wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1SYM
Title	:	3-D SOLUTION STRUCTURE OF REDUCED APO-S100B FROM RAT, NMR, 20 STRUCTURES
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Deposited on	:	1996-05-29

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

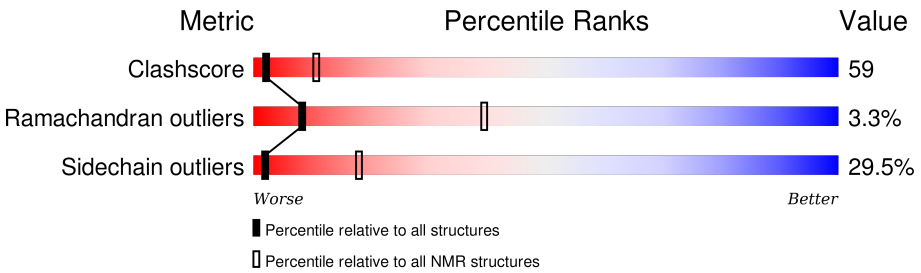
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	92	11% 63% 10% 16%
1	B	92	11% 63% 10% 16%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models).

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:1-A:18, A:25-A:83, B:1-B:18, B:25-B:83 (154)	0.46	17

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 and 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2920 atoms, of which 1418 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called S100B.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	92	1460	471	709	118	155	7	0
1	B	92	1460	471	709	118	155	7	0

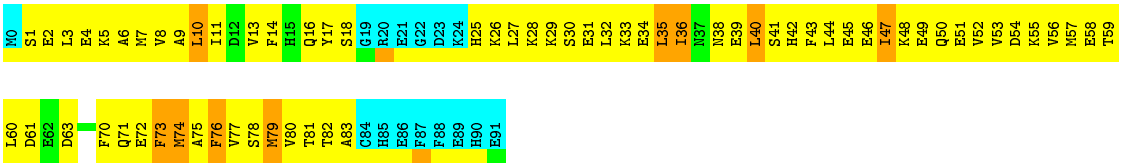
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: S100B

Chain A: 11% 63% 10% 16%



- Molecule 1: S100B

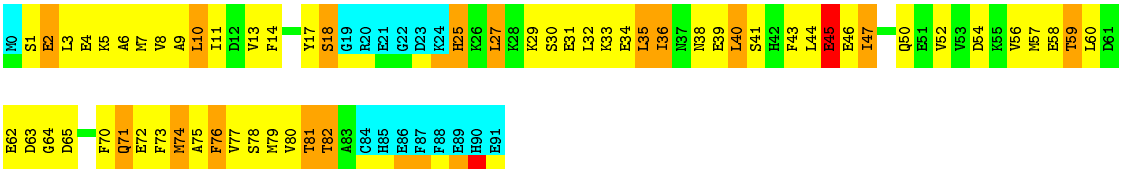
Chain B: 11% 63% 10% 16%

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 17. Colouring as in section 4.1 above.

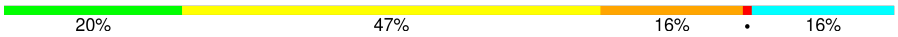
- Molecule 1: S100B

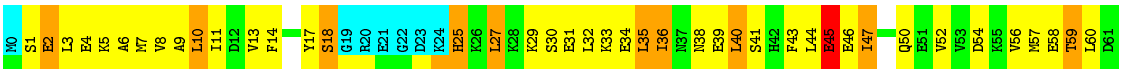
Chain A: 20% 47% 16% • 16%

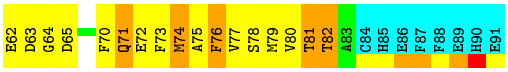


- Molecule 1: S100B

Chain B:


20%
47%
16%
•
16%


M0
S1
E2
L3
E4
K5
A6
M7
V8
A9
L10
I11
D12
V13
F14
Y17
S18
G19
R20
E21
G22
D23
K24
H25
K26
L27
K28
K29
S30
E31
L32
K33
E34
L35
I36
N37
N38
E39
L40
S41
H42
F43
L44
E45
E46
I47
Q50
E51
V52
V53
D54
K55
V56
M57
E58
T59
L60
D61


E62
D63
G64
D65
F70
Q71
E72
F73
M74
A75
F76
V77
S78
M79
V80
T81
T82
A83
C84
H85
E86
F87
F88
E89
H90
E91

5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 20 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 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	A	622	601	601	85±13
1	B	622	601	601	85±13
All	All	24880	24040	24040	2887

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 59.

5 of 1179 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:PHE:CE2	1:B:82:THR:HG23	1.03	1.88	15	1
1:A:82:THR:HG23	1:B:70:PHE:CE2	1.03	1.89	15	1
1:A:36:ILE:CG2	1:A:80:VAL:HG21	1.01	1.85	6	8
1:B:36:ILE:CG2	1:B:80:VAL:HG21	1.01	1.85	6	8
1:A:14:PHE:CZ	1:A:27:LEU:HD23	1.01	1.91	5	5

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	Percentiles
1	A	77/92 (84%)	64±3 (83±4%)	11±2 (14±3%)	3±1 (3±2%)	8 39
1	B	77/92 (84%)	64±3 (83±4%)	11±3 (14±3%)	3±1 (3±2%)	8 39
All	All	3080/3680 (84%)	2543 (83%)	435 (14%)	102 (3%)	8 39

5 of 22 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	47	ILE	17
1	A	47	ILE	17
1	B	40	LEU	10
1	A	40	LEU	10
1	B	42	HIS	5

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	A	71/84 (85%)	50±3 (70±4%)	21±3 (30±4%)	2 18
1	B	71/84 (85%)	50±3 (70±4%)	21±3 (30±4%)	2 18
All	All	2840/3360 (85%)	2001 (70%)	839 (30%)	2 18

5 of 114 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	35	LEU	20
1	A	36	ILE	20
1	B	35	LEU	20
1	B	36	ILE	20
1	A	10	LEU	20

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 carbohydrates 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