



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:17 am BST

PDB ID : 2IW5  
Title : Structural Basis for CoREST-Dependent Demethylation of Nucleosomes by the Human LSD1 Histone Demethylase  
Authors : Yang, M.; Gocke, C.B.; Luo, X.; Borek, D.; Tomchick, D.R.; Machius, M.; Otwinowski, Z.; Yu, H.  
Deposited on : 2006-06-26  
Resolution : 2.57 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

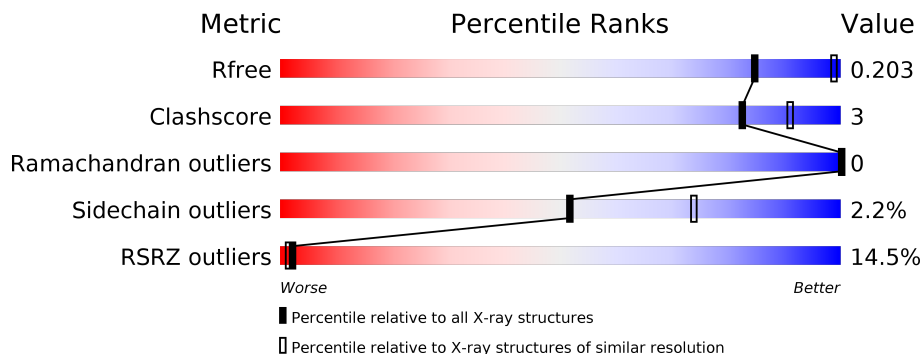
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.57 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	666	 13% 93% 7%
2	B	235	 13% 54% 43%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NH4	A	1842	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6440 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.

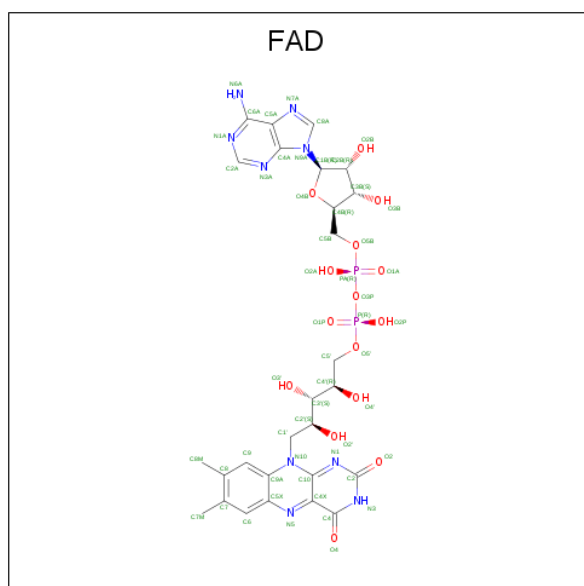
- Molecule 1 is a protein called LYSINE-SPECIFIC HISTONE DEMETHYLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	666	5217	3324	906	967	20	0	0	0

- Molecule 2 is a protein called REST COREPRESSOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	133	1076	676	194	203	3	0	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).

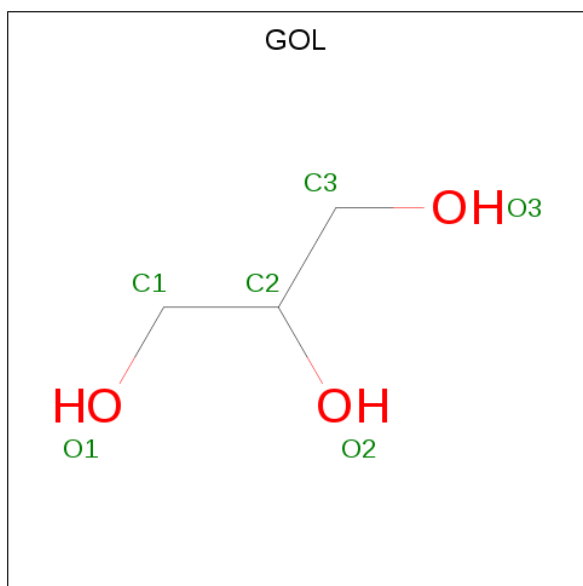


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	53	27	9	15	2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

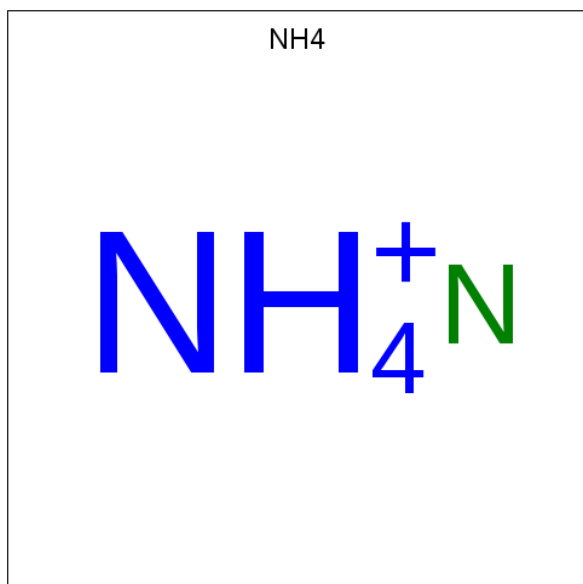
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Cl	0	0
			3	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is AMMONIUM ION (three-letter code: NH4) (formula:  $H_4N$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total N 1 1	0	0

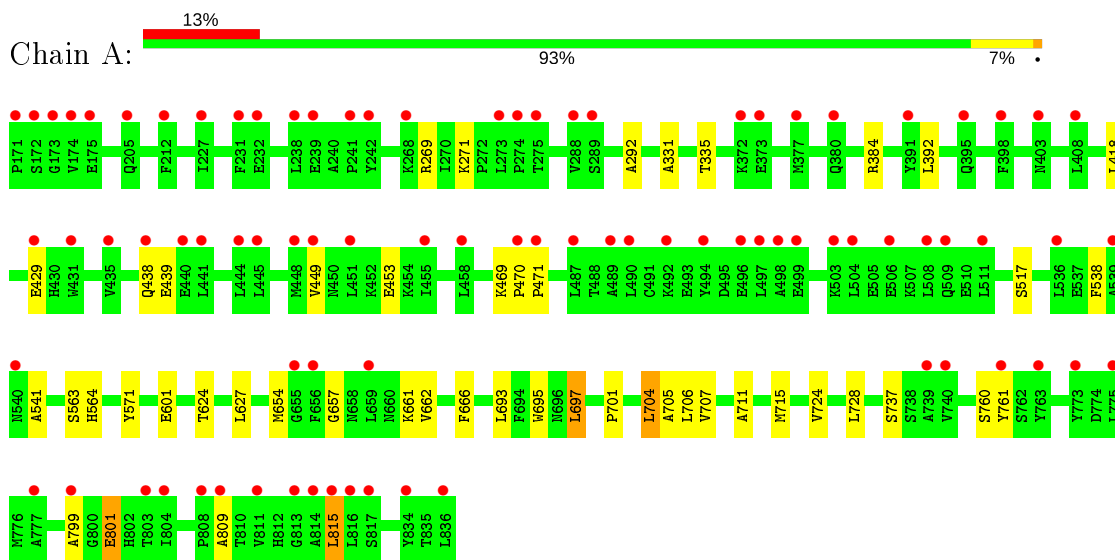
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	77	Total O 77 77	0	0
7	B	1	Total O 1 1	0	0

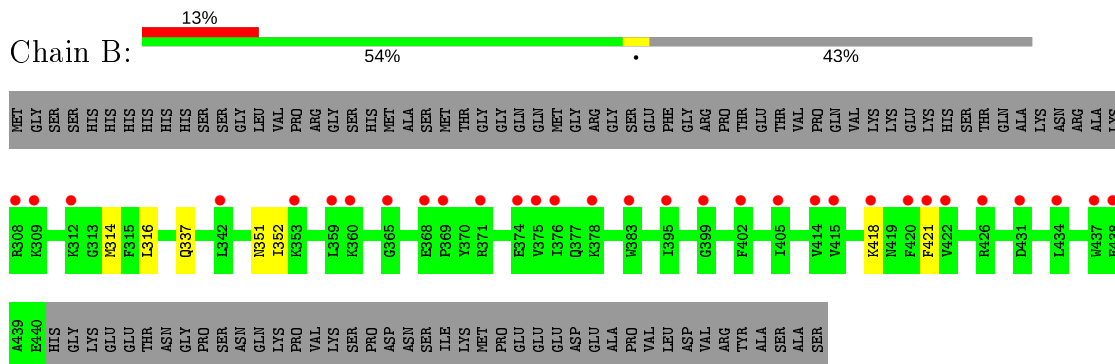
### 3 Residue-property plots [i](#)

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: LYSINE-SPECIFIC HISTONE DEMETHYLASE 1



- Molecule 2: REST COREPRESSOR 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.35Å 178.22Å 234.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.57 49.87 – 2.57	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.00-2.57) 93.2 (49.87-2.57)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.73 (at 2.58Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.203 , 0.212 0.194 , 0.203	Depositor DCC
$R_{free}$ test set	1499 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.7	Xtrriage
Anisotropy	0.475	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 68.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6440	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: GOL, CL, FAD, NH4

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	0.50	0/5331	0.66	2/7232 (0.0%)
2	B	0.42	0/1091	0.55	0/1471
All	All	0.48	0/6422	0.65	2/8703 (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	A	815	LEU	CA-CB-CG	6.60	130.49	115.30
1	A	697	LEU	N-CA-C	5.30	125.32	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	5217	0	5252	30	0
2	B	1076	0	1091	5	0
3	A	53	0	31	2	0
4	A	3	0	0	1	0
5	A	12	0	16	0	0
6	A	1	0	0	0	0
7	A	77	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
All	All	6440	0	6390	32	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 (32) 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)
4:A:1838:CL:CL	4:A:1843:CL:CL	2.19	1.34
1:A:384:ARG:HB3	2:B:314:MET:HE1	1.59	0.85
1:A:801:GLU:HG2	1:A:809:ALA:H	1.48	0.76
1:A:707:VAL:HG11	1:A:715:MET:HG3	1.75	0.67
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.76	0.66
1:A:384:ARG:HB3	2:B:314:MET:CE	2.27	0.65
1:A:335:THR:HG22	1:A:564:HIS:ND1	2.20	0.57
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.41	0.55
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.43	0.54
1:A:470:PRO:HA	1:A:471:PRO:C	2.28	0.53
1:A:711:ALA:O	1:A:715:MET:HG2	2.10	0.52
1:A:624:THR:HG22	1:A:799:ALA:HB3	1.92	0.51
1:A:335:THR:HG22	1:A:564:HIS:CE1	2.47	0.50
1:A:627:LEU:HD22	1:A:654:MET:HE2	1.93	0.50
1:A:661:LYS:HB3	1:A:704:LEU:HD21	1.96	0.47
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.96	0.47
1:A:707:VAL:CG1	1:A:715:MET:HG3	2.45	0.47
1:A:449:VAL:O	1:A:453:GLU:HG2	2.16	0.46
1:A:801:GLU:HG2	1:A:809:ALA:N	2.26	0.45
1:A:269:ARG:HG2	1:A:271:LYS:O	2.17	0.45
1:A:724:VAL:O	1:A:728:LEU:HG	2.17	0.45
1:A:760:SER:HB2	3:A:900:FAD:HM83	2.00	0.44
1:A:292:ALA:HB2	1:A:815:LEU:HD22	2.01	0.43
1:A:693:LEU:HD23	1:A:706:LEU:HD22	2.00	0.43
1:A:662:VAL:HB	1:A:705:ALA:HB3	2.00	0.43
1:A:438:GLN:HG3	2:B:352:ILE:HG22	2.01	0.43
2:B:418:LYS:O	2:B:421:PHE:HB2	2.18	0.43
1:A:801:GLU:CG	1:A:809:ALA:HA	2.45	0.42
1:A:541:ALA:O	1:A:657:GLY:HA3	2.19	0.42
1:A:666:PHE:O	1:A:701:PRO:HG2	2.20	0.42
1:A:439:GLU:HG3	2:B:352:ILE:HD13	2.02	0.41
1:A:331:ALA:HA	3:A:900:FAD:C4X	2.51	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	664/666 (100%)	647 (97%)	17 (3%)	0	100	100
2	B	131/235 (56%)	127 (97%)	4 (3%)	0	100	100
All	All	795/901 (88%)	774 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	566/566 (100%)	554 (98%)	12 (2%)	53	75
2	B	117/203 (58%)	114 (97%)	3 (3%)	46	69
All	All	683/769 (89%)	668 (98%)	15 (2%)	52	74

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	392	LEU
1	A	418	LEU
1	A	429	GLU
1	A	469	LYS
1	A	517	SER

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Mol	Chain	Res	Type
1	A	538	PHE
1	A	563	SER
1	A	571	TYR
1	A	601	GLU
1	A	704	LEU
1	A	737	SER
1	A	801	GLU
2	B	316	LEU
2	B	337	GLN
2	B	351	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	532	HIS
1	A	633	GLN
2	B	348	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

Of 7 ligands modelled in this entry, 1 is modelled with single atom and 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	A	1839	-	5,5,5	0.41	0	5,5,5	0.38	0
3	FAD	A	900	-	51,58,58	1.39	5 (9%)	60,89,89	1.74	8 (13%)
5	GOL	A	1840	-	5,5,5	0.35	0	5,5,5	0.29	0

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
5	GOL	A	1839	-	-	0/4/4/4	-
3	FAD	A	900	-	-	8/30/50/50	0/6/6/6
5	GOL	A	1840	-	-	1/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAD	C10-N1	4.51	1.39	1.33
3	A	900	FAD	C4X-N5	3.93	1.38	1.33
3	A	900	FAD	C2A-N3A	3.73	1.38	1.32
3	A	900	FAD	C4-N3	2.92	1.38	1.33
3	A	900	FAD	C2A-N1A	2.72	1.39	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	FAD	N3A-C2A-N1A	-6.66	118.27	128.68
3	A	900	FAD	C4-N3-C2	6.14	120.33	115.14
3	A	900	FAD	C5'-C4'-C3'	-3.36	105.71	112.20
3	A	900	FAD	C9A-N10-C10	-2.83	118.20	121.91
3	A	900	FAD	C1'-N10-C9A	2.71	120.43	118.29
3	A	900	FAD	C1B-N9A-C4A	-2.64	121.99	126.64
3	A	900	FAD	P-O3P-PA	-2.43	124.49	132.83
3	A	900	FAD	C6-C5X-C9A	2.06	121.76	119.05

There are no chirality outliers.

All (9) torsion outliers are listed below:

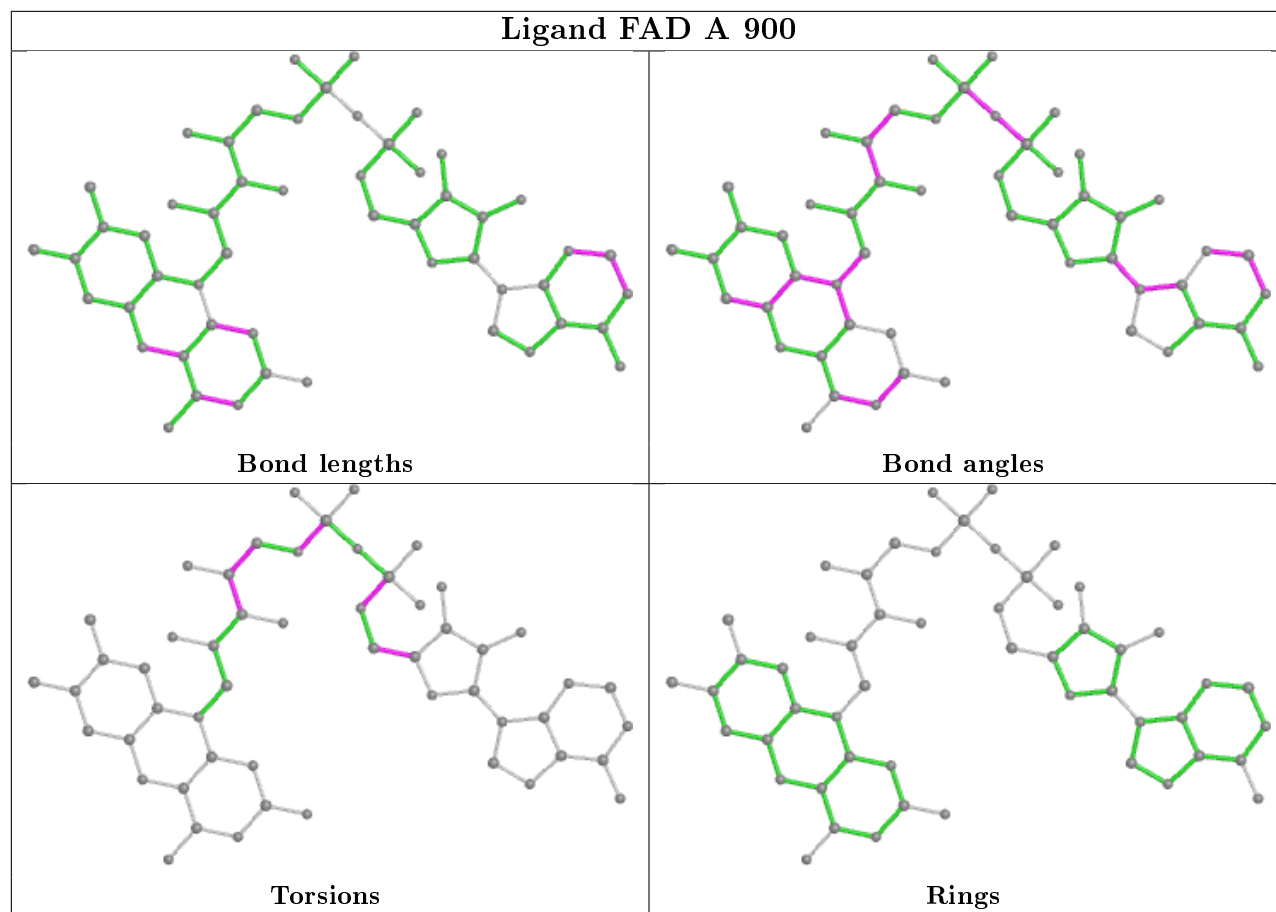
Mol	Chain	Res	Type	Atoms
3	A	900	FAD	C5B-O5B-PA-O1A
3	A	900	FAD	C5'-O5'-P-O3P
3	A	900	FAD	C2'-C3'-C4'-C5'
3	A	900	FAD	C2'-C3'-C4'-O4'
3	A	900	FAD	O3'-C3'-C4'-C5'
3	A	900	FAD	O4B-C4B-C5B-O5B
5	A	1840	GOL	O1-C1-C2-C3
3	A	900	FAD	C5B-O5B-PA-O2A
3	A	900	FAD	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	FAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	666/666 (100%)	1.07	85 (12%) 3 2	18, 70, 84, 105	0
2	B	133/235 (56%)	1.23	31 (23%) 0 0	59, 73, 96, 101	0
All	All	799/901 (88%)	1.10	116 (14%) 2 1	18, 70, 86, 105	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	SER	6.9
2	B	422	VAL	5.6
1	A	836	LEU	4.7
1	A	171	PRO	4.7
2	B	376	ILE	4.2
2	B	375	VAL	4.2
1	A	506	GLU	4.2
1	A	174	VAL	4.1
1	A	508	LEU	4.0
1	A	275	THR	4.0
1	A	238	LEU	3.8
1	A	504	LEU	3.6
2	B	402	PHE	3.5
2	B	309	LYS	3.4
1	A	490	LEU	3.3
1	A	242	TYR	3.3
1	A	273	LEU	3.3
2	B	308	ARG	3.3
1	A	431	TRP	3.3
2	B	437	TRP	3.3
1	A	492	LYS	3.2
1	A	503	LYS	3.2
2	B	378	LYS	3.2
1	A	497	LEU	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	241	PRO	3.1
1	A	451	LEU	3.1
2	B	374	GLU	3.1
1	A	173	GLY	3.1
1	A	403	ASN	3.0
1	A	373	GLU	3.0
1	A	372	LYS	3.0
2	B	399	GLY	3.0
1	A	231	PHE	2.9
1	A	739	ALA	2.9
1	A	814	ALA	2.9
2	B	420	PHE	2.8
1	A	268	LYS	2.8
1	A	441	LEU	2.8
1	A	809	ALA	2.8
2	B	365	GLY	2.7
1	A	496	GLU	2.7
2	B	353	LYS	2.7
2	B	360	LYS	2.7
2	B	371	ARG	2.7
2	B	426	ARG	2.7
1	A	239	GLU	2.7
2	B	312	LYS	2.7
1	A	429	GLU	2.7
1	A	494	TYR	2.7
1	A	232	GLU	2.6
1	A	499	GLU	2.6
1	A	445	LEU	2.6
1	A	212	PHE	2.6
2	B	414	VAL	2.6
2	B	415	VAL	2.6
1	A	455	ILE	2.6
2	B	359	LEU	2.6
1	A	509	GLN	2.6
1	A	444	LEU	2.6
2	B	383	TRP	2.6
1	A	777	ALA	2.5
1	A	740	VAL	2.5
1	A	656	PHE	2.5
1	A	377	MET	2.5
1	A	487	LEU	2.5
2	B	438	GLU	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	274	PRO	2.5
2	B	421	PHE	2.5
1	A	811	VAL	2.4
2	B	342	LEU	2.4
1	A	813	GLY	2.4
1	A	175	GLU	2.4
1	A	438	GLN	2.4
1	A	804	ILE	2.4
1	A	761	TYR	2.4
1	A	763	TYR	2.4
1	A	773	TYR	2.4
1	A	834	TYR	2.4
2	B	369	PRO	2.4
1	A	511	LEU	2.4
1	A	539	ALA	2.3
1	A	817	SER	2.3
1	A	288	VAL	2.3
1	A	380	GLN	2.3
2	B	418	LYS	2.3
1	A	816	LEU	2.3
2	B	368	GLU	2.3
1	A	498	ALA	2.3
1	A	803	THR	2.2
1	A	395	GLN	2.2
1	A	449	VAL	2.2
1	A	808	PRO	2.2
1	A	448	MET	2.2
1	A	471	PRO	2.2
1	A	799	ALA	2.1
1	A	775	LEU	2.1
1	A	289	SER	2.1
1	A	655	GLY	2.1
1	A	489	ALA	2.1
1	A	227	ILE	2.1
1	A	398	PHE	2.1
1	A	408	LEU	2.1
1	A	440	GLU	2.1
1	A	458	LEU	2.1
2	B	434	LEU	2.1
2	B	395	ILE	2.1
2	B	405	ILE	2.1
1	A	659	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	815	LEU	2.1
1	A	540	ASN	2.1
1	A	205	GLN	2.1
1	A	391	TYR	2.0
1	A	435	VAL	2.0
1	A	536	LEU	2.0
2	B	431	ASP	2.0
1	A	470	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

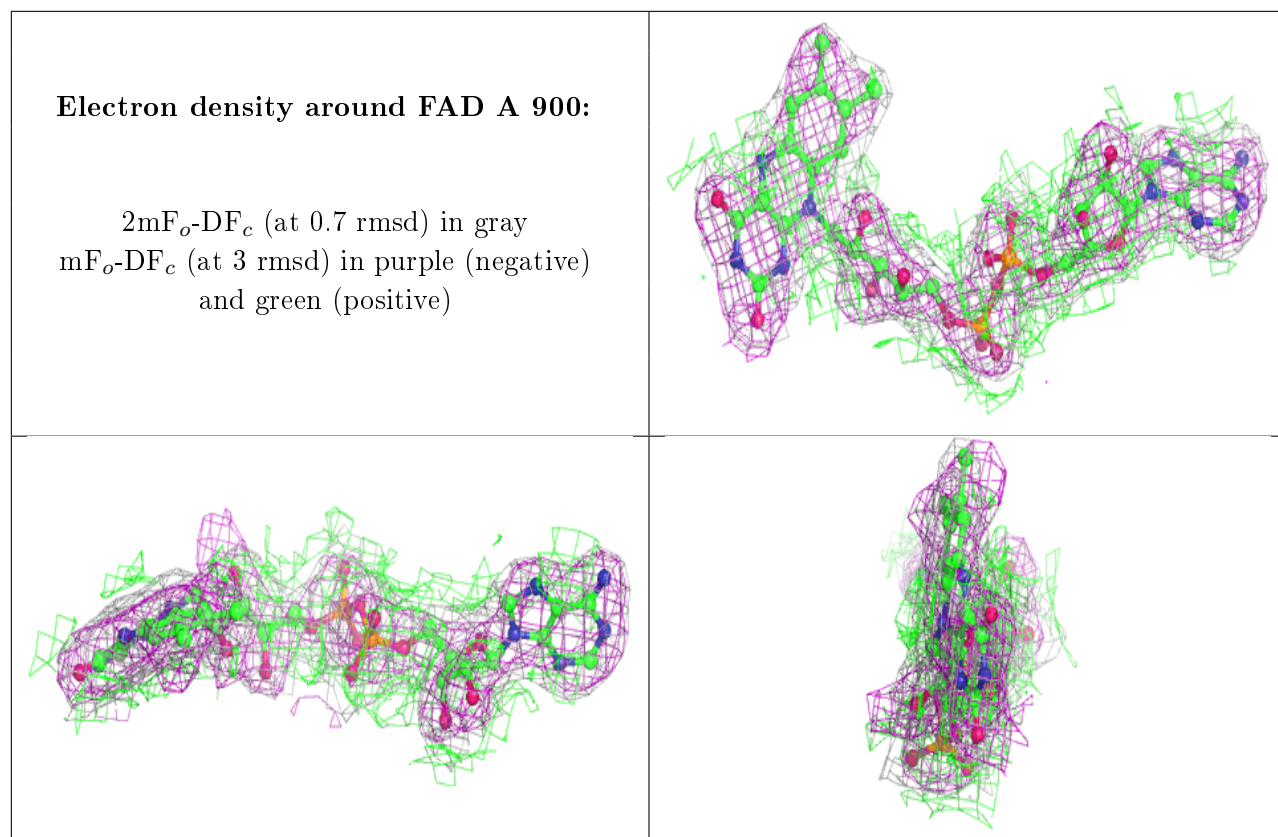
There are no carbohydrates in this entry.

## 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
6	NH4	A	1842	1/1	0.72	0.45	70,70,70,70	0
5	GOL	A	1840	6/6	0.77	0.23	113,114,115,115	0
4	CL	A	1841	1/1	0.83	0.15	92,92,92,92	0
4	CL	A	1838	1/1	0.90	0.29	53,53,53,53	1
4	CL	A	1843	1/1	0.96	0.32	58,58,58,58	1
5	GOL	A	1839	6/6	0.96	0.14	61,62,64,65	0
3	FAD	A	900	53/53	0.98	0.10	38,43,46,47	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.