



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:01 pm GMT

PDB ID : 2Z5Y  
Title : Crystal Structure of Human Monoamine Oxidase A (G110A) with Harmine  
Authors : Son, S.Y.; Ma, J.; Yoshimura, M.; Tsukihara, T.  
Deposited on : 2007-07-20  
Resolution : 2.17 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

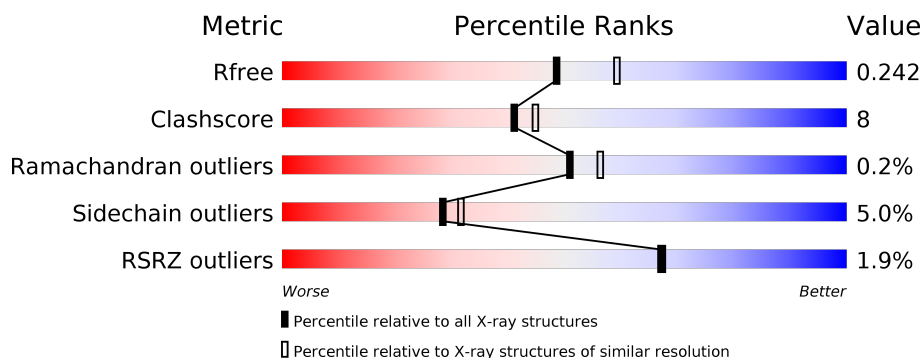
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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))
$R_{free}$	100719	5526 (2.20-2.16)
Clashscore	112137	6386 (2.20-2.16)
Ramachandran outliers	110173	6282 (2.20-2.16)
Sidechain outliers	110143	6282 (2.20-2.16)
RSRZ outliers	101464	5562 (2.20-2.16)

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. 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	513	<div> <div>2%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4397 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.

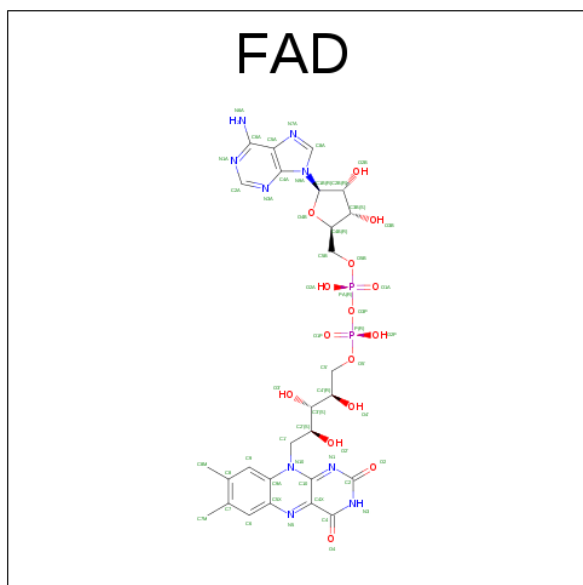
- Molecule 1 is a protein called Amine oxidase [flavin-containing] A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	513	4101	2635	699	746	21	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	GLY	ENGINEERED	UNP P21397

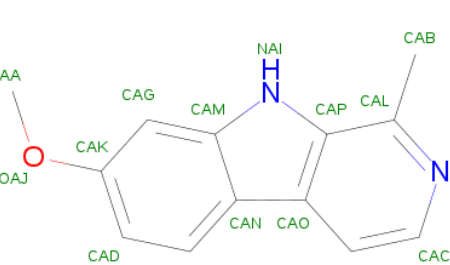
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

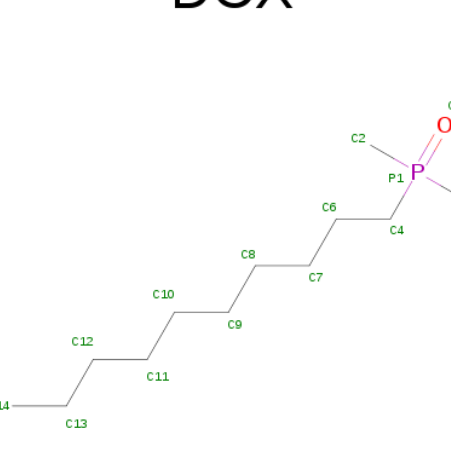
- Molecule 3 is 7-METHOXY-1-METHYL-9H-BETA-CARBOLINE (three-letter code: HRM)

# HRM



The diagram shows a triphenylamine core structure. The central nitrogen atom is bonded to three phenyl rings. The rings are labeled with HRM terms: the left ring has labels CAA, CAJ, CAK, CAD, CAF, and CAM; the bottom ring has labels CAN, CAO, CAE, and CAC; the right ring has labels CAB, CAL, and NAH. The nitrogen atom is also labeled NAI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	13	2	1		

- # DCX
- 
- The ORTEP diagram shows the molecular structure of DCX. The molecule consists of a 12-carbon aliphatic chain (C1-C12) and a phosphorus-containing group (C3-C6, P1, O3, O4). The chain is zig-zagged, with C14 at the end of the main chain. The phosphorus atom (P1) is bonded to C3, C4, C6, and two oxygen atoms (O3 and O4). The oxygen atom O4 is double-bonded to P1, while O3 is single-bonded. The carbon atoms are labeled C1 through C14, and the phosphorus atom is labeled P1. The oxygen atoms are labeled O3 and O4. The structure is shown in a perspective view, with the chain extending from the bottom left towards the top right. The phosphorus group is attached to the chain at C3 and C4. The overall structure is a complex organic molecule with a long aliphatic chain and a phosphorus-containing functional group.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			14	12	1	1		



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			14	12	1	1		

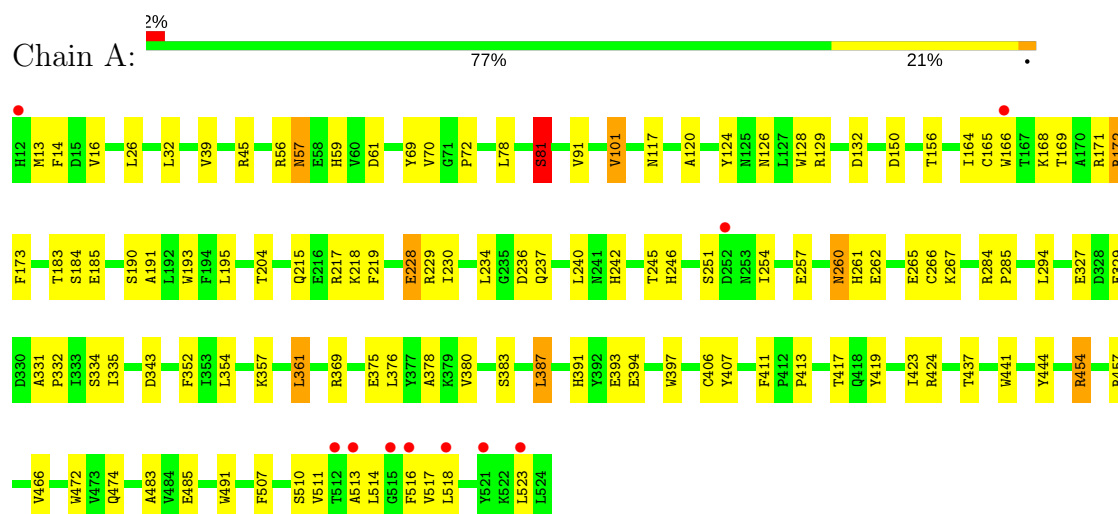
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	199	Total	O	0	0
			199	199		

### 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 ( $\text{RSRZ} > 2$ ). 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: Amine oxidase [flavin-containing] A



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.55Å 217.36Å 54.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.24 – 2.17 44.24 – 2.17	Depositor EDS
% Data completeness (in resolution range)	72.6 (44.24-2.17) 72.6 (44.24-2.17)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.3.0021	Depositor
R, $R_{free}$	0.193 , 0.244 0.191 , 0.242	Depositor DCC
$R_{free}$ test set	1608 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.3	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 35.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4397	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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

### 5.1 Standard geometry

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

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	0.92	3/4203 (0.1%)	0.92	8/5698 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	GLU	CG-CD	5.97	1.60	1.51
1	A	166	TRP	CB-CG	5.62	1.60	1.50
1	A	124	TYR	CE2-CZ	5.40	1.45	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ARG	NE-CZ-NH1	-9.54	115.53	120.30
1	A	45	ARG	NE-CZ-NH2	9.21	124.90	120.30
1	A	81	SER	CB-CA-C	-7.55	95.75	110.10
1	A	454	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	229	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	229	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	81	SER	N-CA-CB	-5.44	102.34	110.50
1	A	343	ASP	CB-CG-OD2	5.06	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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	4101	0	4097	67	0
2	A	53	0	29	2	0
3	A	16	0	12	3	0
4	A	28	0	54	1	0
5	A	199	0	0	2	0
All	All	4397	0	4192	68	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (68) 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:126:ASN:HD22	1:A:129:ARG:HH21	1.33	0.77
1:A:260:ASN:OD1	1:A:262:GLU:OE1	2.03	0.75
1:A:240:LEU:O	1:A:242:HIS:HD2	1.72	0.73
1:A:81:SER:OG	1:A:219:PHE:CE2	2.43	0.71
1:A:454:ARG:HD2	1:A:472:TRP:CH2	2.28	0.69
1:A:14:PHE:O	1:A:266:CYS:HA	1.97	0.65
1:A:424:ARG:HB3	1:A:437:THR:HB	1.79	0.63
1:A:352:PHE:HE2	3:A:700:HRM:HAE	1.67	0.60
1:A:397:TRP:CD1	2:A:600:FAD:HM71	2.38	0.59
1:A:352:PHE:HE2	3:A:700:HRM:CAE	2.15	0.58
1:A:507:PHE:O	1:A:511:VAL:HG22	2.02	0.58
1:A:406:CYS:HB3	1:A:407:TYR:HA	1.84	0.58
1:A:454:ARG:HD2	1:A:472:TRP:CZ2	2.40	0.57
1:A:156:THR:HG22	1:A:413:PRO:HG2	1.88	0.56
1:A:168:LYS:O	1:A:172:ARG:HD3	2.05	0.56
1:A:190:SER:HB2	1:A:413:PRO:HA	1.88	0.56
1:A:378:ALA:HB2	1:A:387:LEU:HD13	1.87	0.56
1:A:294:LEU:HB2	1:A:419:TYR:HB3	1.88	0.54
1:A:257:GLU:OE2	1:A:261:HIS:HD2	1.92	0.53
1:A:406:CYS:CB	1:A:407:TYR:HA	2.41	0.51
1:A:193:TRP:CG	1:A:411:PHE:HB2	2.45	0.51
1:A:491:TRP:HB2	4:A:1:DCX:O4	2.11	0.51
1:A:57:ASN:HD22	1:A:59:HIS:H	1.59	0.50
1:A:26:LEU:HB3	1:A:230:ILE:HG21	1.96	0.48
1:A:260:ASN:CG	1:A:262:GLU:OE1	2.52	0.48
1:A:56:ARG:NH2	1:A:228:GLU:OE1	2.47	0.47
1:A:165:CYS:HB2	1:A:171:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ASN:C	1:A:260:ASN:HD22	2.17	0.46
1:A:457:ARG:NH1	5:A:769:HOH:O	2.36	0.46
1:A:91:VAL:HG21	1:A:215:GLN:O	2.14	0.46
1:A:369:ARG:NH2	1:A:394:GLU:OE1	2.36	0.46
1:A:378:ALA:HA	1:A:383:SER:O	2.15	0.46
1:A:510:SER:O	1:A:513:ALA:HB3	2.14	0.46
1:A:117:ASN:HB3	1:A:120:ALA:HB3	1.98	0.46
1:A:357:LYS:O	1:A:361:LEU:HD12	2.15	0.46
1:A:246:HIS:HB2	1:A:257:GLU:HB3	1.98	0.46
1:A:101:VAL:HG13	1:A:327:GLU:HB3	1.98	0.46
1:A:335:ILE:HD11	3:A:700:HRM:OAJ	2.15	0.45
1:A:518:LEU:HD22	1:A:523:LEU:HB2	1.97	0.45
1:A:376:LEU:O	1:A:380:VAL:HG23	2.16	0.45
1:A:132:ASP:OD1	1:A:204:THR:HG23	2.17	0.45
1:A:260:ASN:ND2	1:A:262:GLU:OE1	2.50	0.45
1:A:70:VAL:HG11	1:A:219:PHE:CZ	2.51	0.45
1:A:16:VAL:HB	1:A:39:VAL:HG13	1.98	0.45
1:A:16:VAL:HG21	1:A:32:LEU:HD13	1.99	0.45
1:A:441:TRP:O	1:A:444:TYR:HB2	2.17	0.45
1:A:81:SER:HG	1:A:219:PHE:HE2	1.56	0.44
1:A:126:ASN:HD22	1:A:129:ARG:NH2	2.10	0.44
1:A:185:GLU:HA	1:A:185:GLU:OE1	2.18	0.43
1:A:329:GLU:HG3	5:A:863:HOH:O	2.17	0.43
1:A:57:ASN:HD22	1:A:59:HIS:N	2.16	0.43
1:A:72:PRO:HB3	1:A:483:ALA:HA	2.00	0.43
1:A:128:TRP:CZ2	1:A:173:PHE:CD2	3.07	0.43
2:A:600:FAD:N1	2:A:600:FAD:H2'	2.34	0.43
1:A:69:TYR:HA	1:A:217:ARG:O	2.18	0.43
1:A:191:ALA:O	1:A:195:LEU:HG	2.19	0.42
1:A:284:ARG:HA	1:A:285:PRO:C	2.39	0.42
1:A:254:ILE:O	1:A:265:GLU:HA	2.19	0.42
1:A:150:ASP:HA	1:A:417:THR:HG21	2.01	0.42
1:A:331:ALA:HA	1:A:332:PRO:HD2	1.93	0.42
1:A:391:HIS:HE1	1:A:393:GLU:OE1	2.02	0.42
1:A:245:THR:OG1	1:A:246:HIS:HD2	2.03	0.41
1:A:391:HIS:CE1	1:A:393:GLU:HG2	2.55	0.41
1:A:218:LYS:HE3	1:A:218:LYS:HB2	1.87	0.41
1:A:183:THR:HG22	1:A:354:LEU:HD22	2.03	0.41
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.85	0.40
1:A:236:ASP:OD1	1:A:237:GLN:NE2	2.55	0.40
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.93	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	511/513 (100%)	489 (96%)	21 (4%)	1 (0%)	51 56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ASP

### 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	439/439 (100%)	417 (95%)	22 (5%)	28 32

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	57	ASN
1	A	81	SER
1	A	101	VAL
1	A	164	ILE
1	A	169	THR
1	A	172	ARG

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Mol	Chain	Res	Type
1	A	184	SER
1	A	251	SER
1	A	260	ASN
1	A	267	LYS
1	A	334	SER
1	A	361	LEU
1	A	375	GLU
1	A	387	LEU
1	A	423	ILE
1	A	466	VAL
1	A	474	GLN
1	A	485	GLU
1	A	514	LEU
1	A	516	PHE
1	A	517	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	126	ASN
1	A	242	HIS
1	A	246	HIS
1	A	260	ASN
1	A	261	HIS
1	A	292	ASN
1	A	296	GLN
1	A	391	HIS
1	A	418	GLN
1	A	461	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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$
4	DCX	A	1	-	12,13,13	0.51	0	13,15,15	0.47	0
4	DCX	A	2	-	12,13,13	0.47	0	13,15,15	0.82	1 (7%)
2	FAD	A	600	-	51,58,58	1.92	12 (23%)	54,89,89	2.17	13 (24%)
3	HRM	A	700	-	17,18,18	1.78	5 (29%)	21,26,26	1.54	4 (19%)

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
4	DCX	A	1	-	-	0/11/11/11	0/0/0/0
4	DCX	A	2	-	-	0/11/11/11	0/0/0/0
2	FAD	A	600	-	-	0/28/50/50	0/6/6/6
3	HRM	A	700	-	-	0/2/2/2	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C4-C4X	-2.78	1.36	1.41
3	A	700	HRM	CAN-CAO	-2.73	1.37	1.45
3	A	700	HRM	CAL-CAP	-2.67	1.39	1.42
2	A	600	FAD	C2B-C1B	-2.65	1.49	1.53
2	A	600	FAD	C1'-N10	-2.44	1.45	1.48
2	A	600	FAD	C4'-C3'	-2.21	1.49	1.53
2	A	600	FAD	C9A-N10	2.11	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	HRM	CAG-CAK	2.16	1.41	1.37
3	A	700	HRM	CAE-CAC	2.23	1.39	1.36
2	A	600	FAD	C2B-C3B	2.33	1.59	1.53
3	A	700	HRM	CAB-CAL	2.43	1.52	1.50
2	A	600	FAD	C7M-C7	2.55	1.56	1.51
2	A	600	FAD	C5'-C4'	3.50	1.57	1.51
2	A	600	FAD	C10-N1	3.84	1.38	1.33
2	A	600	FAD	C4-N3	3.97	1.40	1.33
2	A	600	FAD	O4B-C1B	5.80	1.49	1.41
2	A	600	FAD	C4X-N5	6.06	1.42	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	N3A-C2A-N1A	-8.62	121.35	128.86
2	A	600	FAD	C4-C4X-C10	-3.78	116.91	119.96
3	A	700	HRM	CAA-OAJ-CAK	-3.45	109.95	117.50
3	A	700	HRM	CAE-CAC-NAH	-3.31	120.37	123.80
2	A	600	FAD	C9A-C5X-N5	-2.84	118.01	122.24
2	A	600	FAD	C4X-C10-N10	-2.66	118.67	120.52
4	A	2	DCX	C2-P1-C3	-2.37	103.15	106.45
2	A	600	FAD	C5B-C4B-C3B	-2.14	107.14	115.29
2	A	600	FAD	C4X-C4-N3	-2.05	120.57	123.48
2	A	600	FAD	O2A-PA-O1A	2.09	123.09	112.28
2	A	600	FAD	C1'-N10-C10	2.49	121.05	118.50
2	A	600	FAD	C2A-N1A-C6A	2.53	123.19	118.77
2	A	600	FAD	C5X-C9A-N10	2.61	119.60	117.66
3	A	700	HRM	CAF-CAN-CAM	2.74	121.81	118.17
3	A	700	HRM	CAC-NAH-CAL	2.83	122.37	118.35
2	A	600	FAD	C6-C5X-C9A	2.94	122.81	119.00
2	A	600	FAD	C4-C4X-N5	4.96	124.12	118.68
2	A	600	FAD	C4-N3-C2	7.05	121.33	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	DCX	1	0
2	A	600	FAD	2	0

*Continued on next page...*

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700	HRM	3	0

## 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	513/513 (100%)	-0.18	10 (1%) 67 67	21, 34, 53, 100	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	518	LEU	5.2
1	A	521	TYR	4.7
1	A	516	PHE	3.9
1	A	12	HIS	3.3
1	A	515	GLY	3.0
1	A	513	ALA	3.0
1	A	512	THR	2.7
1	A	523	LEU	2.6
1	A	166	TRP	2.5
1	A	252	ASP	2.5

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DCX	A	2	14/14	0.90	0.16	1.03	64,69,83,84	0
3	HRM	A	700	16/16	0.98	0.12	0.63	29,31,32,34	0
2	FAD	A	600	53/53	0.98	0.13	0.43	14,21,27,29	0
4	DCX	A	1	14/14	0.87	0.14	-	74,76,85,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.