Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2KNG
Title	:	Solution structure of C-domain of Lsr2
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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
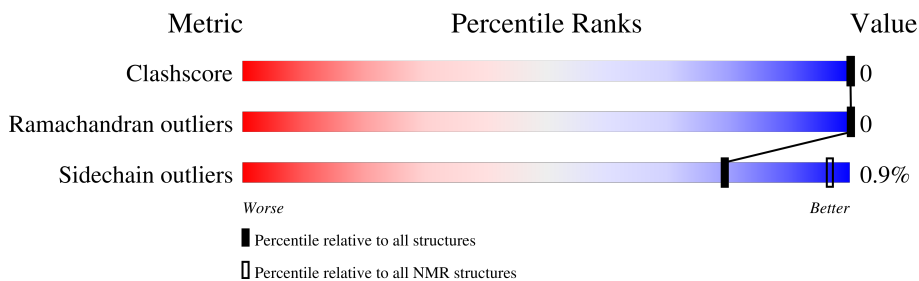with specific help available everywhere you see the (i) symbol.

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Clashscore		0
Ramachandran outliers		0
Sidechain outliers		0.9%

Worse *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#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	A	55	64% • 35%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 4 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:79-A:114 (36)	0.36	4

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 2 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 845 atoms, of which 411 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein lsr2.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	55	845	257	411	99	78	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	LEU	-	expression tag	UNP P65648
A	114	GLU	-	expression tag	UNP P65648
A	115	HIS	-	expression tag	UNP P65648
A	116	HIS	-	expression tag	UNP P65648
A	117	HIS	-	expression tag	UNP P65648
A	118	HIS	-	expression tag	UNP P65648
A	119	HIS	-	expression tag	UNP P65648
A	120	HIS	-	expression tag	UNP P65648

4 Residue-property plots ⓘ

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: Protein lsr2

Chain A:

4.2 Scores per residue for each member of the ensemble
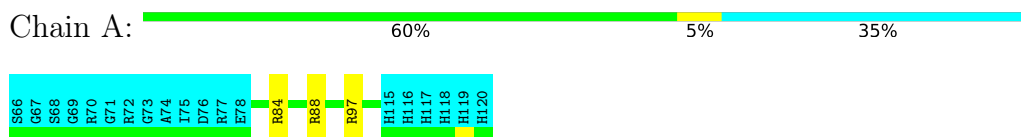
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Protein lsr2

Chain A:

4.2.2 Score per residue for model 2
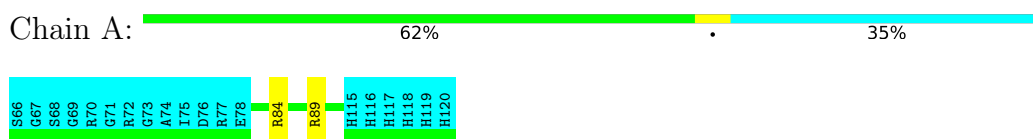
- Molecule 1: Protein lsr2

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Protein lsr2

Chain A:

4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Protein lsr2

Chain A:

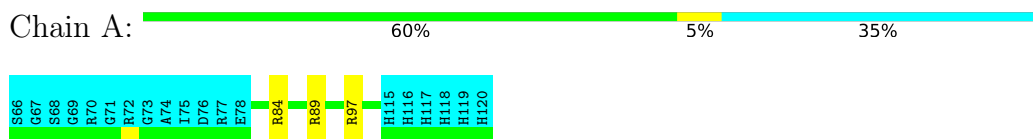### 4.2.5 Score per residue for model 5

• Molecule 1: Protein lsr2

Chain A:

4.2.6 Score per residue for model 6

• Molecule 1: Protein lsr2

Chain A:

4.2.7 Score per residue for model 7

• Molecule 1: Protein lsr2

Chain A:

4.2.8 Score per residue for model 8

• Molecule 1: Protein lsr2

Chain A:
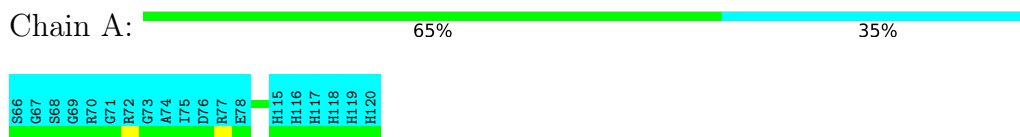
4.2.9 Score per residue for model 9

• Molecule 1: Protein lsr2

Chain A:

4.2.10 Score per residue for model 10

• Molecule 1: Protein lsr2

Chain A:
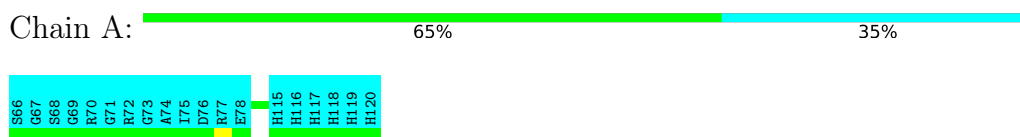
4.2.11 Score per residue for model 11

• Molecule 1: Protein lsr2

Chain A:

4.2.12 Score per residue for model 12

• Molecule 1: Protein lsr2

Chain A:
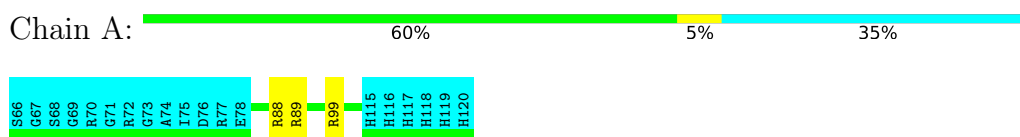
4.2.13　Score per residue for model 13

• Molecule 1: Protein lsr2

Chain A:

4.2.14　Score per residue for model 14

• Molecule 1: Protein lsr2

Chain A:
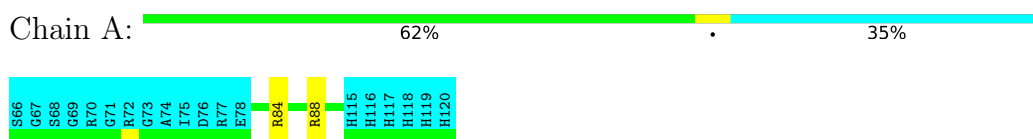
4.2.15　Score per residue for model 15

• Molecule 1: Protein lsr2

Chain A:

4.2.16　Score per residue for model 16

• Molecule 1: Protein lsr2

Chain A:

4.2.17　Score per residue for model 17

• Molecule 1: Protein lsr2

Chain A:

4.2.18   Score per residue for model 18

• Molecule 1: Protein lsr2

Chain A:

S66 G67 S68 G69 R70 G71 R72 G73 A74 I75 D76 R77 E78 R89 H115 H116 H117 H118 H119 H120

4.2.19   Score per residue for model 19

• Molecule 1: Protein lsr2

Chain A:

S66 G67 S68 G69 R70 G71 R72 G73 A74 I75 D76 R77 E78 R89 E114 H115 H116 H117 H118 H119 H120

4.2.20   Score per residue for model 20

• Molecule 1: Protein lsr2

Chain A:

S66 G67 S68 G69 R70 G71 R72 G73 A74 I75 D76 R77 E78 R84 H115 H116 H117 H118 H119 H120

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
Amber	refinement	9

No chemical shift data was provided.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.72±0.01	0±0/288 (0.0± 0.0%)	1.05±0.04	1±1/392 (0.3± 0.2%)
All	All	0.72	0/5760 (0.0%)	1.05	26/7840 (0.3%)

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.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	89	ARG	NE-CZ-NH1	6.57	123.59	120.30	18	13
1	A	84	ARG	NE-CZ-NH1	6.39	123.49	120.30	7	6
1	A	88	ARG	NE-CZ-NH1	6.07	123.34	120.30	2	3
1	A	99	ARG	NE-CZ-NH1	5.30	122.95	120.30	12	1
1	A	89	ARG	NE-CZ-NH2	-5.26	117.67	120.30	11	1
1	A	97	ARG	NE-CZ-NH1	5.20	122.90	120.30	9	2

There are no chirality outliers.

There are no planarity outliers.

6.2 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 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
All	All	5640	5480	5440	-

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 -.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

There are no clashes.

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	Percentiles	
1	A	36/55 (65%)	36±1 (99±2%)	0±1 (1±2%)	0±0 (0±0%)	100	100
All	All	720/1100 (65%)	710 (99%)	10 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 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 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	A	27/41 (66%)	27±1 (99±2%)	0±1 (1±2%)	79	97
All	All	540/820 (66%)	535 (99%)	5 (1%)	79	97

All 4 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	114	GLU	2
1	A	97	ARG	1
1	A	99	ARG	1
1	A	104	VAL	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

No chemical shift data were provided