



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:59 PM GMT

PDB ID : 4GU0  
Title : Crystal structure of LSD2 with H3  
Authors : Chen, F.; Yang, H.; Dong, Z.; Fang, J.; Zhu, T.; Gong, W.; Xu, Y.  
Deposited on : 2012-08-29  
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

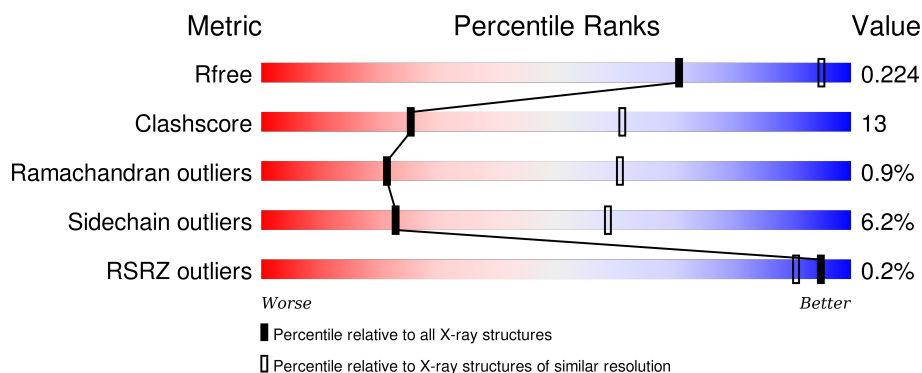
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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.



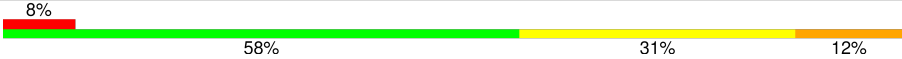
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	776	
1	B	776	
1	C	776	
1	D	776	
2	E	26	

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Mol	Chain	Length	Quality of chain
2	F	26	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (8%), green (58%), yellow (31%), and orange (12%).

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
4	ZN	C	902	-	-	-	X
4	ZN	C	903	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24156 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
1	A	748	Total	C	N	O	S	0	0	0
			5919	3780	1007	1091	41			
1	B	748	Total	C	N	O	S	0	0	0
			5919	3780	1007	1091	41			
1	C	736	Total	C	N	O	S	0	0	0
			5830	3724	992	1073	41			
1	D	735	Total	C	N	O	S	0	0	0
			5822	3718	991	1072	41			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	PRO	-	EXPRESSION TAG	UNP Q8NB78
A	48	LEU	-	EXPRESSION TAG	UNP Q8NB78
A	49	GLY	-	EXPRESSION TAG	UNP Q8NB78
A	50	SER	-	EXPRESSION TAG	UNP Q8NB78
B	47	PRO	-	EXPRESSION TAG	UNP Q8NB78
B	48	LEU	-	EXPRESSION TAG	UNP Q8NB78
B	49	GLY	-	EXPRESSION TAG	UNP Q8NB78
B	50	SER	-	EXPRESSION TAG	UNP Q8NB78
C	47	PRO	-	EXPRESSION TAG	UNP Q8NB78
C	48	LEU	-	EXPRESSION TAG	UNP Q8NB78
C	49	GLY	-	EXPRESSION TAG	UNP Q8NB78
C	50	SER	-	EXPRESSION TAG	UNP Q8NB78
D	47	PRO	-	EXPRESSION TAG	UNP Q8NB78
D	48	LEU	-	EXPRESSION TAG	UNP Q8NB78
D	49	GLY	-	EXPRESSION TAG	UNP Q8NB78
D	50	SER	-	EXPRESSION TAG	UNP Q8NB78

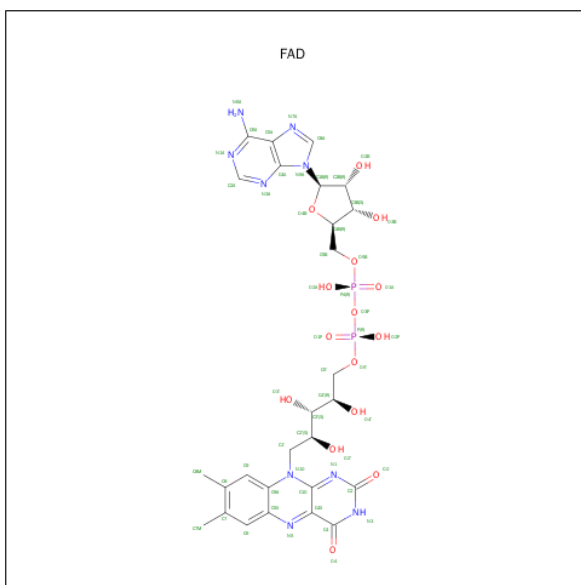
- Molecule 2 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	26	Total	C	N	O	S	0	0	0
			193	115	44	33	1			
2	F	26	Total	C	N	O	S	0	0	0
			193	115	44	33	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	MET	LYS	ENGINEERED MUTATION	UNP P84243
F	4	MET	LYS	ENGINEERED MUTATION	UNP P84243

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total 3	Zn 3	0	0
4	A	3	Total 3	Zn 3	0	0
4	D	3	Total 3	Zn 3	0	0
4	C	3	Total 3	Zn 3	0	0

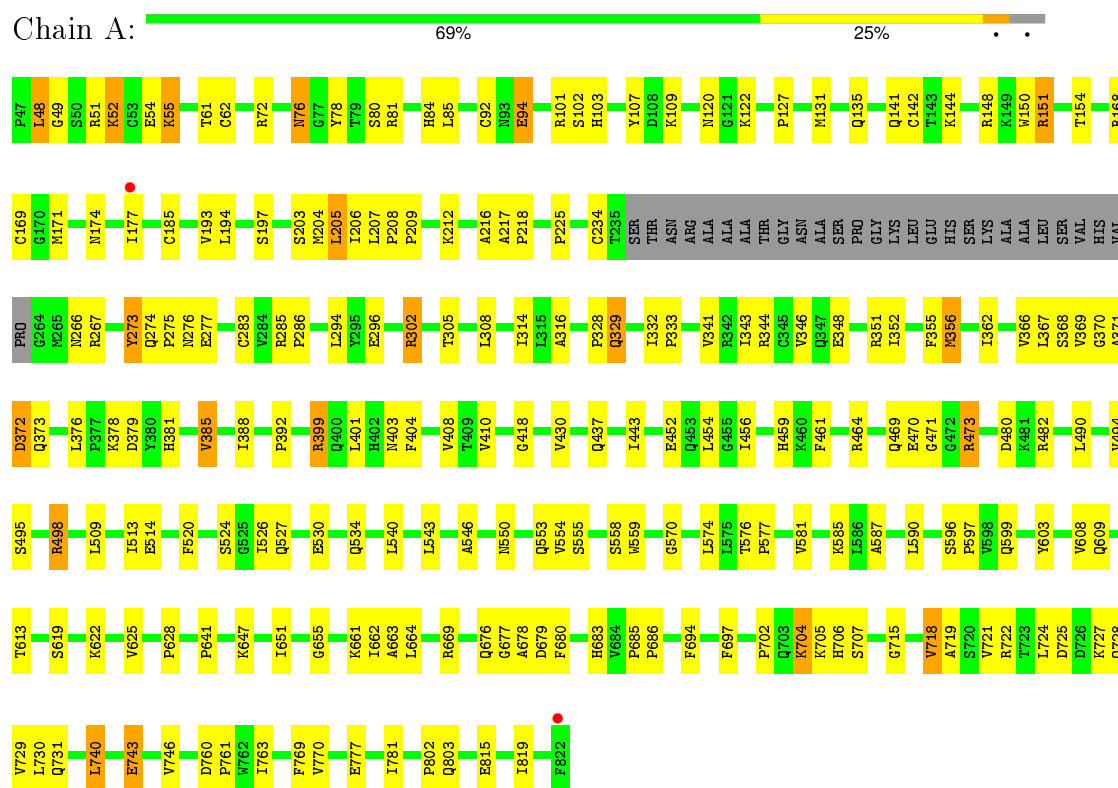
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total 13	O 13	0	0
5	B	10	Total 10	O 10	0	0
5	C	16	Total 16	O 16	0	0
5	D	15	Total 15	O 15	0	0
5	E	1	Total 1	O 1	0	0
5	F	1	Total 1	O 1	0	0

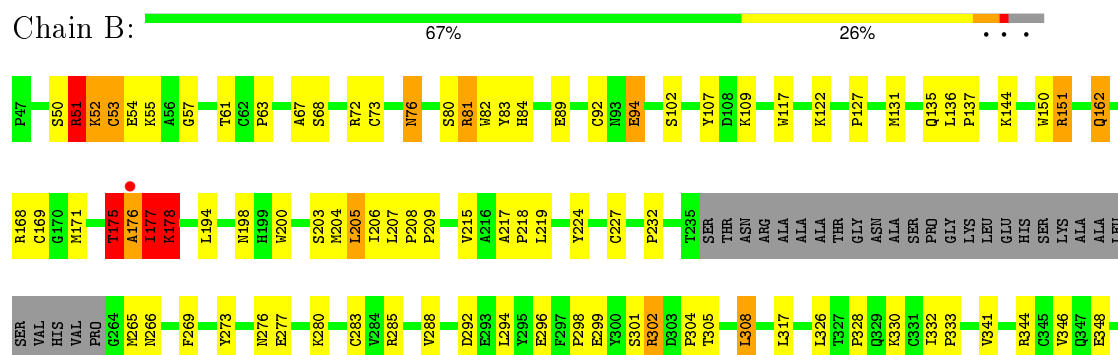
### 3 Residue-property plots

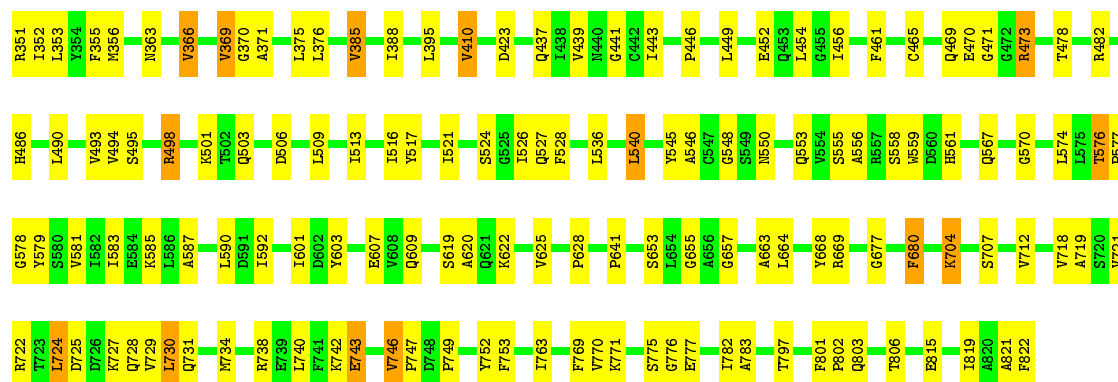
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Lysine-specific histone demethylase 1B

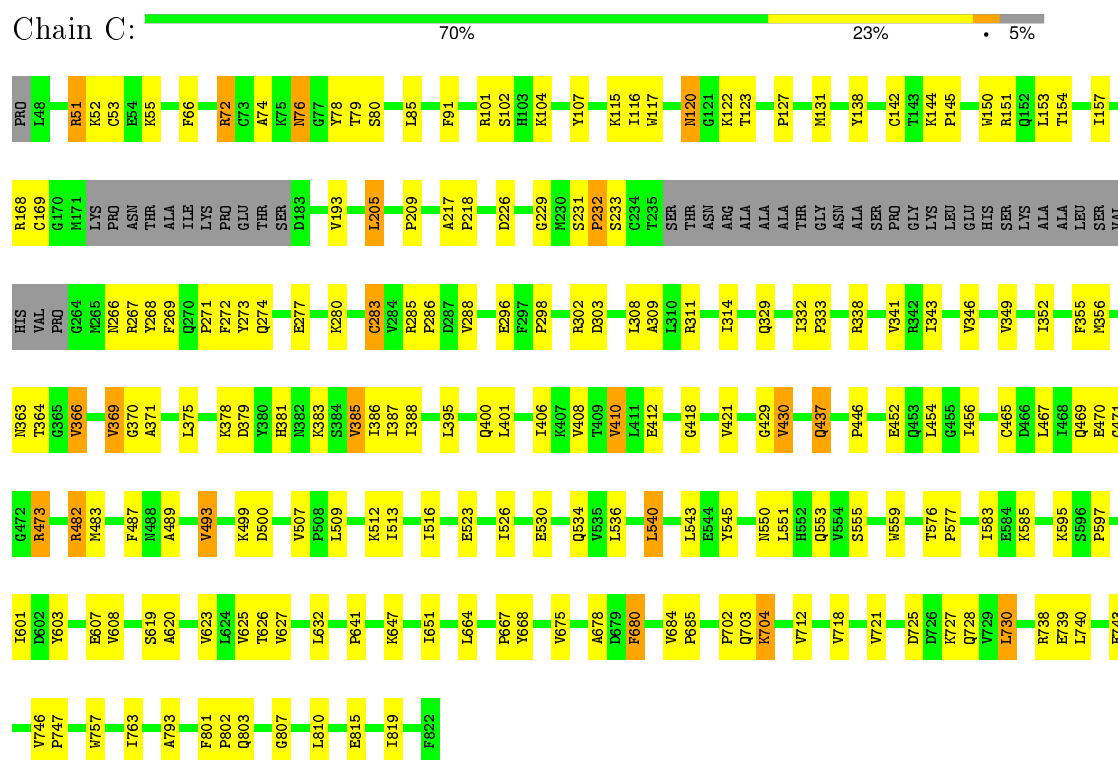


#### • Molecule 1: Lysine-specific histone demethylase 1B

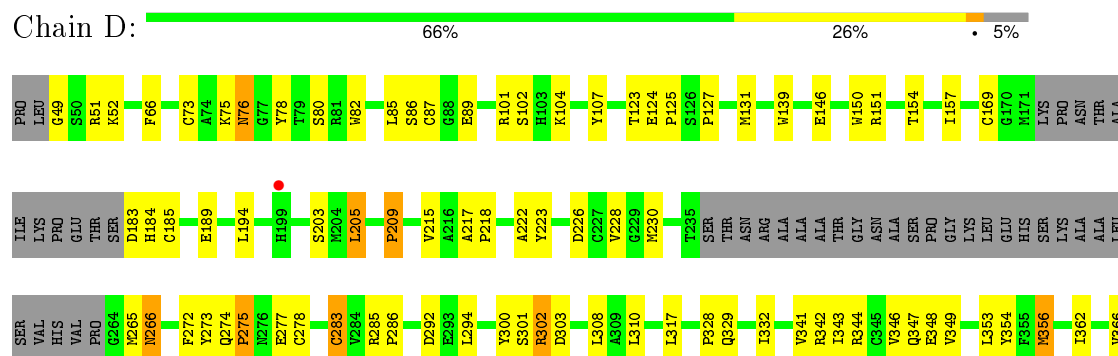




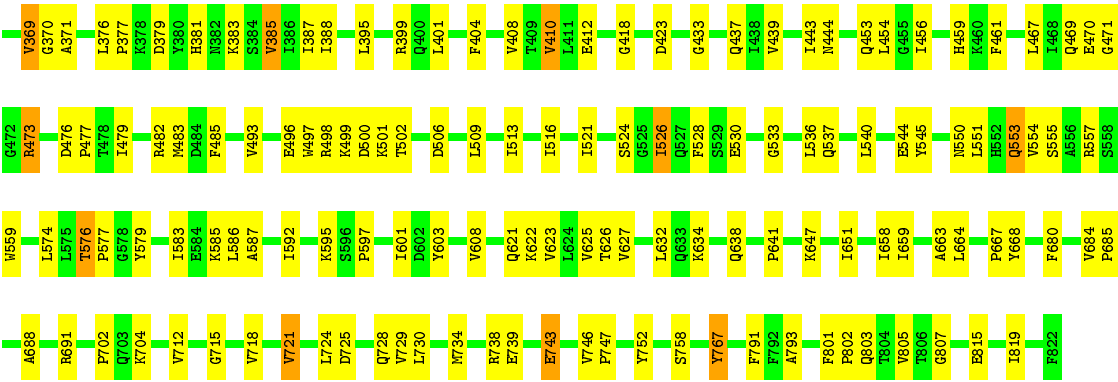
• Molecule 1: Lysine-specific histone demethylase 1B



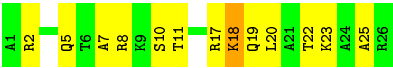
• Molecule 1: Lysine-specific histone demethylase 1B



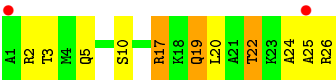




• Molecule 2: Histone H3.3



• Molecule 2: Histone H3.3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.84Å 108.93Å 120.83Å 94.47° 112.34° 117.95°	Depositor
Resolution (Å)	45.06 – 3.10 45.06 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.2 (45.06-3.10) 87.5 (45.06-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_353)	Depositor
R, $R_{free}$	0.204 , 0.221 0.207 , 0.224	Depositor DCC
$R_{free}$ test set	3633 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.0	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 28.1	EDS
Estimated twinning fraction	0.058 for h,-h-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 71966 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	24156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, 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	0.24	0/6067	0.41	0/8221
1	B	0.24	0/6067	0.40	0/8221
1	C	0.24	0/5974	0.40	0/8092
1	D	0.24	0/5966	0.40	0/8081
2	E	0.44	0/193	0.68	0/254
2	F	0.47	0/193	0.73	0/254
All	All	0.24	0/24460	0.41	0/33123

There are no bond length outliers.

There are no bond angle outliers.

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	5919	0	5840	149	0
1	B	5919	0	5840	170	0
1	C	5830	0	5744	139	0
1	D	5822	0	5734	152	0
2	E	193	0	218	10	0
2	F	193	0	218	18	0
3	A	53	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	53	0	30	0	0
3	C	53	0	30	3	0
3	D	53	0	30	2	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	A	13	0	0	4	0
5	B	10	0	0	0	0
5	C	16	0	0	0	0
5	D	15	0	0	1	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	24156	0	23714	604	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 13.

The worst 5 of 604 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:C:72:ARG:HG2	1:C:72:ARG:HH11	1.15	1.11
1:B:302:ARG:HG2	1:D:526:ILE:HD11	1.10	1.10
1:B:203:SER:HA	1:B:302:ARG:HH22	1.19	1.04
3:A:901:FAD:O3B	5:A:1005:HOH:O	1.75	1.01
1:A:276:ASN:HA	2:E:19:GLN:HE21	1.27	0.99

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	744/776 (96%)	682 (92%)	56 (8%)	6 (1%)	24	63
1	B	744/776 (96%)	695 (93%)	38 (5%)	11 (2%)	13	46
1	C	730/776 (94%)	677 (93%)	50 (7%)	3 (0%)	39	75
1	D	729/776 (94%)	678 (93%)	45 (6%)	6 (1%)	24	63
2	E	24/26 (92%)	20 (83%)	4 (17%)	0	100	100
2	F	24/26 (92%)	20 (83%)	3 (12%)	1 (4%)	3	19
All	All	2995/3156 (95%)	2772 (93%)	196 (6%)	27 (1%)	21	61

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	52	LYS
1	A	177	ILE
1	A	373	GLN
1	B	50	SER

### 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	642/662 (97%)	598 (93%)	44 (7%)	19	55
1	B	642/662 (97%)	601 (94%)	41 (6%)	22	57
1	C	631/662 (95%)	598 (95%)	33 (5%)	29	65
1	D	630/662 (95%)	596 (95%)	34 (5%)	27	64
2	E	18/18 (100%)	15 (83%)	3 (17%)	3	11
2	F	18/18 (100%)	14 (78%)	4 (22%)	1	5
All	All	2581/2684 (96%)	2422 (94%)	159 (6%)	23	59

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	501	LYS

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Mol	Chain	Res	Type
1	C	122	LYS
1	D	680	PHE
1	B	576	THR
1	B	730	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	593	GLN
1	C	120	ASN
1	D	706	HIS
1	B	609	GLN
1	B	706	HIS

### 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 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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
3	FAD	A	901	-	48,58,58	2.34	23 (47%)	54,89,89	2.16	13 (24%)
3	FAD	B	901	-	48,58,58	2.35	23 (47%)	54,89,89	2.15	14 (25%)
3	FAD	C	901	-	48,58,58	2.34	23 (47%)	54,89,89	2.15	13 (24%)
3	FAD	D	901	-	48,58,58	2.34	23 (47%)	54,89,89	2.15	14 (25%)

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
3	FAD	A	901	-	-	0/30/50/50	0/6/6/6
3	FAD	B	901	-	-	0/30/50/50	0/6/6/6
3	FAD	C	901	-	-	0/30/50/50	0/6/6/6
3	FAD	D	901	-	-	0/30/50/50	0/6/6/6

The worst 5 of 92 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	FAD	C10-N10	-5.12	1.33	1.39
3	C	901	FAD	C10-N10	-5.11	1.33	1.39
3	D	901	FAD	C10-N10	-5.08	1.33	1.39
3	A	901	FAD	C10-N10	-5.01	1.33	1.39
3	C	901	FAD	PA-O5B	-4.36	1.39	1.59

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	901	FAD	N3A-C2A-N1A	-8.10	122.69	128.89
3	B	901	FAD	N3A-C2A-N1A	-8.06	122.72	128.89
3	A	901	FAD	N3A-C2A-N1A	-8.03	122.74	128.89
3	C	901	FAD	N3A-C2A-N1A	-8.01	122.76	128.89
3	A	901	FAD	C4A-C5A-N7A	-3.02	106.70	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	FAD	3	0
3	C	901	FAD	3	0
3	D	901	FAD	2	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 ⓘ

### 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	748/776 (96%)	-0.36	2 (0%) 94 88	51, 76, 115, 151	0
1	B	748/776 (96%)	-0.36	1 (0%) 95 91	52, 78, 114, 156	0
1	C	736/776 (94%)	-0.40	0 100 100	42, 68, 104, 154	0
1	D	735/776 (94%)	-0.41	1 (0%) 95 91	45, 71, 107, 163	0
2	E	26/26 (100%)	0.33	0 100 100	83, 110, 143, 162	0
2	F	26/26 (100%)	0.51	2 (7%) 16 5	92, 110, 139, 149	0
All	All	3019/3156 (95%)	-0.37	6 (0%) 95 91	42, 73, 113, 163	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	822	PHE	4.2
1	B	176	ALA	2.8
1	A	177	ILE	2.7
2	F	25	ALA	2.4
2	F	1	ALA	2.4

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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(Å <sup>2</sup> )	Q<0.9
4	ZN	C	903	1/1	0.76	0.42	6.15	147,147,147,147	0
4	ZN	C	902	1/1	0.97	0.20	2.26	71,71,71,71	0
4	ZN	A	902	1/1	0.99	0.19	0.77	77,77,77,77	0
3	FAD	A	901	53/53	0.92	0.21	0.53	56,67,82,172	0
3	FAD	B	901	53/53	0.95	0.21	0.44	52,65,73,124	0
4	ZN	D	903	1/1	0.99	0.17	0.44	63,63,63,63	0
3	FAD	C	901	53/53	0.94	0.20	0.29	43,52,61,75	0
3	FAD	D	901	53/53	0.95	0.20	0.06	45,55,65,95	0
4	ZN	B	903	1/1	0.99	0.15	-0.01	53,53,53,53	0
4	ZN	D	902	1/1	0.99	0.16	-0.08	69,69,69,69	0
4	ZN	A	904	1/1	0.99	0.13	-0.19	65,65,65,65	0
4	ZN	B	904	1/1	0.99	0.11	-0.93	67,67,67,67	0
4	ZN	B	902	1/1	0.99	0.13	-0.96	57,57,57,57	0
4	ZN	D	904	1/1	0.87	0.08	-1.12	95,95,95,95	0
4	ZN	A	903	1/1	0.99	0.11	-1.36	53,53,53,53	0
4	ZN	C	904	1/1	0.99	0.09	-1.37	96,96,96,96	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.