



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 09:18 AM EDT

PDB ID : 4FWE  
Title : Native structure of LSD2 /AOF1/KDM1b in spacegroup of C2221 at 2.13Å  
Authors : Zhang, Q.; Chen, Z.  
Deposited on : 2012-07-01  
Resolution : 2.13 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

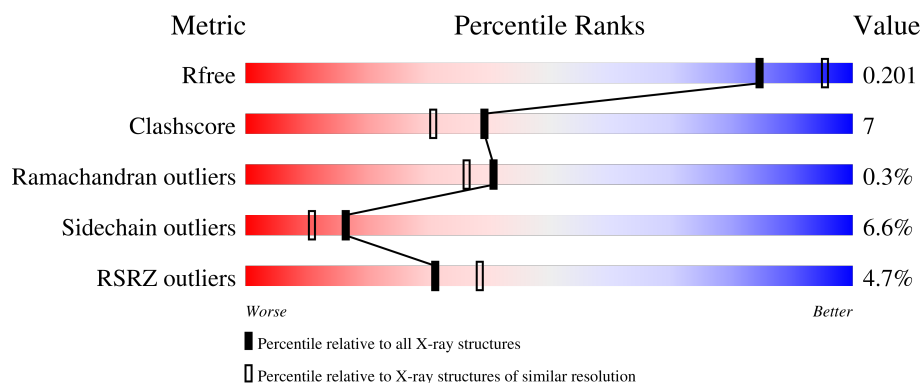
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 of 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	796	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6155 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 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	750	5850	3741	996	1072	41	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	expression tag	UNP Q8NB78
A	28	HIS	-	expression tag	UNP Q8NB78
A	29	MET	-	expression tag	UNP Q8NB78

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

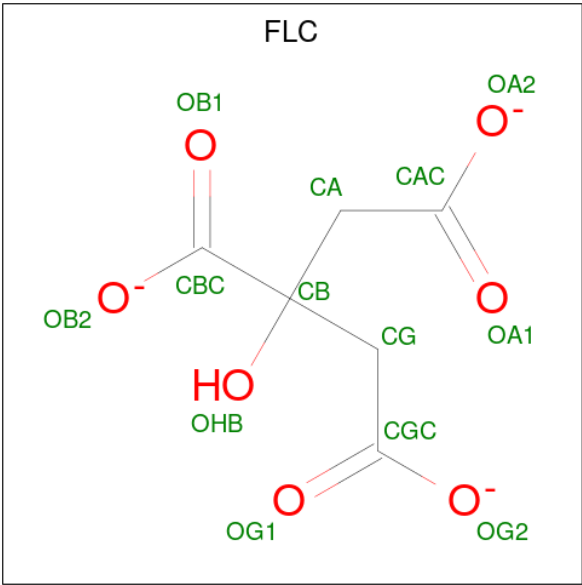
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		

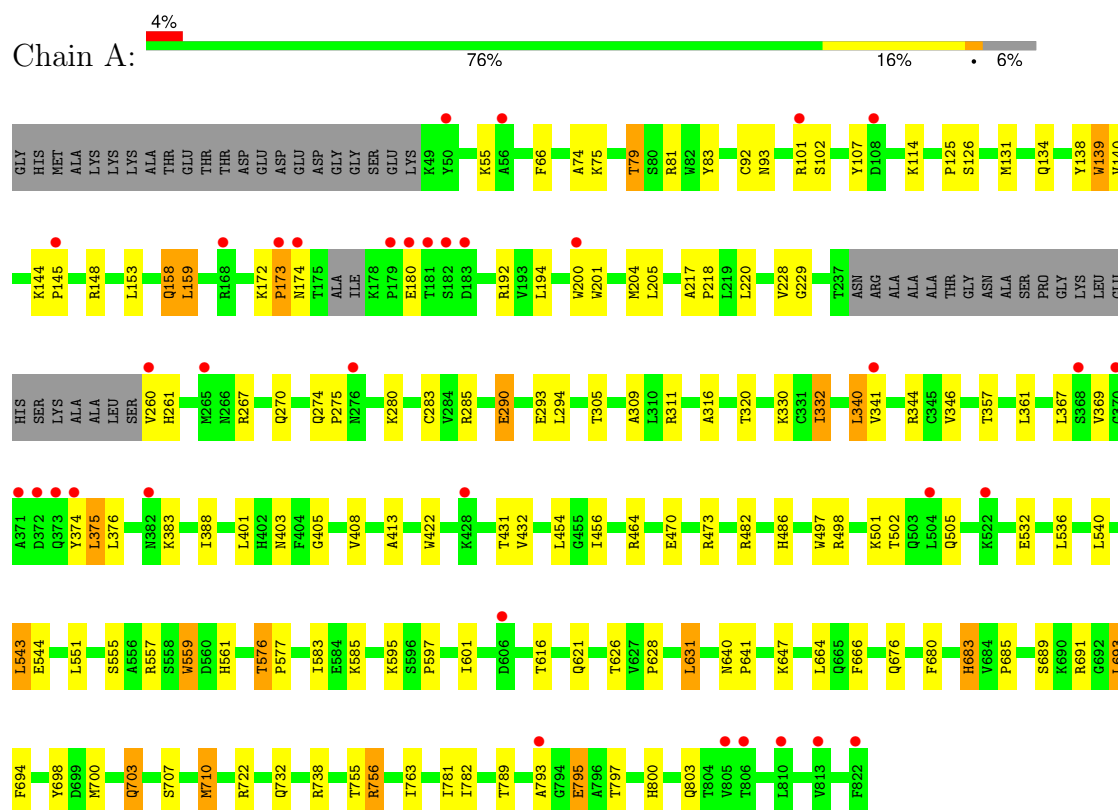
- Molecule 5 is water.

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

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 1B



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.69Å 96.27Å 182.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.13 29.95 – 2.11	Depositor EDS
% Data completeness (in resolution range)	94.0 (50.00-2.13) 93.0 (29.95-2.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.203 , 0.246 0.203 , 0.201	Depositor DCC
$R_{free}$ test set	2265 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.2	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.031 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6155	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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: FAD, FLC, ZN

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	0.54	6/6000 (0.1%)	0.63	2/8145 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	TRP	CD2-CE2	5.38	1.47	1.41
1	A	422	TRP	CD2-CE2	5.26	1.47	1.41
1	A	559	TRP	CD2-CE2	5.25	1.47	1.41
1	A	200	TRP	CD2-CE2	5.21	1.47	1.41
1	A	497	TRP	CD2-CE2	5.08	1.47	1.41
1	A	139	TRP	CD2-CE2	5.07	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	631	LEU	CA-CB-CG	-6.82	99.61	115.30
1	A	664	LEU	CA-CB-CG	5.83	128.70	115.30

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	5850	0	5681	86	0
2	A	3	0	0	0	0
3	A	53	0	31	1	0
4	A	13	0	5	0	0
5	A	236	0	0	7	0
All	All	6155	0	5717	86	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 7.

All (86) 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:79:THR:HG21	1:A:92:CYS:HB2	1.70	0.74
1:A:473:ARG:HH11	1:A:473:ARG:HG3	1.54	0.73
1:A:502:THR:H	1:A:505:GLN:HE21	1.38	0.71
1:A:738:ARG:HD2	5:A:1175:HOH:O	1.92	0.70
1:A:260:VAL:HG12	1:A:261:HIS:H	1.59	0.68
1:A:375:LEU:HD22	1:A:403:ASN:HB3	1.77	0.66
1:A:158:GLN:HG3	5:A:1028:HOH:O	1.95	0.66
1:A:698:TYR:HB2	1:A:710[A]:MET:HG3	1.79	0.65
1:A:700:MET:HA	1:A:700:MET:CE	2.28	0.64
1:A:502:THR:H	1:A:505:GLN:NE2	1.96	0.62
1:A:172:LYS:CB	1:A:173:PRO:HD2	2.29	0.62
1:A:261:HIS:CE1	1:A:267:ARG:HG2	2.37	0.60
1:A:134:GLN:HG2	5:A:1224:HOH:O	2.02	0.59
1:A:470:GLU:OE1	1:A:683:HIS:HE1	1.85	0.59
1:A:544:GLU:HG2	1:A:551:LEU:HG	1.86	0.57
1:A:229:GLY:HA2	1:A:305:THR:HG23	1.86	0.57
1:A:700:MET:HA	1:A:700:MET:HE2	1.85	0.57
1:A:220:LEU:HD13	1:A:228:VAL:HG11	1.87	0.56
1:A:698:TYR:HB3	1:A:700:MET:HE1	1.88	0.56
1:A:700:MET:SD	1:A:710[A]:MET:HG2	2.47	0.55
1:A:285:ARG:NH1	1:A:290:GLU:OE2	2.41	0.54
1:A:454:LEU:HD21	1:A:585:LYS:HG2	1.89	0.54
1:A:413:ALA:O	1:A:595:LYS:HA	2.09	0.53
1:A:139:TRP:CE2	1:A:340:LEU:HD13	2.44	0.53
1:A:501:LYS:HA	1:A:505:GLN:NE2	2.24	0.52
1:A:698:TYR:HB3	1:A:700:MET:CE	2.39	0.52
1:A:316:ALA:O	1:A:320:THR:HG23	2.09	0.52
1:A:79:THR:CG2	1:A:92:CYS:HB2	2.39	0.51
1:A:782:ILE:HG22	1:A:797:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:GLU:HG2	1:A:803:GLN:CA	2.40	0.51
1:A:543:LEU:HD21	1:A:559:TRP:CZ3	2.46	0.51
1:A:217:ALA:HB3	1:A:218:PRO:HD3	1.91	0.51
1:A:383:LYS:HA	1:A:621:GLN:OE1	2.10	0.51
1:A:74:ALA:HB2	1:A:79:THR:HG23	1.92	0.50
1:A:81:ARG:HD2	1:A:83:TYR:CZ	2.46	0.50
1:A:332:ILE:HD11	1:A:346:VAL:HG13	1.92	0.50
1:A:561:HIS:HE1	5:A:1143:HOH:O	1.94	0.49
1:A:205:LEU:HD11	1:A:341:VAL:HG23	1.95	0.49
1:A:274:GLN:HB3	1:A:275:PRO:HD2	1.94	0.49
1:A:666:PHE:O	1:A:707:SER:OG	2.31	0.48
1:A:293:GLU:OE2	1:A:311:ARG:HD3	2.13	0.48
1:A:501:LYS:HD2	1:A:505:GLN:NE2	2.29	0.47
1:A:138:TYR:CG	1:A:159:LEU:HB2	2.50	0.47
1:A:220:LEU:HD13	1:A:228:VAL:CG1	2.44	0.47
1:A:800:HIS:HD2	5:A:1030:HOH:O	1.98	0.47
1:A:473:ARG:HG3	1:A:473:ARG:NH1	2.26	0.46
1:A:81:ARG:HD2	1:A:83:TYR:CE1	2.49	0.46
1:A:229:GLY:HA3	1:A:309:ALA:HB2	1.96	0.46
1:A:261:HIS:HB3	1:A:270:GLN:HG2	1.98	0.46
1:A:703:GLN:HE21	1:A:703:GLN:HA	1.79	0.46
1:A:280:LYS:HE3	1:A:283:CYS:SG	2.55	0.46
1:A:693:LEU:HD22	1:A:694:PHE:CE2	2.51	0.45
1:A:401:LEU:HB2	1:A:408:VAL:HG11	1.98	0.45
1:A:722:ARG:HH11	1:A:722:ARG:HB3	1.81	0.45
1:A:102:SER:HA	1:A:107:TYR:CG	2.51	0.45
1:A:374:TYR:CD1	1:A:405:GLY:HA2	2.52	0.45
1:A:205:LEU:HD11	1:A:341:VAL:CG2	2.47	0.45
1:A:140:VAL:HG21	1:A:153:LEU:HD11	1.99	0.45
1:A:388:ILE:CD1	1:A:601:ILE:HD11	2.47	0.44
1:A:498:ARG:HD2	1:A:557:ARG:HA	1.98	0.44
1:A:126:SER:HB2	5:A:1185:HOH:O	2.18	0.44
1:A:640:ASN:HA	1:A:641:PRO:C	2.38	0.44
1:A:79:THR:HG21	1:A:93:ASN:H	1.83	0.44
1:A:700:MET:SD	1:A:710[B]:MET:HE2	2.59	0.43
1:A:795:GLU:HG2	1:A:803:GLN:N	2.32	0.43
1:A:144:LYS:HA	1:A:145:PRO:HD3	1.93	0.43
1:A:685:PRO:HB3	1:A:691:ARG:HA	2.00	0.43
1:A:66:PHE:HZ	1:A:131:MET:HB3	1.84	0.42
1:A:482:ARG:NH1	1:A:532:GLU:OE2	2.51	0.42
1:A:628:PRO:HG2	1:A:763:ILE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:THR:HG21	1:A:375:LEU:HB3	2.02	0.42
1:A:626:THR:HG22	1:A:793:ALA:HB3	2.02	0.42
1:A:486:HIS:HB2	5:A:1205:HOH:O	2.19	0.42
1:A:576:THR:HB	1:A:577:PRO:HD3	2.02	0.42
1:A:647:LYS:NZ	1:A:781:ILE:O	2.53	0.41
1:A:228:VAL:CG1	1:A:228:VAL:O	2.67	0.41
1:A:595:LYS:C	1:A:597:PRO:HD3	2.39	0.41
1:A:229:GLY:HA2	1:A:305:THR:CG2	2.50	0.41
1:A:473:ARG:HH11	1:A:473:ARG:CG	2.30	0.41
1:A:803:GLN:O	3:A:904:FAD:H1'2	2.20	0.41
1:A:464:ARG:HH12	1:A:676:GLN:HB2	1.85	0.41
1:A:755:THR:C	1:A:756:ARG:HG2	2.41	0.41
1:A:114:LYS:HG3	1:A:125:PRO:HB2	2.03	0.41
1:A:502:THR:N	1:A:505:GLN:HE21	2.10	0.41
1:A:555:SER:O	1:A:559:TRP:HB3	2.20	0.40
1:A:456:ILE:HB	1:A:577:PRO:HG3	2.02	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	745/796 (94%)	707 (95%)	36 (5%)	2 (0%)	41 36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	GLU
1	A	173	PRO

### 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	619/678 (91%)	577 (93%)	42 (7%)	16	10

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	75	LYS
1	A	79	THR
1	A	101	ARG
1	A	148	ARG
1	A	158	GLN
1	A	159	LEU
1	A	174	ASN
1	A	192	ARG
1	A	194	LEU
1	A	204	MET
1	A	290	GLU
1	A	294	LEU
1	A	330	LYS
1	A	332	ILE
1	A	340	LEU
1	A	344	ARG
1	A	361	LEU
1	A	367	LEU
1	A	369	VAL
1	A	375	LEU
1	A	376	LEU
1	A	431	THR
1	A	432	VAL
1	A	536	LEU
1	A	540	LEU
1	A	543	LEU
1	A	576	THR
1	A	583	ILE
1	A	616	THR

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Mol	Chain	Res	Type
1	A	631	LEU
1	A	680	PHE
1	A	683	HIS
1	A	689	SER
1	A	693	LEU
1	A	703	GLN
1	A	710[A]	MET
1	A	710[B]	MET
1	A	732	GLN
1	A	756	ARG
1	A	789	THR
1	A	795	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	135	GLN
1	A	141	GLN
1	A	198	ASN
1	A	334	HIS
1	A	459	HIS
1	A	488	ASN
1	A	503	GLN
1	A	505	GLN
1	A	550	ASN
1	A	552	HIS
1	A	640	ASN
1	A	683	HIS
1	A	703	GLN
1	A	800	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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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$
4	FLC	A	905	-	12,12,12	1.10	0	17,17,17	5.17	6 (35%)
3	FAD	A	904	-	54,58,58	1.14	4 (7%)	71,89,89	1.60	13 (18%)

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	FLC	A	905	-	-	5/16/16/16	-
3	FAD	A	904	-	-	1/30/50/50	0/6/6/6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	904	FAD	C4X-N5	4.09	1.39	1.30
3	A	904	FAD	PA-O3P	3.23	1.63	1.59
3	A	904	FAD	C1'-C2'	2.72	1.56	1.52
3	A	904	FAD	C10-N1	2.48	1.38	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	905	FLC	OHB-CB-CBC	-12.19	91.67	108.96
4	A	905	FLC	OHB-CB-CA	-11.56	83.00	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	905	FLC	OHB-CB-CG	-10.11	86.32	109.38
3	A	904	FAD	C4B-O4B-C1B	-5.92	104.50	109.92
3	A	904	FAD	N3A-C2A-N1A	-5.41	121.33	128.67
4	A	905	FLC	CG-CB-CBC	4.80	120.65	110.03
4	A	905	FLC	CA-CB-CBC	4.77	120.59	110.03
3	A	904	FAD	C4-N3-C2	-3.67	119.13	125.64
4	A	905	FLC	CG-CB-CA	3.37	117.96	109.31
3	A	904	FAD	C10-C4X-N5	-3.13	118.41	124.81
3	A	904	FAD	C4X-C10-N10	3.01	120.80	116.48
3	A	904	FAD	C4-C4X-N5	2.91	122.22	118.21
3	A	904	FAD	C4X-C4-N3	2.81	120.39	113.25
3	A	904	FAD	C9A-C5X-N5	-2.62	119.68	122.45
3	A	904	FAD	C5'-C4'-C3'	-2.43	107.63	112.22
3	A	904	FAD	C1B-N9A-C4A	-2.08	122.98	126.64
3	A	904	FAD	C4A-C5A-N7A	-2.05	107.17	109.34
3	A	904	FAD	O2A-PA-O3P	-2.04	101.76	107.27
3	A	904	FAD	O4-C4-C4X	-2.03	121.19	126.53

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	905	FLC	CAC-CA-CB-CBC
4	A	905	FLC	CAC-CA-CB-OHB
4	A	905	FLC	CBC-CB-CG-CGC
3	A	904	FAD	PA-O3P-P-O5'
4	A	905	FLC	CA-CB-CBC-OB1
4	A	905	FLC	CA-CB-CBC-OB2

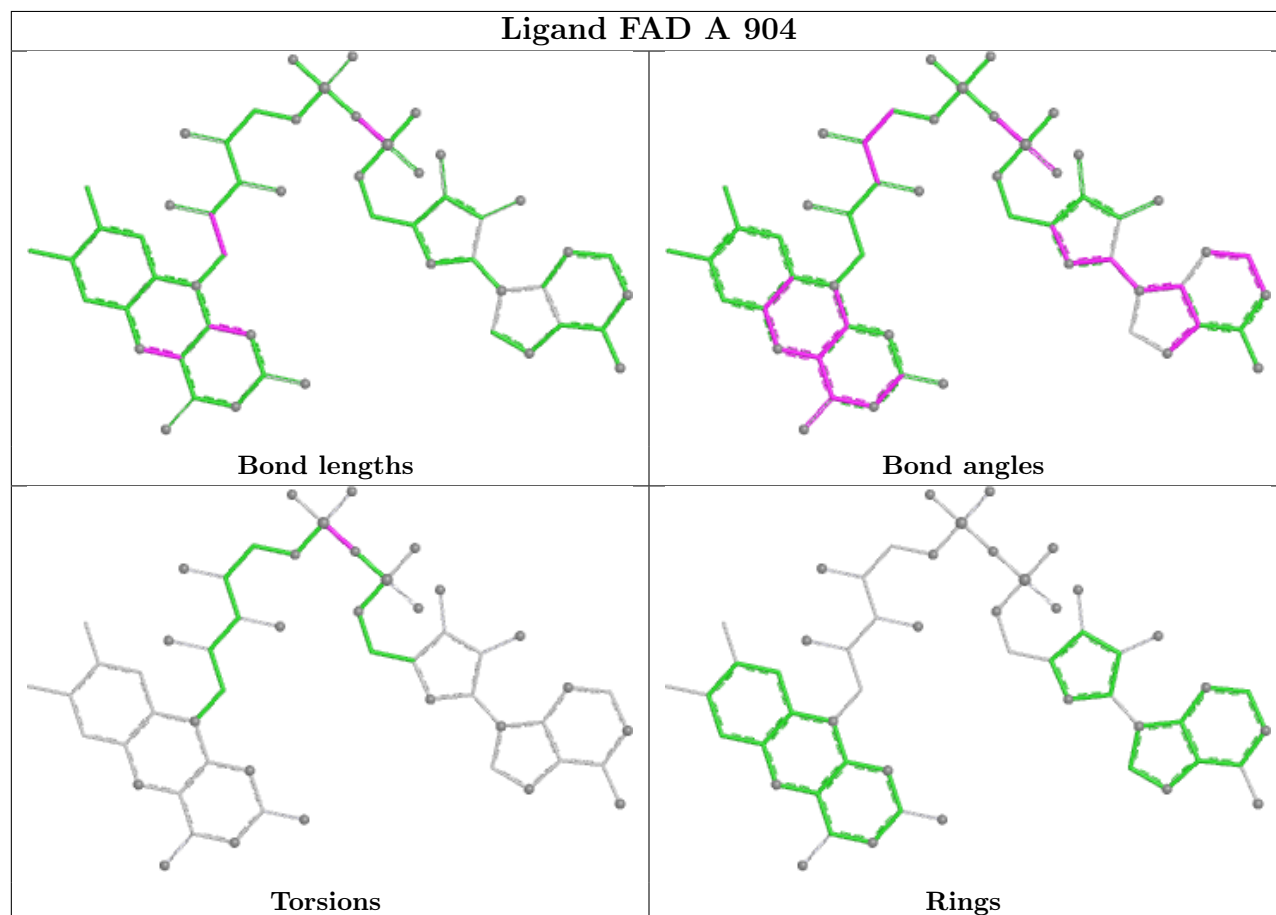
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	904	FAD	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

### 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	750/796 (94%)	0.19	35 (4%) 31 38	32, 48, 70, 114	1 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	PRO	5.7
1	A	822	PHE	5.0
1	A	181	THR	4.6
1	A	504	LEU	4.5
1	A	180	GLU	4.5
1	A	370	GLY	4.2
1	A	50	TYR	4.2
1	A	200	TRP	4.0
1	A	56	ALA	4.0
1	A	374	TYR	4.0
1	A	182	SER	3.8
1	A	373	GLN	3.7
1	A	522	LYS	3.6
1	A	173	PRO	3.6
1	A	371	ALA	3.5
1	A	265	MET	3.4
1	A	382	ASN	3.3
1	A	183	ASP	3.0
1	A	168	ARG	2.9
1	A	260	VAL	2.8
1	A	606	ASP	2.7
1	A	810	LEU	2.7
1	A	341	VAL	2.7
1	A	813	VAL	2.6
1	A	368	SER	2.5
1	A	174	ASN	2.4
1	A	805	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	428	LYS	2.3
1	A	276	ASN	2.2
1	A	793	ALA	2.2
1	A	101	ARG	2.2
1	A	806	THR	2.2
1	A	145	PRO	2.1
1	A	372	ASP	2.1
1	A	108	ASP	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](#)

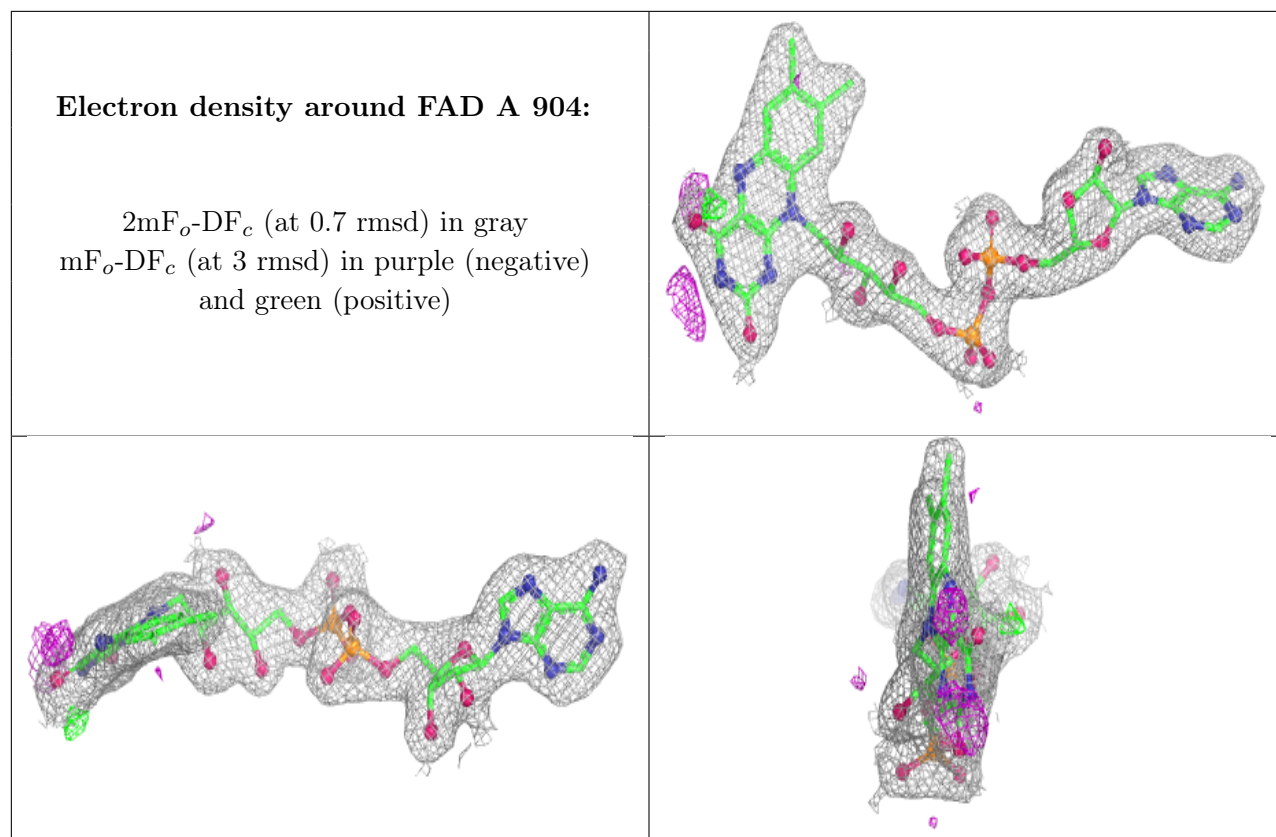
There are no monosaccharides in this entry.

## 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
4	FLC	A	905	13/13	0.91	0.15	55,60,64,65	0
3	FAD	A	904	53/53	0.97	0.13	29,34,38,39	0
2	ZN	A	903	1/1	0.99	0.04	48,48,48,48	0
2	ZN	A	901	1/1	0.99	0.07	55,55,55,55	0
2	ZN	A	902	1/1	0.99	0.07	49,49,49,49	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.