

Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 01:29 PM EDT

PDB ID	:	2L3D
Title	:	The solution structure of the short form SWIRM domain of LSD1
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Deposited on	:	2010-09-13

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/NMRValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

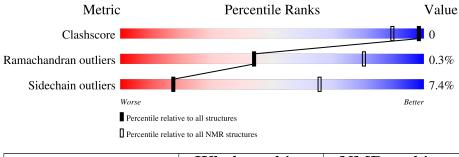
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $SOLUTION\ NMR$

The overall completeness of chemical shifts assignment was not calculated.

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	NMR archive		
Metric	$(\# {\rm Entries})$	(# Entries)		
Clashscore	158937	12864		
Ramachandran outliers	154571	11451		
Sidechain outliers	154315	11428		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 <=5%

Mol	Chain	Length	Quality of chain		
1	А	102	75%	•	24%



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues							
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model				
1	A:12-A:89 (78)	0.95	15				

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters. No single-model clusters were found.

Cluster number	Models
1	3, 4, 7, 8, 9, 11, 12, 14, 16, 17, 18
2	2, 13, 15, 19, 20
3	1, 6
4	5, 10



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1664 atoms, of which 833 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Lysine-specific histone demethylase 1A.

Mol	Chain	Residues		Atoms					Trace
1	Δ	102	Total	С	Η	Ν	0	S	0
	A	102	1664	531	833	149	149	2	U

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	GLY	-	expression tag	UNP O60341
А	2	SER	-	expression tag	UNP O60341

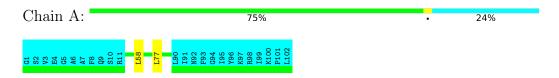


4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Lysine-specific histone demethylase 1A

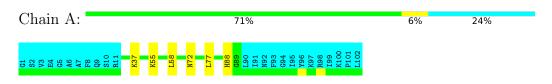


4.2 Scores per residue for each member of the ensemble

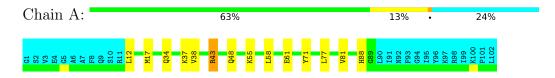
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Lysine-specific histone demethylase 1A



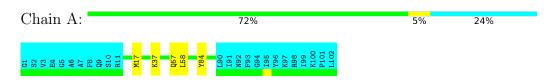
4.2.2 Score per residue for model 2





4.2.3 Score per residue for model 3

• Molecule 1: Lysine-specific histone demethylase 1A



4.2.4 Score per residue for model 4

• Molecule 1: Lysine-specific histone demethylase 1A

Chain A:	7			7	71%	5%•	24%
G1 S2 V3 E4 G5 G5 A7 A7 F8 F8 S10 S10 S10	R16 Q33	F41 I42 R43	L58	R87	L90 191 N92 F93 F95 G94 C95 K199 K100 F101 L102		

4.2.5 Score per residue for model 5

• Molecule 1: Lysine-specific histone demethylase 1A

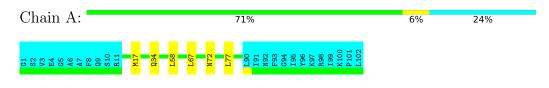
Chain A:	73%	•	24%
G1 822 822 846 846 810 810 811	L58 N72 L77 L77 F93 F93 F93 F93 F93 F93 F93 F93 F93 F93		

4.2.6 Score per residue for model 6

• Molecule 1: Lysine-specific histone demethylase 1A

Chain A:	68%	8% •	24%
G1 S2 E4 A6 A6 A7 A7 S10 S10 S10 S11 S11 S11	920 45 45 45 45 45 163 163 193 193 193 193 193 193 193 193 193 19	L102	

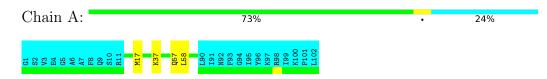
4.2.7 Score per residue for model 7





4.2.8 Score per residue for model 8

• Molecule 1: Lysine-specific histone demethylase 1A



4.2.9 Score per residue for model 9

• Molecule 1: Lysine-specific histone demethylase 1A

Chain A:	71%				6%	24%	
G1 S2 C3 C3 C5 C5 A7 A7 A7 C1 C3 C1 C C1 C C1 C C C C C C C C C C	F25 R43	K55 I E e	E68 E68	L77	L90 191 N92 F93 G94 C94 C96 K97 K97 K96 K97 K100 F101 L102		

4.2.10 Score per residue for model 10

• Molecule 1: Lysine-specific histone demethylase 1A

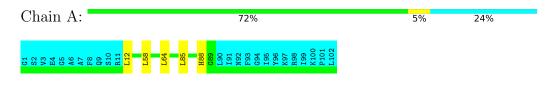
Chain A:	71%	6%	24%	
G1 S2 C2 G5 G5 A7 A7 S10 S10 S10 S10	T46 L47 L64 L77 L77 L77 L77 L77 T94 T99 R98 R94 T99 R94 T99 R95 R93 R95 R93 R95 R93 R95 R93 L100 L101 L101			

4.2.11 Score per residue for model 11

• Molecule 1: Lysine-specific histone demethylase 1A

Chain A:			6%	2	24%											
G1 S2 G5 G5 A6 A7 F8 S10 S10 R11	K37 1 58	N72	L85 E86 B87	H88 H88 C89	L90	191 N92	193 694 105	796 X	K97 R98	199 K100	L102					

4.2.12 Score per residue for model 12





4.2.13 Score per residue for model 13

• Molecule 1: Lysine-specific histone demethylase 1A



4.2.14 Score per residue for model 14

• Molecule 1: Lysine-specific histone demethylase 1A

Chain A:				72%	5%	24%
61 S2 V3 V3 65 65 A7 A7 78 09 810 810 811	H14 Q20	R43 1.58	L77	L90 191 N92 R93 R97 K97 R95 R95 R90 L101 L102		

4.2.15 Score per residue for model 15 (medoid)

• Molecule 1: Lysine-specific histone demethylase 1A

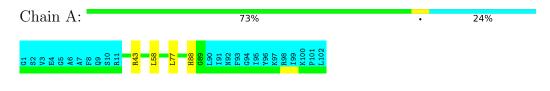
Chain A:	71%	6%	24%
G1 S2 F4 G5 A7 A7 A7 C5 C5 C10 S10 S10 S10	M17 q34 156 156 156 156 156 457 156 159 196 191 196 198 198 198 198 198 198 198 198 198 198		

4.2.16 Score per residue for model 16

• Molecule 1: Lysine-specific histone demethylase 1A

Chain A:	71%	6%	24%	
G1 S2 C3 G5 G5 A7 A7 A7 C3 C10 S10 S10	420 837 837 837 839 839 839 839 849 849 849 849 849 849 849 849 849 84			

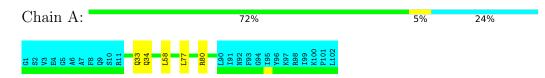
4.2.17 Score per residue for model 17





4.2.18 Score per residue for model 18

• Molecule 1: Lysine-specific histone demethylase 1A



4.2.19 Score per residue for model 19

• Molecule 1: Lysine-specific histone demethylase 1A

Chain A:	66%	11%	24%
G1 S2 S2 55 65 65 7 7 8 10 810 811	H14 1118 1118 1118 1118 1118 1118 1118 1	694 195 196 198 198 198 199 101 102	

4.2.20 Score per residue for model 20

Chain A:	74%	·	24%
G1 S2 S2 G5 A7 A7 A7 S10 S110 S110	E21 E22 E28 E28 E28 E30 E30 E30 E30 E30 E30 E30 E30 E30 E30		



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: structures with the least restraint violations.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	
Amber	refinement	

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

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 (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol Chain		B	Sond lengths	I	Bond angles
	Unam	RMSZ	$\#Z{>}5$	RMSZ	#Z > 5
1	А	$0.71 {\pm} 0.01$	$0{\pm}0/659~(~0.0{\pm}~0.0\%)$	$0.92{\pm}0.02$	$0{\pm}0/898~(~0.0{\pm}~0.0\%)$
All	All	0.71	0/13180~(~0.0%)	0.92	5/17960~(~0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mal	Chain	Dec	Tuno	pe Atoms		Observed(°)		Mod	lels
Mol	Chain	nes	Type	Atoms		Observed(*)	$Ideal(^{o})$	Worst	Total
1	А	43	ARG	NE-CZ-NH1	6.28	123.44	120.30	4	3
1	А	45	ARG	NE-CZ-NH1	5.34	122.97	120.30	6	1
1	А	80	ARG	NE-CZ-NH1	5.09	122.84	120.30	18	1

There are no chirality outliers.

There are no planarity outliers.

$6.2 \quad \text{Too-close contacts} (i)$

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	А	642	632	632	0±1
All	All	12840	12640	12640	5

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 0.

All unique clashes are listed below, sorted by their clash magnitude.



Atom-1	Atom 2	Clash(Å)	Distance(Å)	Mod	lels
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:38:VAL:HG23	1:A:71:TYR:CD2	0.52	2.39	2	2
1:A:67:LEU:HD13	1:A:72:ASN:ND2	0.49	2.23	13	1
1:A:39:PHE:CE2	1:A:81:VAL:HG22	0.42	2.50	19	1
1:A:46:THR:HG23	1:A:82:HIS:CE1	0.41	2.50	10	1

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	Perce	ntiles
1	A	78/102~(76%)	$74\pm2~(95\pm2\%)$	$4\pm1~(5\pm2\%)$	0±0 (0±1%)	44	80
All	All	1560/2040~(76%)	1483 (95%)	73 (5%)	4 (0%)	44	80

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	89	GLY	2
1	А	55	LYS	1
1	А	14	HIS	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	А	72/91~(79%)	$67\pm2(93\pm3\%)$	$5\pm2~(7\pm3\%)$	17	65
All	All	1440/1820~(79%)	1333 (93%)	107 (7%)	17	65

All 32 unique residues with a non-rotameric side chain are listed below. They are sorted by the frequency of occurrence in the ensemble.



Mol	Chain	Res	Type	Models (Total)
1	А	58	LEU	16
1	А	77	LEU	11
1	А	37	LYS	7
1	А	17	MET	7
1	А	88	HIS	6
1	А	55	LYS	6
1	А	72	ASN	5
1	А	34	GLN	4
1	А	43	ARG	4
1	А	12	LEU	3
1	А	57	GLN	3
1	А	87	ARG	3
1	А	20	GLN	3
1	А	64	LEU	3
1	А	80	ARG	3
1	А	85	LEU	3
1	А	67	LEU	3
1	А	33	GLN	2
1	А	47	LEU	2
1	А	48	GLN	1
1	А	61	GLU	1
1	А	81	VAL	1
1	А	84	TYR	1
1	А	16	ARG	1
1	А	41	PHE	1
1	А	45	ARG	1
1	А	63	THR	1
1	А	25	PHE	1
1	А	68	GLU	1
1	А	14	HIS	1
1	А	18	THR	1
1	А	21	GLU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

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



6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



7 Chemical shift validation (i)

No chemical shift data were provided

