



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:31 am BST

PDB ID : 3GMC  
Title : Crystal Structure of 2-Methyl-3-hydroxypyridine-5-carboxylic acid Oxygenase with substrate bound  
Authors : McCulloch, K.M.; Mukherjee, T.; Begley, T.P.; Ealick, S.E.  
Deposited on : 2009-03-13  
Resolution : 2.10 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

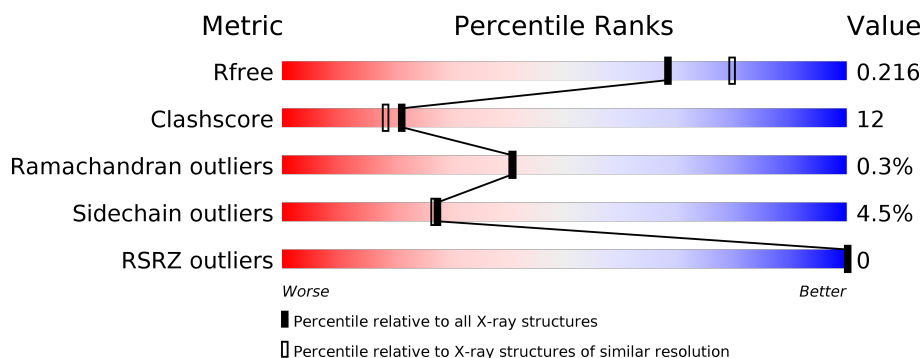
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	415	
1	B	415	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6579 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 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2865	1807	512	532	14			
1	B	369	Total	C	N	O	S	0	0	0
			2865	1807	512	532	14			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	EXPRESSION TAG	UNP Q988D3
A	-34	GLY	-	EXPRESSION TAG	UNP Q988D3
A	-33	SER	-	EXPRESSION TAG	UNP Q988D3
A	-32	HIS	-	EXPRESSION TAG	UNP Q988D3
A	-31	HIS	-	EXPRESSION TAG	UNP Q988D3
A	-30	HIS	-	EXPRESSION TAG	UNP Q988D3
A	-29	HIS	-	EXPRESSION TAG	UNP Q988D3
A	-28	HIS	-	EXPRESSION TAG	UNP Q988D3
A	-27	HIS	-	EXPRESSION TAG	UNP Q988D3
A	-26	ASP	-	EXPRESSION TAG	UNP Q988D3
A	-25	ILE	-	EXPRESSION TAG	UNP Q988D3
A	-24	THR	-	EXPRESSION TAG	UNP Q988D3
A	-23	SER	-	EXPRESSION TAG	UNP Q988D3
A	-22	LEU	-	EXPRESSION TAG	UNP Q988D3
A	-21	TYR	-	EXPRESSION TAG	UNP Q988D3
A	-20	LYS	-	EXPRESSION TAG	UNP Q988D3
A	-19	LYS	-	EXPRESSION TAG	UNP Q988D3
A	-18	ALA	-	EXPRESSION TAG	UNP Q988D3
A	-17	GLY	-	EXPRESSION TAG	UNP Q988D3
A	-16	SER	-	EXPRESSION TAG	UNP Q988D3
A	-15	ALA	-	EXPRESSION TAG	UNP Q988D3
A	-14	ALA	-	EXPRESSION TAG	UNP Q988D3
A	-13	ALA	-	EXPRESSION TAG	UNP Q988D3
A	-12	VAL	-	EXPRESSION TAG	UNP Q988D3
A	-11	LEU	-	EXPRESSION TAG	UNP Q988D3

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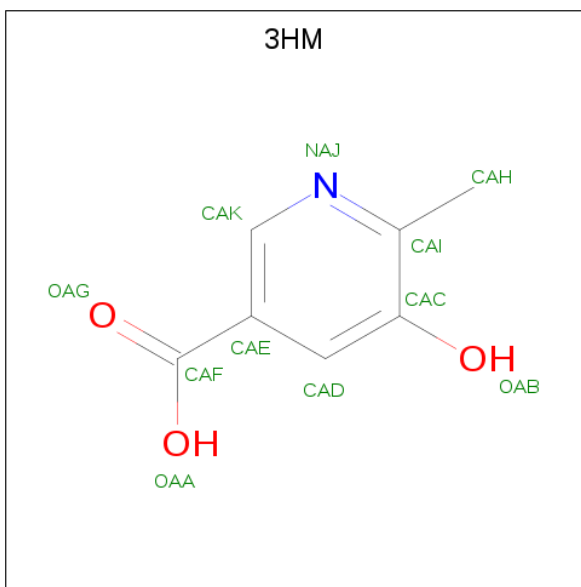
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLU	-	EXPRESSION TAG	UNP Q988D3
A	-9	GLU	-	EXPRESSION TAG	UNP Q988D3
A	-8	ASN	-	EXPRESSION TAG	UNP Q988D3
A	-7	LEU	-	EXPRESSION TAG	UNP Q988D3
A	-6	TYR	-	EXPRESSION TAG	UNP Q988D3
A	-5	PHE	-	EXPRESSION TAG	UNP Q988D3
A	-4	GLY	-	EXPRESSION TAG	UNP Q988D3
A	-3	GLY	-	EXPRESSION TAG	UNP Q988D3
A	-2	SER	-	EXPRESSION TAG	UNP Q988D3
A	-1	PHE	-	EXPRESSION TAG	UNP Q988D3
A	0	THR	-	EXPRESSION TAG	UNP Q988D3
B	-35	MET	-	EXPRESSION TAG	UNP Q988D3
B	-34	GLY	-	EXPRESSION TAG	UNP Q988D3
B	-33	SER	-	EXPRESSION TAG	UNP Q988D3
B	-32	HIS	-	EXPRESSION TAG	UNP Q988D3
B	-31	HIS	-	EXPRESSION TAG	UNP Q988D3
B	-30	HIS	-	EXPRESSION TAG	UNP Q988D3
B	-29	HIS	-	EXPRESSION TAG	UNP Q988D3
B	-28	HIS	-	EXPRESSION TAG	UNP Q988D3
B	-27	HIS	-	EXPRESSION TAG	UNP Q988D3
B	-26	ASP	-	EXPRESSION TAG	UNP Q988D3
B	-25	ILE	-	EXPRESSION TAG	UNP Q988D3
B	-24	THR	-	EXPRESSION TAG	UNP Q988D3
B	-23	SER	-	EXPRESSION TAG	UNP Q988D3
B	-22	LEU	-	EXPRESSION TAG	UNP Q988D3
B	-21	TYR	-	EXPRESSION TAG	UNP Q988D3
B	-20	LYS	-	EXPRESSION TAG	UNP Q988D3
B	-19	LYS	-	EXPRESSION TAG	UNP Q988D3
B	-18	ALA	-	EXPRESSION TAG	UNP Q988D3
B	-17	GLY	-	EXPRESSION TAG	UNP Q988D3
B	-16	SER	-	EXPRESSION TAG	UNP Q988D3
B	-15	ALA	-	EXPRESSION TAG	UNP Q988D3
B	-14	ALA	-	EXPRESSION TAG	UNP Q988D3
B	-13	ALA	-	EXPRESSION TAG	UNP Q988D3
B	-12	VAL	-	EXPRESSION TAG	UNP Q988D3
B	-11	LEU	-	EXPRESSION TAG	UNP Q988D3
B	-10	GLU	-	EXPRESSION TAG	UNP Q988D3
B	-9	GLU	-	EXPRESSION TAG	UNP Q988D3
B	-8	ASN	-	EXPRESSION TAG	UNP Q988D3
B	-7	LEU	-	EXPRESSION TAG	UNP Q988D3
B	-6	TYR	-	EXPRESSION TAG	UNP Q988D3
B	-5	PHE	-	EXPRESSION TAG	UNP Q988D3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	EXPRESSION TAG	UNP Q988D3
B	-3	GLY	-	EXPRESSION TAG	UNP Q988D3
B	-2	SER	-	EXPRESSION TAG	UNP Q988D3
B	-1	PHE	-	EXPRESSION TAG	UNP Q988D3
B	0	THR	-	EXPRESSION TAG	UNP Q988D3

- # FAD
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- The image displays the chemical structure of Flavin Adenine Dinucleotide (FAD), a crucial coenzyme. The structure is composed of several interconnected parts:
- Flavin Mononucleotide (FMN) Core:** This includes the isoalloxazine ring system (top left) and the ribitol chain (middle). The ribitol chain is a five-carbon chain with hydroxyl groups at C2, C3, and C4. The C1 position is linked to the ribose sugar of the adenine nucleotide.
  - Adenine Nucleotide:** This part consists of a ribose sugar (bottom left) and an adenine base (bottom right). The ribose sugar is linked to the FMN core via its C1 position. The adenine base is a purine derivative with an amino group at C6.
  - Phosphate Groups:** The structure shows two phosphate groups (P1 and P2) linked by a pyrophosphate bridge. The first phosphate group (P1) is linked to the ribitol chain at C5, and the second phosphate group (P2) is linked to the ribose sugar at C5. The pyrophosphate bridge is formed by the condensation of the two phosphate groups, releasing a water molecule.
- The overall structure is a complex molecule with a high degree of stereochemical specificity, as indicated by the wedge and dash notation used throughout the diagram.

- Molecule 3 is 5-hydroxy-6-methylpyridine-3-carboxylic acid (three-letter code: 3HM) (formula:  $\text{C}_7\text{H}_7\text{NO}_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	7	1	3		
3	B	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 4 is water.

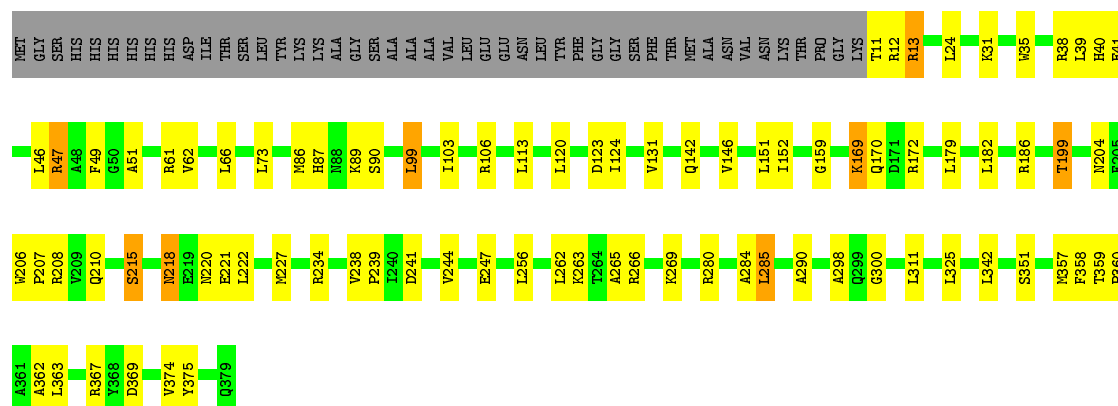
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	366	Total	O	0	0
			366	366		
4	B	355	Total	O	0	0
			355	355		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

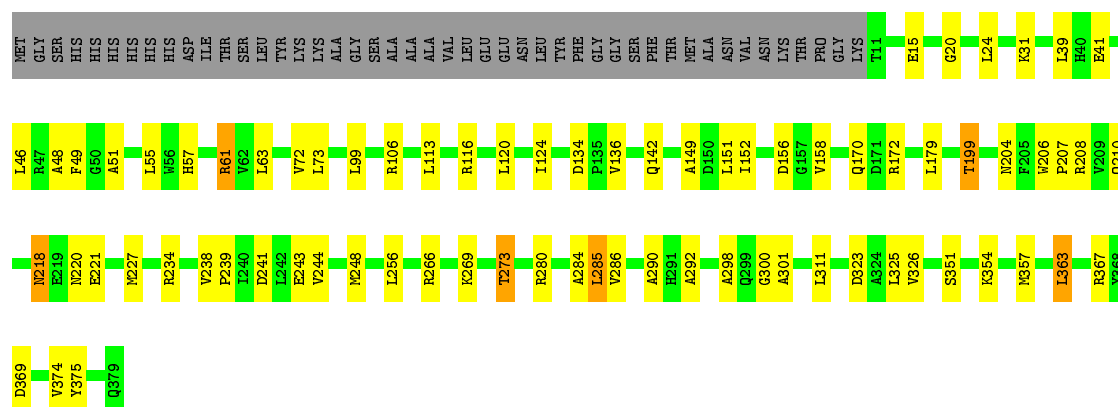
- Molecule 1: 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase

Chain A: 



- Molecule 1: 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.49Å 129.54Å 89.10Å 90.00° 122.60° 90.00°	Depositor
Resolution (Å)	49.04 – 2.10 75.59 – 2.08	Depositor EDS
% Data completeness (in resolution range)	90.7 (49.04-2.10) 90.6 (75.59-2.08)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.08Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.188 , 0.222 0.183 , 0.216	Depositor DCC
$R_{free}$ test set	3181 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtriage
Anisotropy	1.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6579	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 5.20% 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: 3HM, 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	0.31	0/2931	0.60	1/3981 (0.0%)
1	B	0.31	0/2931	0.60	1/3981 (0.0%)
All	All	0.31	0/5862	0.60	2/7962 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	THR	N-CA-C	-6.01	94.77	111.00
1	A	199	THR	N-CA-C	-5.51	96.11	111.00

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	2865	0	2824	78	0
1	B	2865	0	2824	68	0
2	A	53	0	31	1	0
2	B	53	0	31	2	0
3	A	11	0	5	1	0
3	B	11	0	5	1	0
4	A	366	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	355	0	0	11	1
All	All	6579	0	5720	140	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 12.

All (140) 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:B:208:ARG:HD2	1:B:210:GLN:HE21	1.18	1.01
1:A:218:ASN:HD22	1:A:220:ASN:H	1.12	0.98
1:B:218:ASN:HD22	1:B:220:ASN:H	1.14	0.95
1:A:208:ARG:HH11	1:A:210:GLN:NE2	1.74	0.86
1:B:208:ARG:HD2	1:B:210:GLN:NE2	1.92	0.84
1:A:358:PHE:HB3	1:A:363:LEU:HD11	1.62	0.80
1:A:298:ALA:HB2	3:A:381:3HM:HAHA	1.64	0.80
1:A:61:ARG:HD3	1:A:369:ASP:OD1	1.82	0.79
1:A:170:GLN:HE22	1:B:172:ARG:HH11	1.29	0.79
1:A:300:GLY:HA3	2:A:380:FAD:H1'2	1.65	0.78
1:A:218:ASN:ND2	1:A:221:GLU:H	1.83	0.76
1:A:172:ARG:HH11	1:B:170:GLN:HE22	1.34	0.75
1:B:300:GLY:HA3	2:B:380:FAD:H1'2	1.69	0.75
1:B:298:ALA:HB2	3:B:381:3HM:HAHA	1.67	0.74
1:A:46:LEU:HD11	1:A:124:ILE:HG21	1.69	0.74
1:A:47:ARG:NH1	1:A:47:ARG:HB2	2.01	0.74
1:B:61:ARG:HD3	1:B:369:ASP:OD1	1.87	0.73
1:A:169:LYS:NZ	1:A:169:LYS:HB2	2.04	0.73
1:B:210:GLN:HE22	1:B:244:VAL:HG22	1.57	0.68
1:A:218:ASN:ND2	1:A:220:ASN:H	1.90	0.67
1:B:234:ARG:HD2	1:B:241:ASP:OD2	1.95	0.67
1:B:116:ARG:CZ	1:B:120:LEU:HD21	2.24	0.67
1:B:218:ASN:ND2	1:B:221:GLU:H	1.93	0.67
1:B:208:ARG:HH11	1:B:210:GLN:NE2	1.94	0.66
1:B:46:LEU:HD11	1:B:124:ILE:HG21	1.78	0.66
1:B:218:ASN:ND2	1:B:220:ASN:H	1.91	0.64
1:A:218:ASN:HD21	1:A:221:GLU:H	1.46	0.64
1:B:351:SER:HA	1:B:354:LYS:HE2	1.80	0.64
1:A:238:VAL:HA	1:A:239:PRO:C	2.18	0.63
1:A:269:LYS:HD3	4:B:505:HOH:O	1.98	0.62
1:A:208:ARG:HH11	1:A:210:GLN:HE22	1.45	0.62
1:B:244:VAL:HG21	4:B:413:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:GLY:O	1:B:24:LEU:HD23	2.00	0.61
1:B:227:MET:HE2	4:B:552:HOH:O	2.00	0.61
1:A:169:LYS:HZ3	1:A:169:LYS:HB2	1.63	0.61
1:A:204:ASN:HB2	1:A:210:GLN:O	2.01	0.61
1:A:234:ARG:HB3	1:A:244:VAL:HG21	1.82	0.60
1:A:208:ARG:NH1	1:A:210:GLN:NE2	2.49	0.60
1:B:238:VAL:HA	1:B:239:PRO:C	2.22	0.59
1:B:208:ARG:CD	1:B:210:GLN:HE21	2.06	0.59
1:B:273:THR:HG21	4:B:607:HOH:O	2.02	0.58
1:A:218:ASN:HD22	1:A:220:ASN:N	1.93	0.58
1:A:234:ARG:HD2	1:A:241:ASP:OD2	2.04	0.58
1:A:13:ARG:NH1	1:A:13:ARG:HB2	2.20	0.57
1:B:243:GLU:HG2	4:B:491:HOH:O	2.03	0.57
1:A:39:LEU:HD23	1:A:40:HIS:N	2.20	0.56
1:B:284:ALA:HB2	1:B:325:LEU:HD13	1.87	0.56
1:B:311:LEU:HD11	1:B:325:LEU:HD22	1.87	0.56
4:A:593:HOH:O	1:B:269:LYS:HD3	2.05	0.56
1:B:273:THR:HB	4:B:533:HOH:O	2.05	0.55
1:A:208:ARG:HH22	1:A:247:GLU:CD	2.10	0.55
1:A:170:GLN:NE2	1:B:172:ARG:HH11	2.03	0.55
1:A:208:ARG:NH1	1:A:210:GLN:HE22	2.04	0.55
1:A:38:ARG:HG3	1:A:123:ASP:OD2	2.07	0.54
1:A:172:ARG:HH11	1:B:170:GLN:NE2	2.04	0.53
1:A:41:GLU:HG2	1:A:46:LEU:HD23	1.91	0.53
1:B:116:ARG:O	1:B:120:LEU:HD23	2.08	0.53
1:A:13:ARG:HD2	4:A:439:HOH:O	2.09	0.53
1:B:151:LEU:C	1:B:152:ILE:HD12	2.29	0.52
1:B:273:THR:HG23	1:B:292:ALA:HB3	1.92	0.52
1:A:284:ALA:HB2	1:A:325:LEU:HD13	1.92	0.52
1:B:266:ARG:HH11	1:B:266:ARG:HG3	1.74	0.52
1:B:218:ASN:HD21	1:B:221:GLU:H	1.58	0.52
1:B:363:LEU:O	1:B:367:ARG:HG3	2.08	0.52
1:B:208:ARG:HH11	1:B:210:GLN:HE22	1.57	0.51
1:A:103:ILE:HD13	1:A:215:SER:HB3	1.93	0.51
1:A:49:PHE:O	1:A:106:ARG:HD2	2.11	0.51
1:B:41:GLU:HG2	1:B:46:LEU:HD23	1.93	0.51
1:A:182:LEU:HD21	1:A:265:ALA:CB	2.40	0.51
1:A:47:ARG:HH11	1:A:47:ARG:HB2	1.75	0.50
1:A:210:GLN:HE22	1:A:244:VAL:CG1	2.25	0.50
1:A:170:GLN:HE22	1:B:172:ARG:NH1	2.06	0.50
1:A:47:ARG:HH11	1:A:47:ARG:CB	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ALA:HB1	4:B:529:HOH:O	2.11	0.50
1:A:363:LEU:O	1:A:367:ARG:HG3	2.11	0.50
1:A:151:LEU:C	1:A:152:ILE:HD12	2.32	0.49
1:B:134:ASP:CG	1:B:136:VAL:HG12	2.33	0.49
1:A:172:ARG:NH1	1:B:170:GLN:HE22	2.07	0.49
1:B:323:ASP:O	1:B:326:VAL:HG22	2.13	0.49
1:B:374:VAL:HG22	1:B:375:TYR:N	2.28	0.49
1:A:244:VAL:HG11	4:A:393:HOH:O	2.13	0.49
1:B:204:ASN:HB2	1:B:210:GLN:O	2.13	0.48
1:A:186:ARG:HD2	1:A:222:LEU:HB2	1.94	0.48
1:B:351:SER:O	1:B:357:MET:HG3	2.13	0.48
1:B:241:ASP:O	1:B:244:VAL:HG12	2.14	0.47
1:A:39:LEU:C	1:A:39:LEU:HD23	2.35	0.47
1:B:116:ARG:NE	1:B:120:LEU:HD21	2.29	0.47
1:A:266:ARG:HH11	1:A:266:ARG:HG3	1.80	0.47
1:A:351:SER:O	1:A:357:MET:HG3	2.15	0.47
1:A:179:LEU:HB2	1:A:227:MET:HG2	1.96	0.46
1:B:208:ARG:HG2	1:B:248:MET:SD	2.54	0.46
1:B:285:LEU:HB3	1:B:290:ALA:HB2	1.97	0.46
1:B:99:LEU:HD13	1:B:99:LEU:C	2.35	0.46
1:A:47:ARG:HB2	1:A:47:ARG:CZ	2.45	0.46
1:B:39:LEU:HD23	1:B:39:LEU:C	2.35	0.46
1:B:49:PHE:O	1:B:106:ARG:HD2	2.15	0.46
1:B:273:THR:CG2	1:B:292:ALA:HB3	2.47	0.45
1:A:146:VAL:HG12	4:A:653:HOH:O	2.17	0.44
1:A:182:LEU:HD13	1:A:262:LEU:HD12	1.99	0.44
1:B:179:LEU:HD23	1:B:179:LEU:N	2.32	0.44
1:A:311:LEU:HD11	1:A:325:LEU:HD22	2.00	0.44
1:A:47:ARG:NH1	1:A:47:ARG:CB	2.75	0.44
1:B:156:ASP:N	1:B:156:ASP:OD1	2.49	0.44
1:A:359:THR:HB	1:A:360:PRO:CD	2.48	0.43
1:A:266:ARG:HD3	4:A:611:HOH:O	2.18	0.43
1:A:285:LEU:HB3	1:A:290:ALA:HB2	1.99	0.43
1:B:15:GLU:HG2	1:B:149:ALA:HB2	2.00	0.43
1:B:286:VAL:HA	4:B:583:HOH:O	2.17	0.43
1:A:11:THR:O	1:A:11:THR:HG23	2.18	0.43
1:A:218:ASN:HD21	1:A:221:GLU:N	2.14	0.43
1:B:57:HIS:HE1	4:B:683:HOH:O	2.01	0.43
1:B:134:ASP:OD1	1:B:136:VAL:HG12	2.19	0.43
1:A:210:GLN:HE22	1:A:244:VAL:HG13	1.83	0.42
1:A:62:VAL:O	1:A:66:LEU:HG	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:VAL:HA	4:B:607:HOH:O	2.18	0.42
1:A:206:TRP:CG	1:A:207:PRO:HA	2.54	0.42
1:A:38:ARG:HD2	1:A:40:HIS:CE1	2.55	0.42
1:B:63:LEU:HD13	1:B:72:VAL:HG21	2.02	0.42
1:A:159:GLY:HA2	4:A:739:HOH:O	2.19	0.42
1:A:99:LEU:C	1:A:99:LEU:HD13	2.40	0.42
1:A:206:TRP:CD1	1:A:207:PRO:HA	2.55	0.42
1:A:374:VAL:HG22	1:A:375:TYR:N	2.35	0.42
1:A:86:MET:HE2	1:A:87:HIS:N	2.35	0.41
1:B:206:TRP:CG	1:B:207:PRO:HA	2.55	0.41
1:A:342:LEU:HD23	1:A:362:ALA:HA	2.01	0.41
1:A:208:ARG:HD2	1:A:210:GLN:HE21	1.86	0.41
1:B:31:LYS:HG2	1:B:120:LEU:HB3	2.01	0.41
1:B:266:ARG:NH1	1:B:266:ARG:HG3	2.35	0.41
1:A:263:LYS:HG2	4:A:613:HOH:O	2.21	0.41
1:A:89:LYS:HD3	1:A:90:SER:N	2.36	0.41
1:B:301:ALA:HB3	2:B:380:FAD:O2	2.21	0.41
1:A:12:ARG:HB3	1:A:35:TRP:CZ3	2.56	0.41
1:A:31:LYS:HD2	1:A:35:TRP:O	2.20	0.40
1:A:359:THR:HB	1:A:360:PRO:HD2	2.02	0.40
1:B:206:TRP:CD1	1:B:207:PRO:HA	2.56	0.40
1:A:131:VAL:HG12	1:A:131:VAL:O	2.22	0.40
1:A:358:PHE:HB3	1:A:363:LEU:CD1	2.44	0.40
1:A:31:LYS:HE2	4:A:585:HOH:O	2.22	0.40
1:B:218:ASN:HD22	1:B:220:ASN:N	1.97	0.40
1:B:227:MET:HE1	4:B:481:HOH:O	2.20	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:B:704:HOH:O	4:B:704:HOH:O[2_554]	2.14	0.06

## 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	367/415 (88%)	353 (96%)	13 (4%)	1 (0%)	41	41
1	B	367/415 (88%)	354 (96%)	12 (3%)	1 (0%)	41	41
All	All	734/830 (88%)	707 (96%)	25 (3%)	2 (0%)	41	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	ALA
1	A	51	ALA

### 5.3.2 Protein sidechains ⓘ

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	297/333 (89%)	282 (95%)	15 (5%)	24	22
1	B	297/333 (89%)	285 (96%)	12 (4%)	31	32
All	All	594/666 (89%)	567 (96%)	27 (4%)	27	27

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	24	LEU
1	A	47	ARG
1	A	73	LEU
1	A	99	LEU
1	A	113	LEU
1	A	120	LEU
1	A	142	GLN
1	A	169	LYS
1	A	199	THR
1	A	215	SER

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Mol	Chain	Res	Type
1	A	218	ASN
1	A	256	LEU
1	A	280	ARG
1	A	285	LEU
1	B	55	LEU
1	B	61	ARG
1	B	73	LEU
1	B	113	LEU
1	B	142	GLN
1	B	199	THR
1	B	218	ASN
1	B	256	LEU
1	B	273	THR
1	B	280	ARG
1	B	285	LEU
1	B	363	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	97	ASN
1	A	142	GLN
1	A	170	GLN
1	A	210	GLN
1	A	218	ASN
1	A	356	ASN
1	B	57	HIS
1	B	97	ASN
1	B	142	GLN
1	B	170	GLN
1	B	210	GLN
1	B	218	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 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	A	380	-	51,58,58	2.54	14 (27%)	60,89,89	2.23	12 (20%)
3	3HM	A	381	-	8,11,11	2.31	1 (12%)	10,15,15	1.51	3 (30%)
2	FAD	B	380	-	51,58,58	2.52	14 (27%)	60,89,89	2.24	13 (21%)
3	3HM	B	381	-	8,11,11	2.32	1 (12%)	10,15,15	1.48	3 (30%)

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	A	380	-	-	15/30/50/50	0/6/6/6
3	3HM	A	381	-	-	0/0/4/4	0/1/1/1
2	FAD	B	380	-	-	17/30/50/50	0/6/6/6
3	3HM	B	381	-	-	0/0/4/4	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	380	FAD	C4X-N5	6.39	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	380	FAD	C4X-N5	6.34	1.42	1.33
3	B	381	3HM	CAE-CAF	6.21	1.53	1.47
3	A	381	3HM	CAE-CAF	6.20	1.53	1.47
2	A	380	FAD	C10-N1	6.17	1.41	1.33
2	A	380	FAD	C4X-C10	6.16	1.45	1.38
2	B	380	FAD	C4X-C10	6.11	1.44	1.38
2	B	380	FAD	C10-N1	6.05	1.41	1.33
2	B	380	FAD	C2A-N3A	5.71	1.41	1.32
2	A	380	FAD	C2A-N3A	5.70	1.41	1.32
2	A	380	FAD	C9A-N10	5.50	1.46	1.38
2	B	380	FAD	C9A-N10	5.34	1.45	1.38
2	B	380	FAD	C4-N3	4.90	1.41	1.33
2	A	380	FAD	C4-N3	4.83	1.41	1.33
2	A	380	FAD	C5X-N5	4.39	1.42	1.35
2	A	380	FAD	C1'-N10	4.21	1.52	1.48
2	B	380	FAD	C1'-N10	4.20	1.52	1.48
2	A	380	FAD	C2A-N1A	4.13	1.41	1.33
2	B	380	FAD	C5X-N5	4.11	1.42	1.35
2	B	380	FAD	C2A-N1A	3.93	1.41	1.33
2	B	380	FAD	C4A-N3A	3.64	1.40	1.35
2	A	380	FAD	C4A-N3A	3.42	1.40	1.35
2	A	380	FAD	C6-C7	2.94	1.45	1.37
2	B	380	FAD	C6-C7	2.93	1.45	1.37
2	A	380	FAD	C9-C9A	2.76	1.46	1.40
2	B	380	FAD	C9-C9A	2.69	1.46	1.40
2	A	380	FAD	C8-C7	2.50	1.47	1.40
2	B	380	FAD	C8-C7	2.48	1.47	1.40
2	A	380	FAD	C9-C8	2.35	1.43	1.37
2	B	380	FAD	C9-C8	2.19	1.43	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	380	FAD	O2A-PA-O5B	8.70	148.13	107.75
2	A	380	FAD	O2A-PA-O5B	8.57	147.53	107.75
2	A	380	FAD	C4-N3-C2	7.29	121.30	115.14
2	B	380	FAD	C4-N3-C2	7.19	121.22	115.14
2	B	380	FAD	N3A-C2A-N1A	-6.77	118.10	128.68
2	A	380	FAD	N3A-C2A-N1A	-6.73	118.16	128.68
2	B	380	FAD	C4X-N5-C5X	5.07	121.83	116.77
2	A	380	FAD	C4X-N5-C5X	5.05	121.81	116.77
2	A	380	FAD	O2A-PA-O1A	-3.69	94.01	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	380	FAD	O2A-PA-O1A	-3.55	94.71	112.24
2	B	380	FAD	C4-C4X-N5	3.04	122.07	118.60
2	A	380	FAD	C4-C4X-N5	2.98	122.00	118.60
2	A	380	FAD	C4-C4X-C10	-2.82	118.08	119.95
2	B	380	FAD	C4-C4X-C10	-2.79	118.11	119.95
3	A	381	3HM	CAE-CAD-CAC	-2.71	118.52	120.68
3	B	381	3HM	CAE-CAD-CAC	-2.68	118.55	120.68
2	A	380	FAD	C2B-C3B-C4B	2.61	107.71	102.64
2	B	380	FAD	C2B-C3B-C4B	2.57	107.64	102.64
2	B	380	FAD	C4X-C4-N3	-2.55	119.94	123.43
2	A	380	FAD	C4X-C4-N3	-2.46	120.06	123.43
3	A	381	3HM	CAD-CAE-CAK	2.40	119.49	117.11
3	B	381	3HM	CAD-CAE-CAK	2.34	119.42	117.11
2	B	380	FAD	C3B-C2B-C1B	2.28	104.41	100.98
3	A	381	3HM	CAE-CAK-NAJ	-2.25	120.62	124.32
2	A	380	FAD	C3B-C2B-C1B	2.22	104.32	100.98
3	B	381	3HM	CAE-CAK-NAJ	-2.21	120.68	124.32
2	A	380	FAD	C1'-N10-C10	2.11	120.30	118.41
2	B	380	FAD	C1B-N9A-C4A	-2.10	122.94	126.64
2	B	380	FAD	C10-C4X-N5	-2.08	119.82	121.26
2	B	380	FAD	C9A-C5X-N5	-2.02	119.19	122.36
2	A	380	FAD	C9A-C5X-N5	-2.01	119.22	122.36

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	380	FAD	C5B-O5B-PA-O1A
2	A	380	FAD	C3'-C4'-C5'-O5'
2	A	380	FAD	O4'-C4'-C5'-O5'
2	A	380	FAD	C5'-O5'-P-O1P
2	A	380	FAD	C5'-O5'-P-O2P
2	A	380	FAD	C5'-O5'-P-O3P
2	B	380	FAD	C5B-O5B-PA-O1A
2	B	380	FAD	C3'-C4'-C5'-O5'
2	B	380	FAD	O4'-C4'-C5'-O5'
2	B	380	FAD	C5'-O5'-P-O1P
2	B	380	FAD	C5'-O5'-P-O2P
2	B	380	FAD	C5'-O5'-P-O3P
2	A	380	FAD	O4B-C4B-C5B-O5B
2	A	380	FAD	C3B-C4B-C5B-O5B
2	B	380	FAD	O4B-C4B-C5B-O5B

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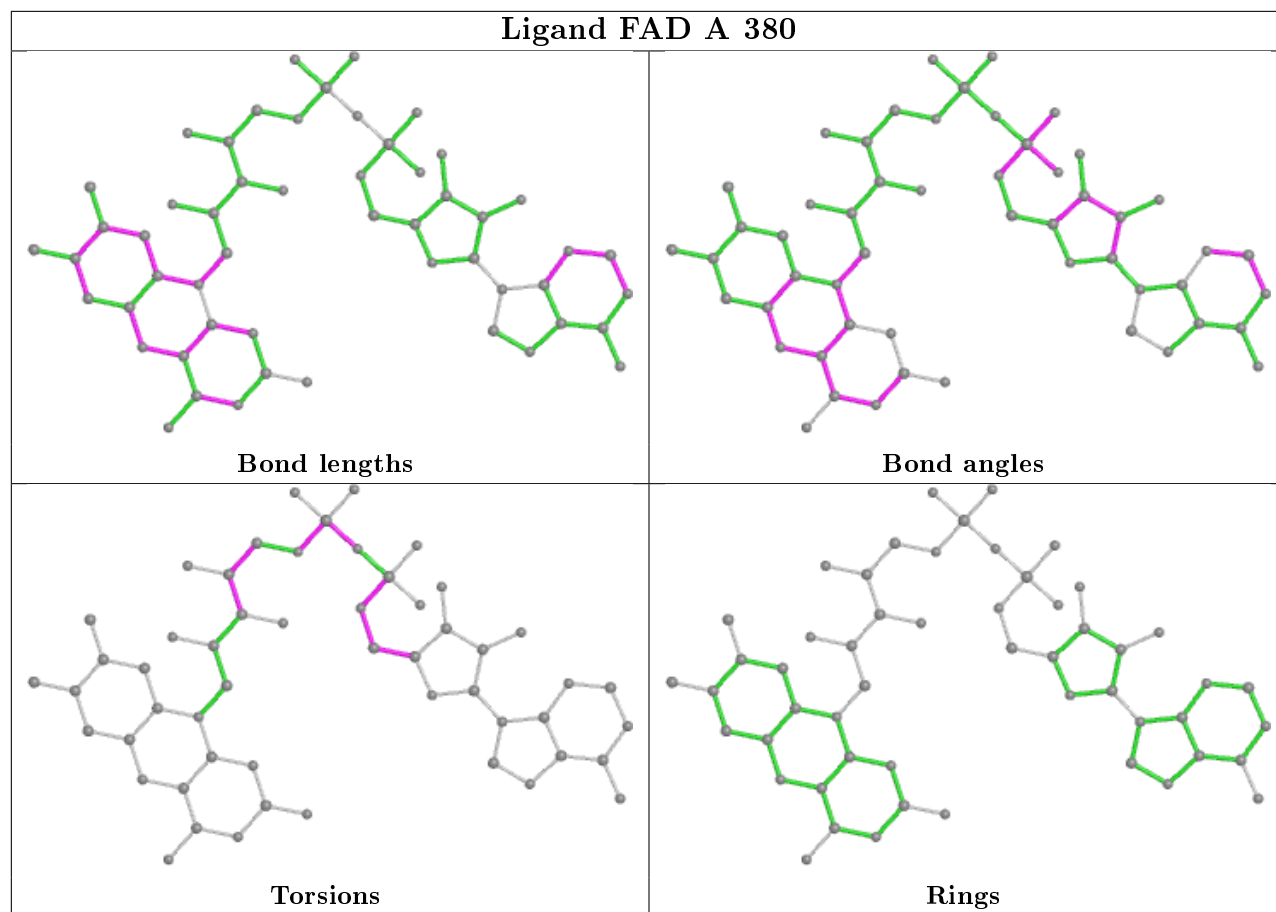
Mol	Chain	Res	Type	Atoms
2	B	380	FAD	C3B-C4B-C5B-O5B
2	A	380	FAD	C4B-C5B-O5B-PA
2	B	380	FAD	C4B-C5B-O5B-PA
2	A	380	FAD	C5B-O5B-PA-O3P
2	B	380	FAD	C5B-O5B-PA-O3P
2	A	380	FAD	PA-O3P-P-O2P
2	B	380	FAD	PA-O3P-P-O2P
2	A	380	FAD	C5B-O5B-PA-O2A
2	B	380	FAD	C5B-O5B-PA-O2A
2	A	380	FAD	C2'-C3'-C4'-O4'
2	B	380	FAD	C2'-C3'-C4'-O4'
2	B	380	FAD	C2'-C3'-C4'-C5'
2	A	380	FAD	C2'-C3'-C4'-C5'
2	A	380	FAD	PA-O3P-P-O1P
2	B	380	FAD	PA-O3P-P-O1P
2	B	380	FAD	C1'-C2'-C3'-O3'
2	B	380	FAD	O3'-C3'-C4'-C5'

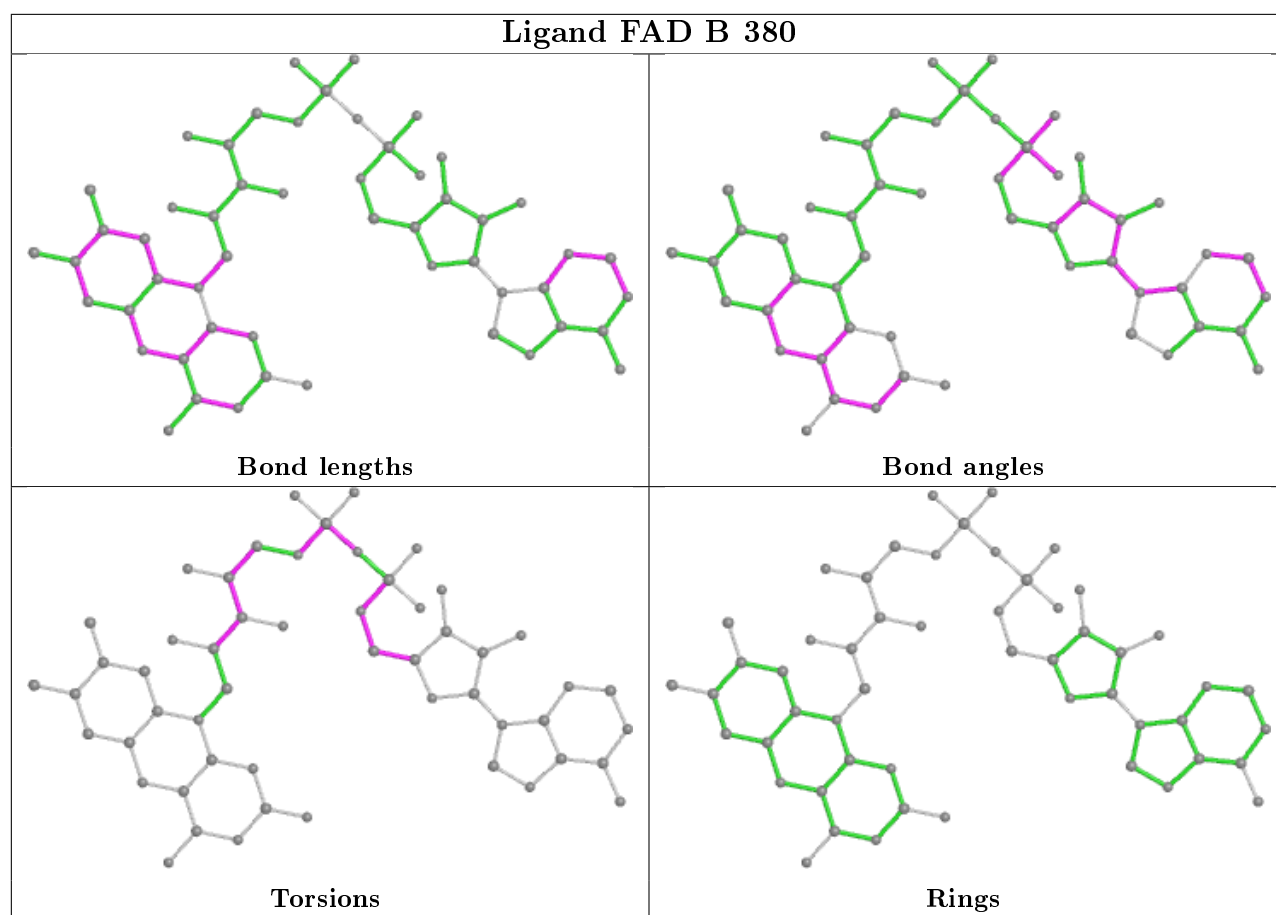
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	380	FAD	1	0
3	A	381	3HM	1	0
2	B	380	FAD	2	0
3	B	381	3HM	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 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	369/415 (88%)	-0.29	0 100 100	13, 21, 34, 48	0
1	B	369/415 (88%)	-0.31	0 100 100	12, 21, 34, 46	0
All	All	738/830 (88%)	-0.30	0 100 100	12, 21, 34, 48	0

There are no RSRZ outliers to report.

### 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 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.

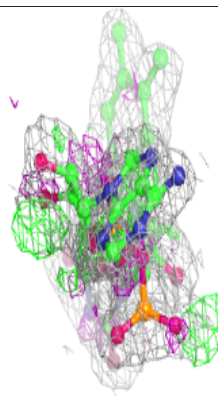
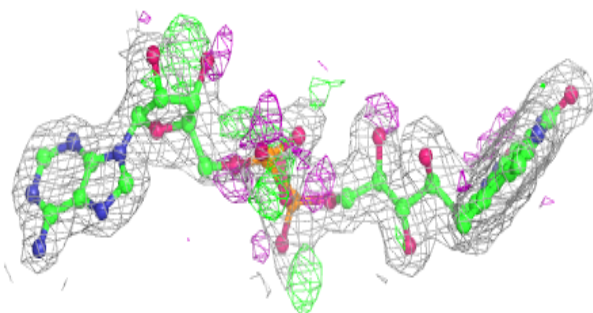
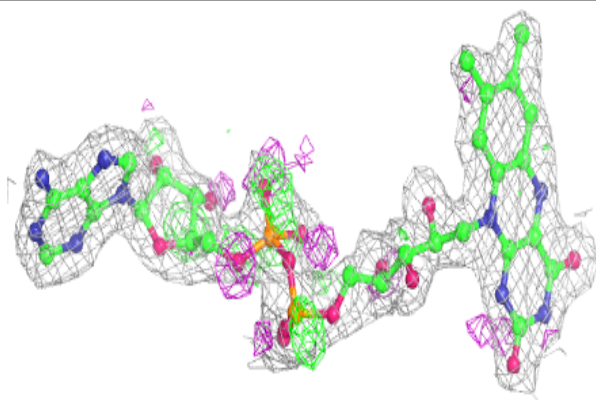
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	3HM	A	381	11/11	0.83	0.20	43,45,46,47	0
3	3HM	B	381	11/11	0.86	0.19	39,42,43,44	0
2	FAD	B	380	53/53	0.94	0.14	20,23,32,36	0
2	FAD	A	380	53/53	0.94	0.15	20,24,31,36	0

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.

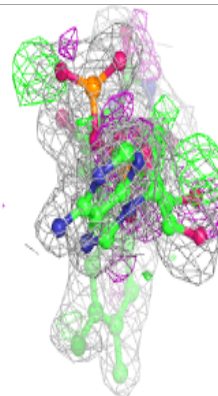
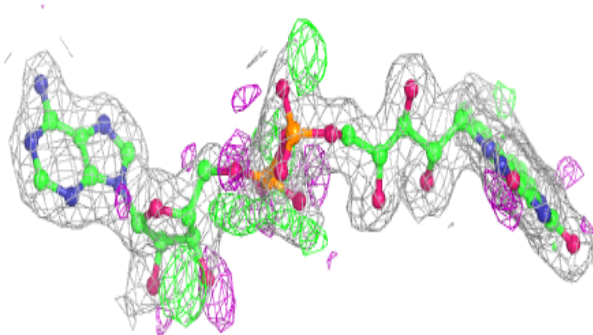
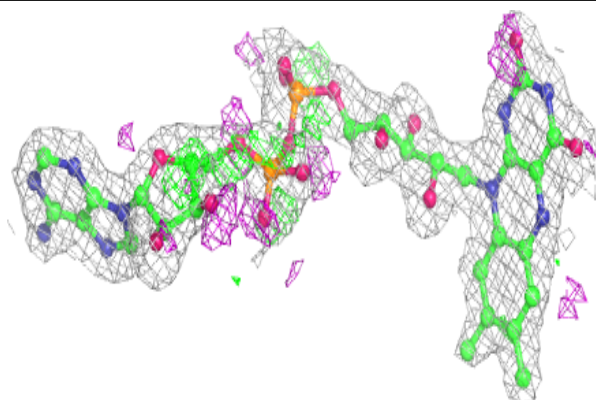
**Electron density around FAD B 380:**

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



**Electron density around FAD A 380:**

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



## 6.5 Other polymers

There are no such residues in this entry.