wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1JR5
Title	:	Solution Structure of the Anti-Sigma Factor AsiA Homodimer
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Deposited on	:	2001-08-10

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:

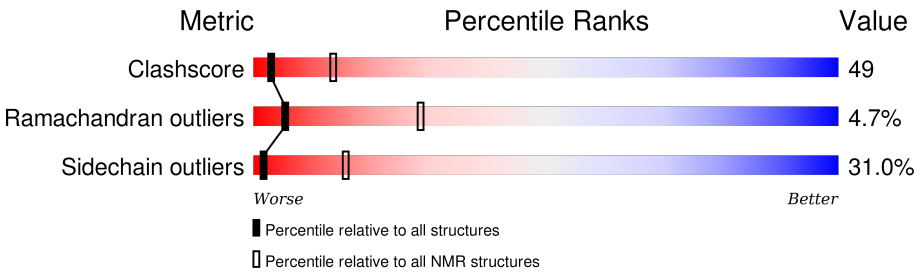
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	90	31% 53% 13% ••
1	B	90	30% 54% 14% •

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 14 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:2-A:90, B:1-B:90 (179)	0.31	14

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 5 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 6, 7, 8, 13, 21
2	2, 3, 10, 20, 22
3	12, 15, 17, 23
4	5, 9, 16
5	4, 11, 14
Single-model clusters	18; 19; 24; 25

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2990 atoms, of which 1498 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 10 KDA Anti-Sigma Factor.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	90	1495	471	749	128	145	2	0
1	B	90	1495	471	749	128	145	2	0

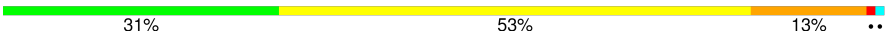
4 Residue-property plots (i)

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: 10 KDA Anti-Sigma Factor

Chain A:



- Molecule 1: 10 KDA Anti-Sigma Factor

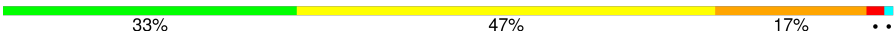
Chain B:

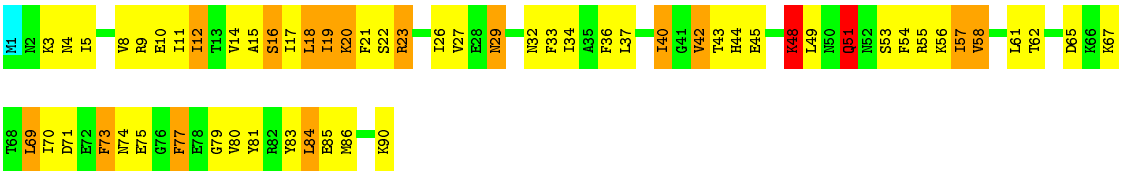
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 14. Colouring as in section 4.1 above.

- Molecule 1: 10 KDA Anti-Sigma Factor

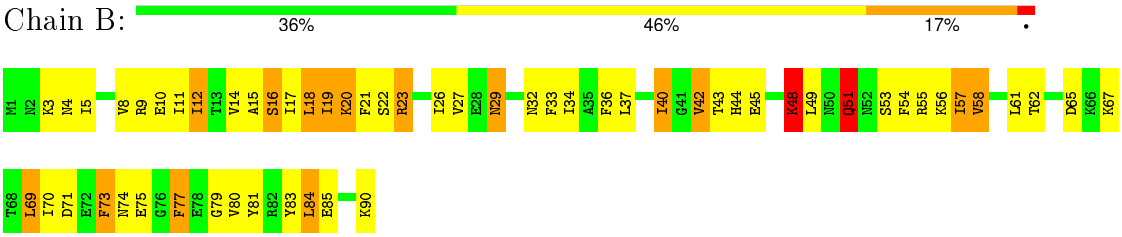
Chain A:





- Molecule 1: 10 KDA Anti-Sigma Factor

Chain B:


36%
46%
17%
M1 M2 K3 N4 I5 V8 R9 E10 I11 I12 T13 V14 A15 S16 I17 L18 I19 K20 F21 S22 R23 I26 V27 E28 M29 N32 F33 I34 A35 F36 L37 I40 G41 V42 T43 H44 E45 K48 L49 N50 Q51 N52 S53 F54 R55 K56 I57 V58 L61 T62 D65 K66 K67
T68 L69 I70 D71 E72 F73 N74 E75 G76 F77 E78 G79 V80 Y81 R82 Y83 L84 E85 K90

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing, molecular dynamics, torsion angle and cartesian dynamics.*

Of the 50 calculated structures, 25 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
CNS	structure solution	1.0
CNS	refinement	1.0

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	738	738	737	78±7
1	B	746	749	748	77±8
All	All	37100	37175	37125	3663

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 49.

5 of 525 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ILE:HD12	1:B:17:ILE:HD12	1.03	1.30	8	25
1:B:19:ILE:HD12	1:B:27:VAL:HG11	0.95	1.35	24	24
1:A:19:ILE:HD12	1:A:27:VAL:HG11	0.94	1.35	24	24
1:A:14:VAL:HG12	1:B:17:ILE:HD11	0.93	1.40	1	25
1:A:17:ILE:HD11	1:B:14:VAL:HG12	0.91	1.40	1	25

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	88/90 (98%)	72±2 (82±2%)	12±2 (13±2%)	4±1 (5±1%)	5 28
1	B	88/90 (98%)	72±2 (82±2%)	11±2 (13±2%)	4±1 (5±1%)	5 28
All	All	4400/4500 (98%)	3617 (82%)	575 (13%)	208 (5%)	5 28

5 of 16 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	45	GLU	25
1	B	45	GLU	25
1	B	74	ASN	24
1	A	74	ASN	24
1	B	48	LYS	24

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	82/83 (99%)	57±2 (69±3%)	25±2 (31±3%)	2 16
1	B	83/83 (100%)	57±3 (69±3%)	26±3 (31±3%)	2 16
All	All	4125/4150 (99%)	2846 (69%)	1279 (31%)	2 16

5 of 119 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	57	ILE	25
1	B	40	ILE	25
1	B	57	ILE	25
1	B	12	ILE	25
1	A	58	VAL	25

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