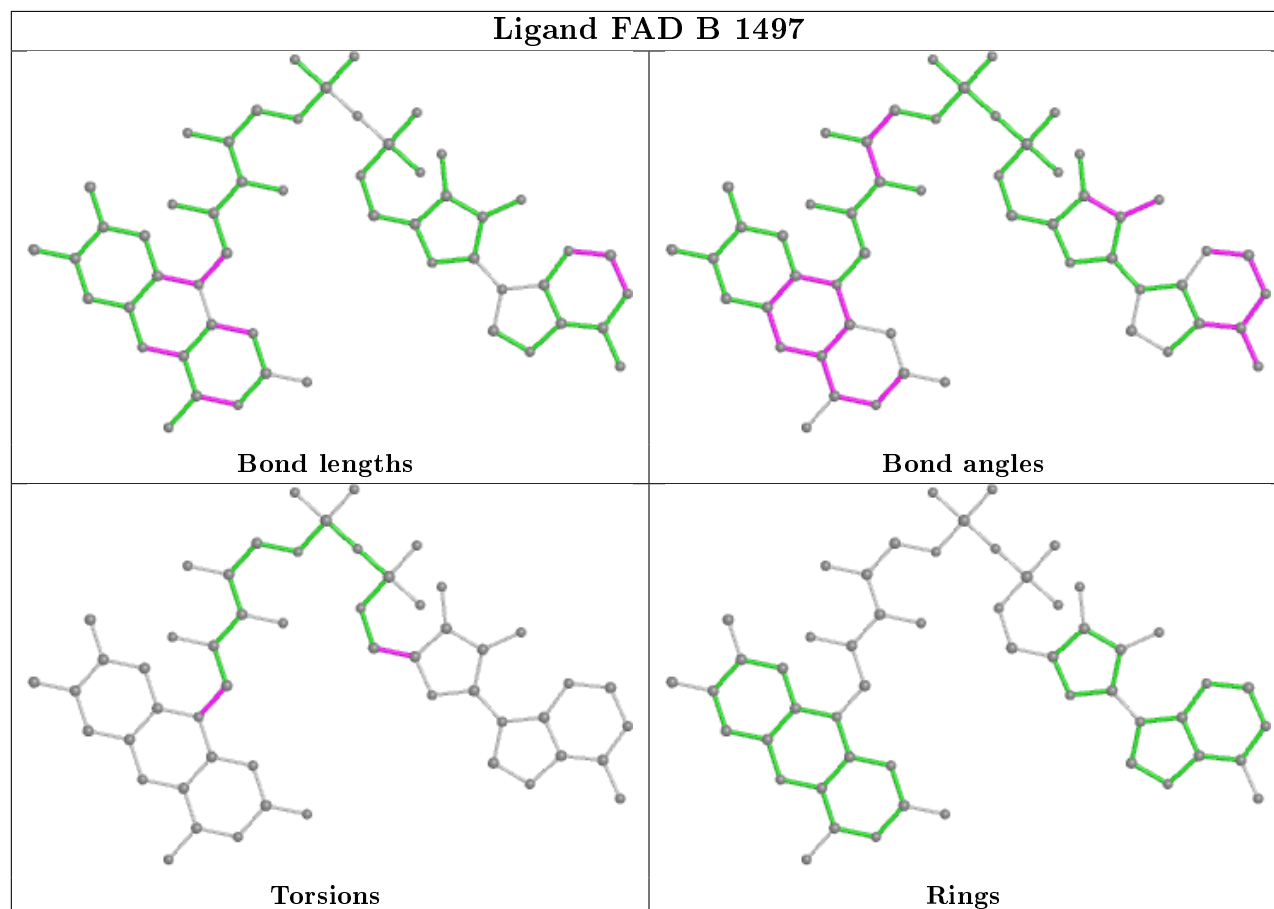
There are no ring outliers.

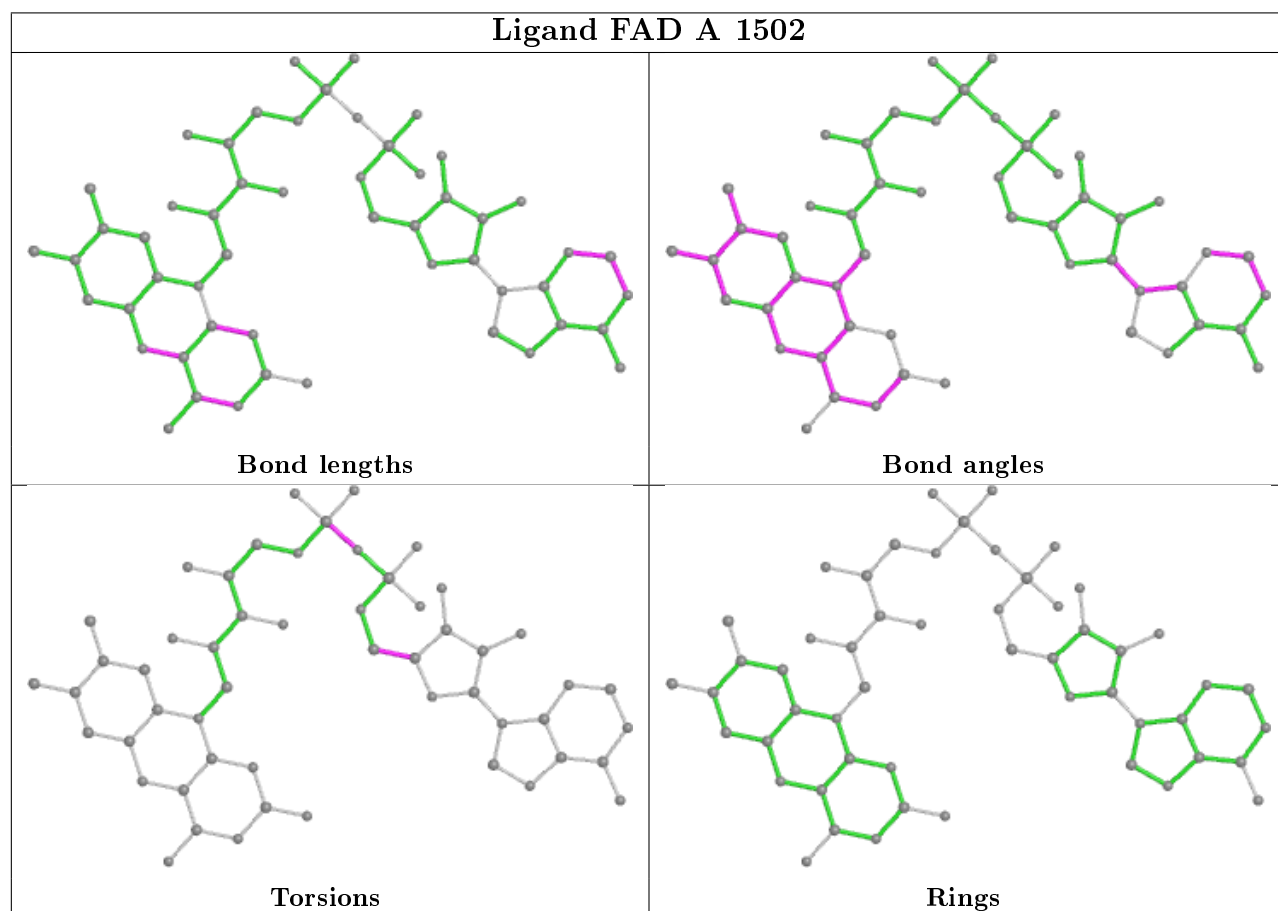
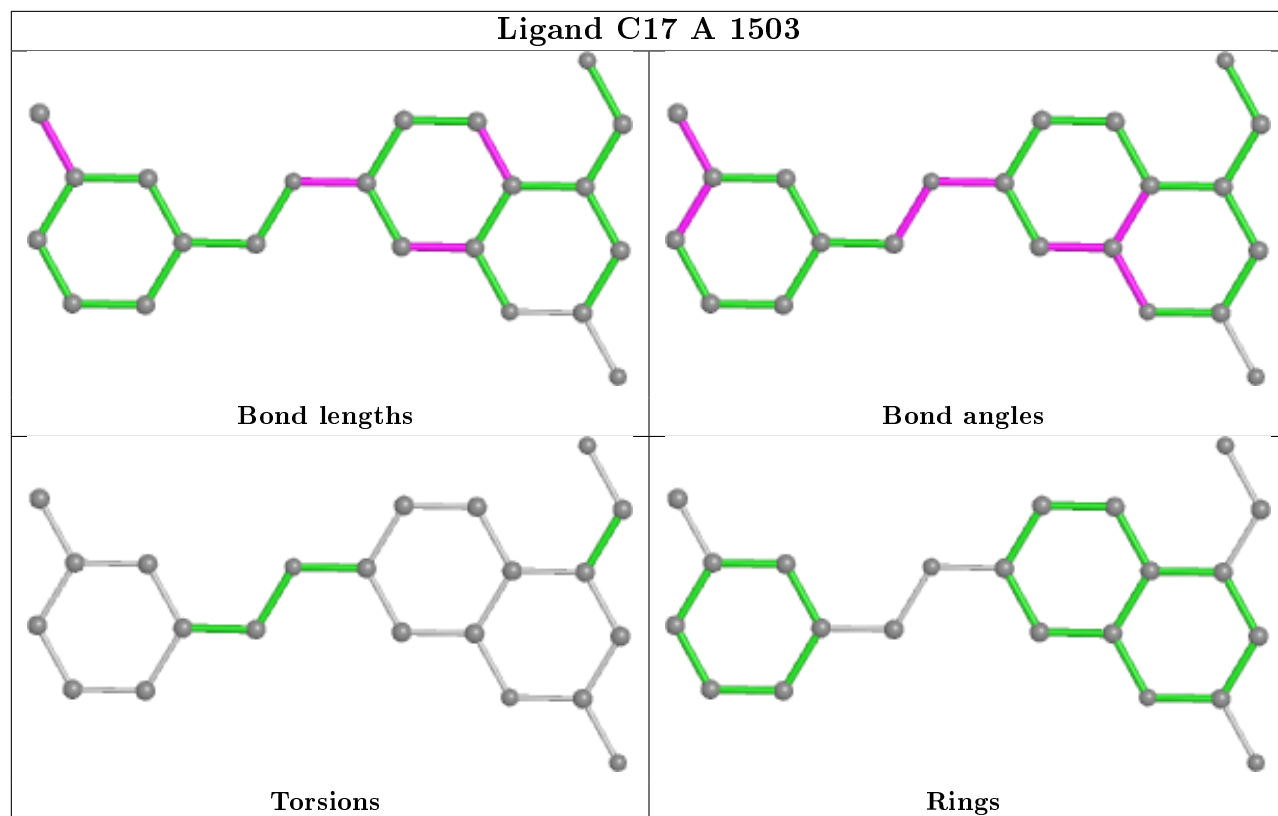
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1497	FAD	1	0
3	A	1503	C17	4	0
2	A	1502	FAD	1	0
3	B	1498	C17	4	0

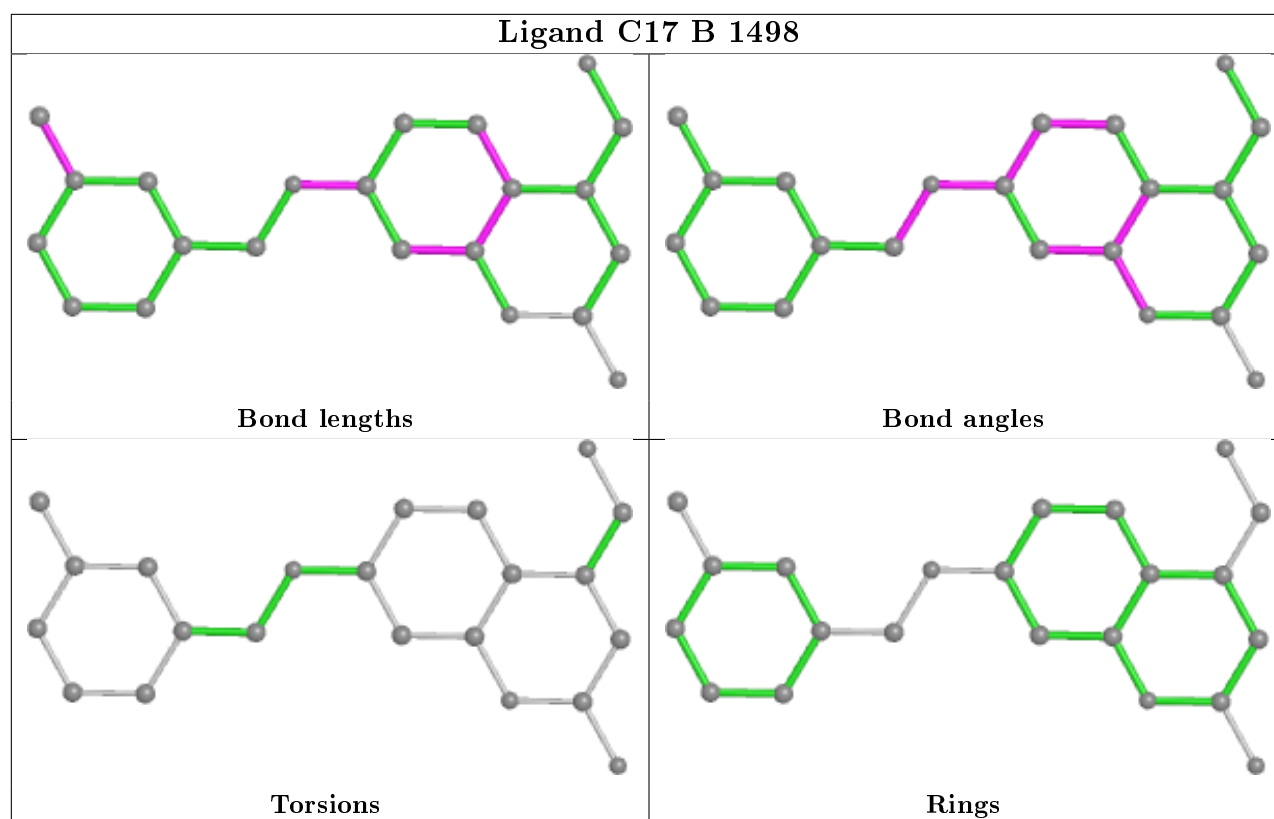
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	499/520 (95%)	-0.28	11 (2%) 62 60	12, 21, 36, 70	0
1	B	494/520 (95%)	-0.19	7 (1%) 75 74	12, 20, 34, 57	0
All	All	993/1040 (95%)	-0.23	18 (1%) 68 66	12, 20, 35, 70	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	500	THR	5.8
1	A	498	LEU	4.8
1	B	496	ILE	4.7
1	B	495	LEU	4.3
1	A	495	LEU	3.4
1	A	499	THR	3.4
1	B	494	ARG	3.2
1	B	107	TRP	3.0
1	A	501	ILE	2.8
1	B	243	GLU	2.7
1	A	107	TRP	2.5
1	B	242	ARG	2.4
1	A	497	GLY	2.3
1	A	494	ARG	2.2
1	A	27	GLY	2.2
1	A	496	ILE	2.2
1	A	242	ARG	2.2
1	B	354	ARG	2.1

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

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

## 6.3 Carbohydrates [i](#)

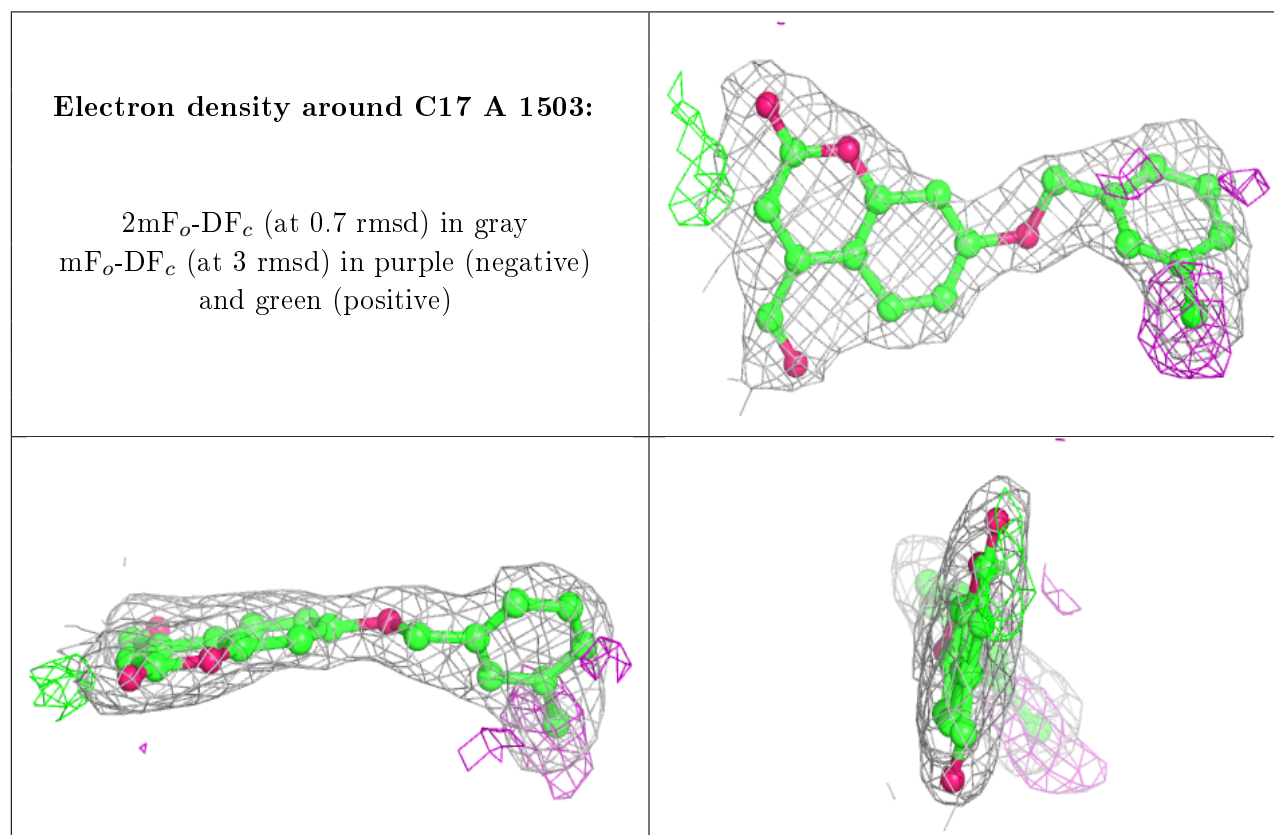
There are no carbohydrates in this entry.

## 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<sup>th</sup> 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.

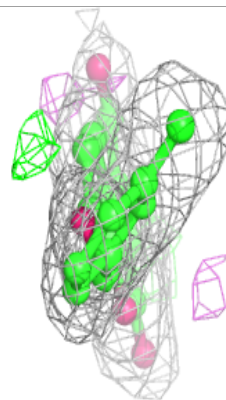
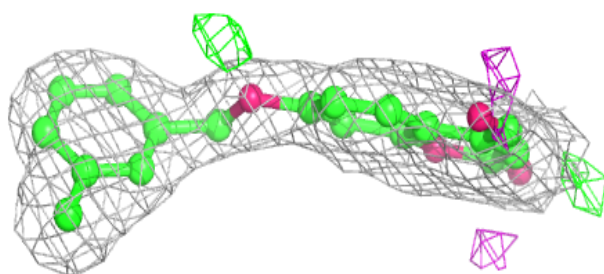
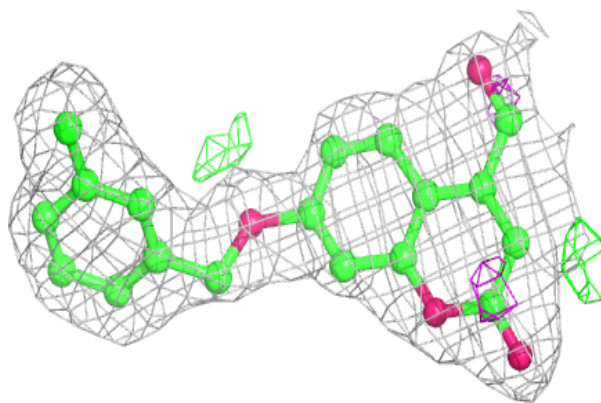
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	C17	A	1503	22/22	0.88	0.16	35,36,38,42	0
3	C17	B	1498	22/22	0.92	0.12	33,35,36,38	0
2	FAD	B	1497	53/53	0.98	0.13	10,14,18,19	0
2	FAD	A	1502	53/53	0.99	0.10	12,15,17,18	0

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.

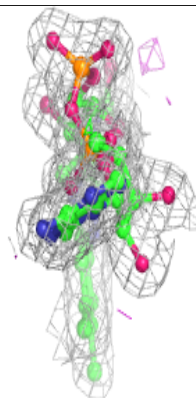
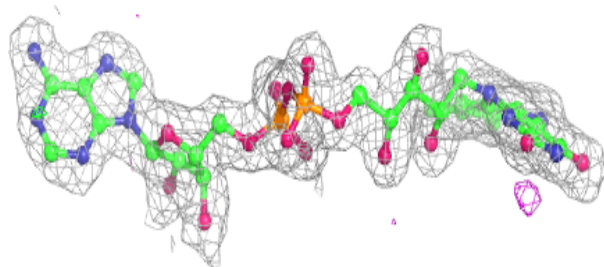
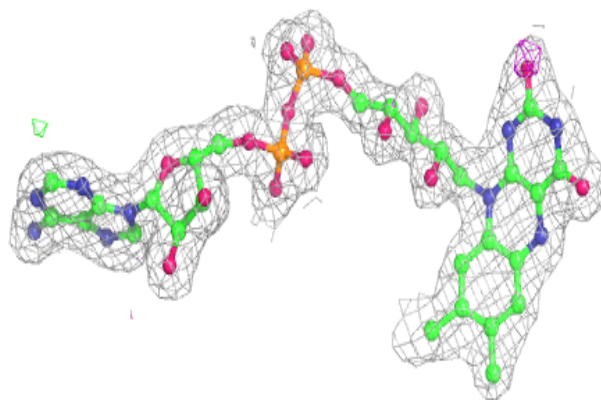


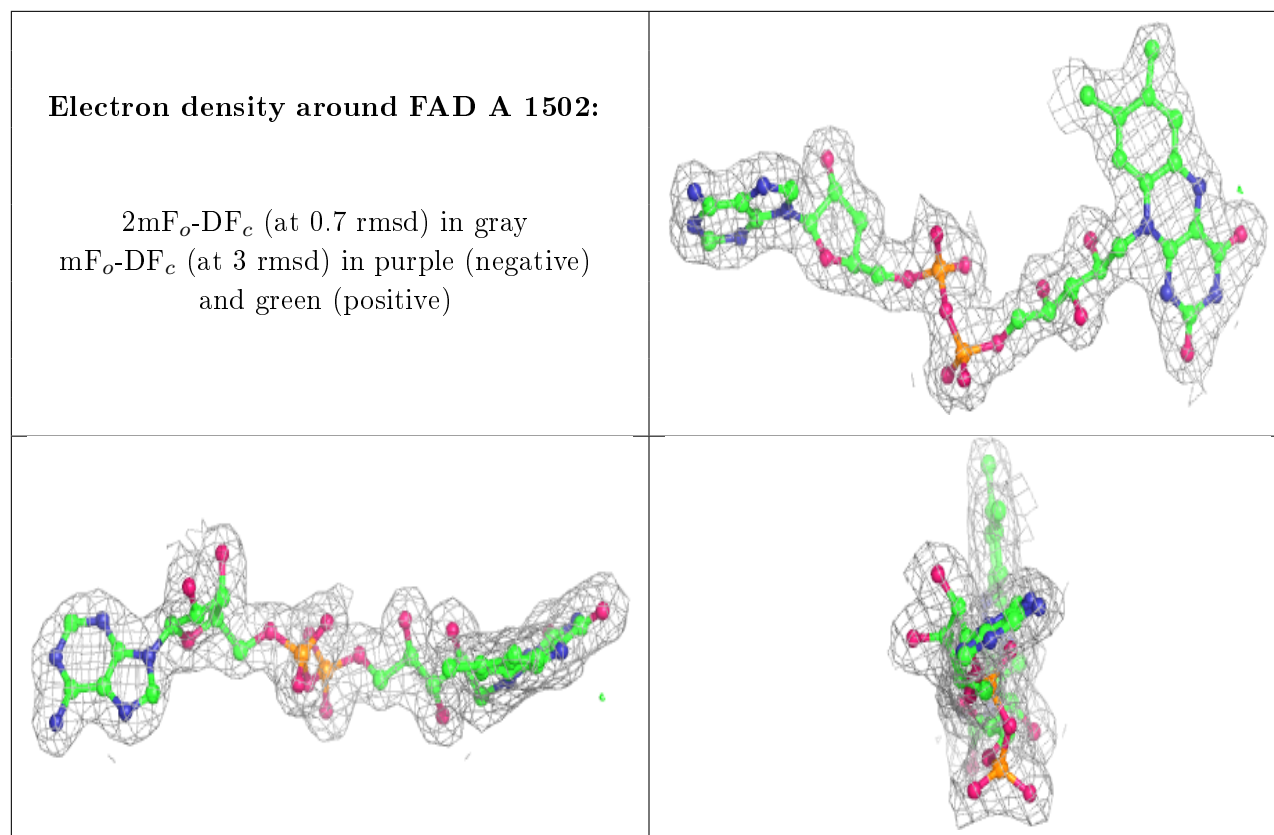
**Electron density around C17 B 1498:**

$2mF_o-DF_c$  (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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.