Full wwPDB NMR Structure Validation Report (i)

Feb 27, 2022 – 08:14 PM EST

PDB ID	:	2DIN
Title	:	Solution structure of the Myb_DNA-binding domain of human Cell division cycle 5-like protein
Authors	:	Yoneyama, M.; Tochio, N.; Koshiba, S.; Inoue, M.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2006-03-30

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

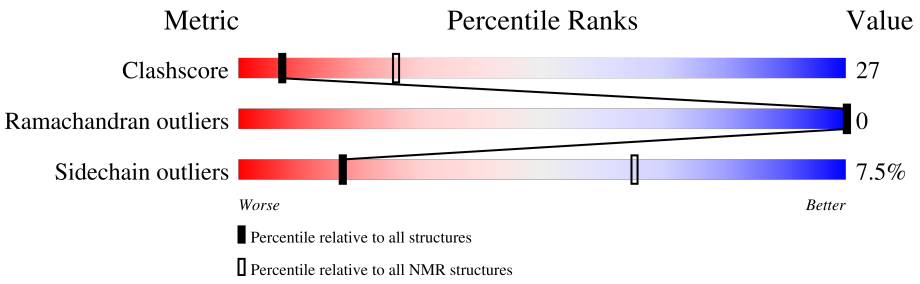
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	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	66	39% 23% • 36%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 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:15-A:56 (42)	0.12	1

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 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1017 atoms, of which 506 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	66	1017	317	506	92	100	2	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q99459
A	2	SER	-	cloning artifact	UNP Q99459
A	3	SER	-	cloning artifact	UNP Q99459
A	4	GLY	-	cloning artifact	UNP Q99459
A	5	SER	-	cloning artifact	UNP Q99459
A	6	SER	-	cloning artifact	UNP Q99459
A	7	GLY	-	cloning artifact	UNP Q99459
A	61	SER	-	cloning artifact	UNP Q99459
A	62	GLY	-	cloning artifact	UNP Q99459
A	63	PRO	-	cloning artifact	UNP Q99459
A	64	SER	-	cloning artifact	UNP Q99459
A	65	SER	-	cloning artifact	UNP Q99459
A	66	GLY	-	cloning artifact	UNP Q99459

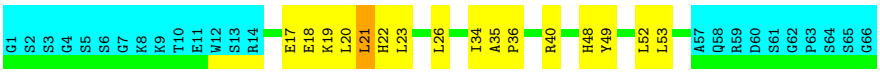
4 Residue-property plots (i)

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: Cell division cycle 5-like protein

Chain A: 39% 23% • 36%



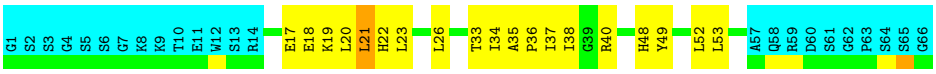
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Cell division cycle 5-like protein

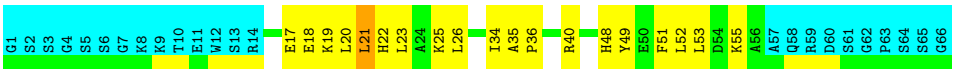
Chain A: 35% 27% • 36%



4.2.2 Score per residue for model 2

• Molecule 1: Cell division cycle 5-like protein

Chain A: 35% 27% • 36%



4.2.3 Score per residue for model 3

- Molecule 1: Cell division cycle 5-like protein

Chain A: 35% 27% • 36%

G1 S2 S3 G4 S5 S6 G7 K8 K9 T10 E11 W12 S13 R14 E17 E18 K19 L20 L21 H22 L23 A24 K25 L26 T29 Q30 I34 A35 P36 I37 I38 G39 R40 H48 Y49 L52 L53 A57 Q58 R59 D60 S61 G62 P63 S64 S65 G66

4.2.4 Score per residue for model 4

- Molecule 1: Cell division cycle 5-like protein

Chain A: 29% 32% • 36%

G1 S2 S3 G4 S5 S6 G7 K8 K9 T10 E11 W12 S13 R14 E15 E16 E17 E18 K19 L20 L21 H22 L23 A24 K25 L26 T29 Q30 W31 I34 A35 P36 R40 Q44 C45 L46 E47 H48 Y49 L52 L53 A57 Q58 R59 D60 S61 G62 P63 S64 S65 G66

4.2.5 Score per residue for model 5

- Molecule 1: Cell division cycle 5-like protein

Chain A: 36% 26% • 36%

G1 S2 S3 G4 S5 S6 G7 K8 K9 T10 E11 W12 S13 R14 E17 E18 K19 L20 L21 H22 L23 A24 K25 L26 R32 T33 I34 A35 P36 I37 I38 Y49 L52 L53 A57 Q58 R59 D60 S61 G62 P63 S64 S65 G66

4.2.6 Score per residue for model 6

- Molecule 1: Cell division cycle 5-like protein

Chain A: 36% 26% • 36%

G1 S2 S3 G4 S5 S6 G7 K8 K9 T10 E11 W12 S13 R14 E17 E18 K19 L20 L21 H22 L23 L26 M27 P28 W31 I34 A35 P36 R40 L46 E47 H48 Y49 L53 A57 Q58 R59 D60 S61 G62 P63 S64 S65 G66

4.2.7 Score per residue for model 7

- Molecule 1: Cell division cycle 5-like protein

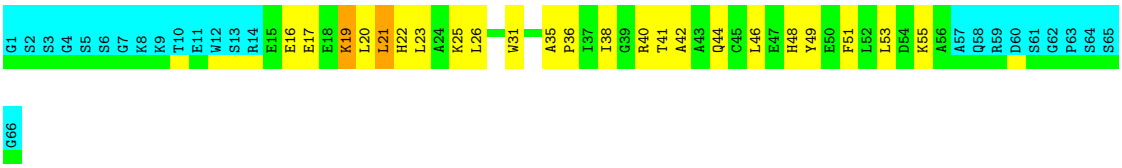
Chain A: 36% 26% • 36%

G1 S2 S3 G4 S5 S6 G7 K8 K9 T10 E11 W12 S13 R14 E15 E16 E17 L20 L21 H22 L23 A24 K25 L26 T29 Q30 I34 A35 P36 R40 H48 Y49 L52 L53 A57 Q58 R59 D60 S61 G62 P63 S64 S65 G66

4.2.8 Score per residue for model 8

- Molecule 1: Cell division cycle 5-like protein

Chain A: 29% 32% • 36%



4.2.9 Score per residue for model 9

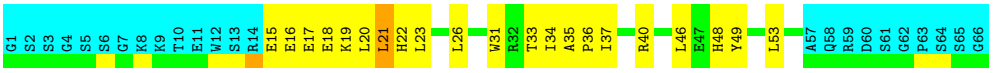
- Molecule 1: Cell division cycle 5-like protein

Chain A: 35% 26% • 36%

4.2.10 Score per residue for model 10

- Molecule 1: Cell division cycle 5-like protein

Chain A: 32% 30% • 36%



4.2.11 Score per residue for model 11

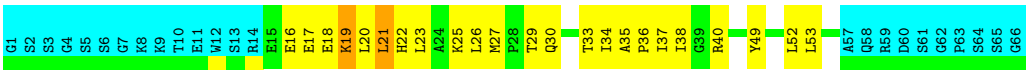
- Molecule 1: Cell division cycle 5-like protein

Chain A: 38% 23% • 36%

4.2.12 Score per residue for model 12

- Molecule 1: Cell division cycle 5-like protein

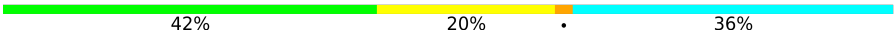
Chain A: 29% 32% • 36%

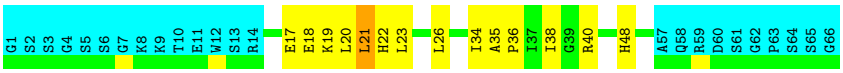


4.2.13 Score per residue for model 13

- Molecule 1: Cell division cycle 5-like protein

Chain A:

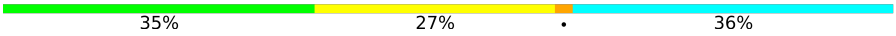


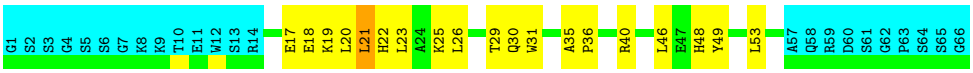


4.2.14 Score per residue for model 14

- Molecule 1: Cell division cycle 5-like protein

Chain A:

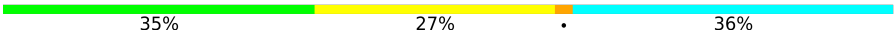


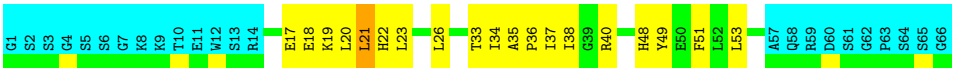


4.2.15 Score per residue for model 15

- Molecule 1: Cell division cycle 5-like protein

Chain A:

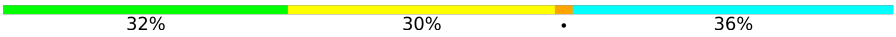


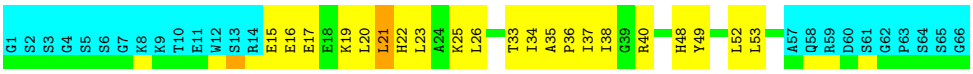


4.2.16 Score per residue for model 16

- Molecule 1: Cell division cycle 5-like protein

Chain A:

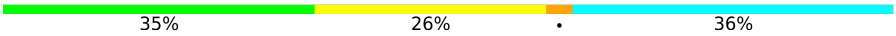


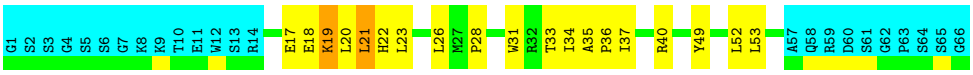


4.2.17 Score per residue for model 17

- Molecule 1: Cell division cycle 5-like protein

Chain A:

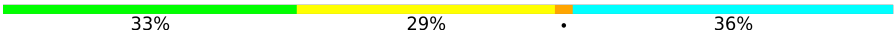


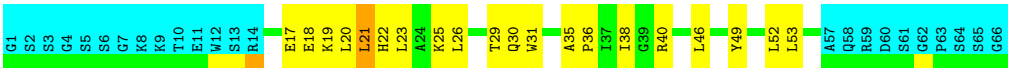


4.2.18 Score per residue for model 18

- Molecule 1: Cell division cycle 5-like protein

Chain A:

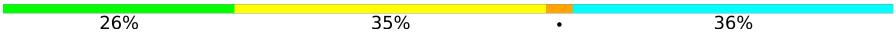


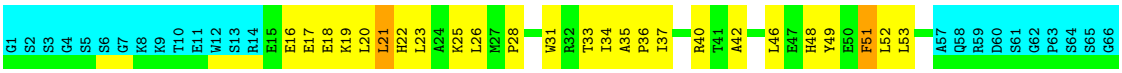


4.2.19 Score per residue for model 19

- Molecule 1: Cell division cycle 5-like protein

Chain A:

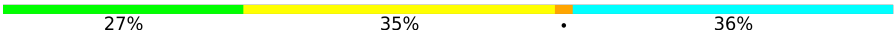


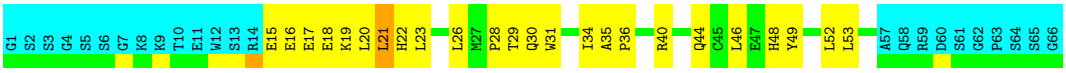


4.2.20 Score per residue for model 20

- Molecule 1: Cell division cycle 5-like protein

Chain A:





5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function, 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	2.0.17
CYANA	refinement	2.0.17

No chemical shift data was provided.

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	344	352	350	18±2
All	All	6880	7040	7000	369

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:HIS:CD2	1:A:26:LEU:HD11	0.92	1.99	15	20
1:A:31:TRP:CZ2	1:A:46:LEU:HD13	0.74	2.17	14	8
1:A:21:LEU:HD21	1:A:52:LEU:HD13	0.73	1.58	7	12
1:A:23:LEU:HD13	1:A:34:ILE:HG23	0.71	1.62	9	16
1:A:49:TYR:HA	1:A:52:LEU:HD12	0.68	1.65	7	9
1:A:33:THR:HG22	1:A:37:ILE:CD1	0.63	2.23	1	7
1:A:22:HIS:CD2	1:A:26:LEU:CD1	0.63	2.79	15	18
1:A:35:ALA:HB3	1:A:36:PRO:HD3	0.62	1.71	1	20
1:A:23:LEU:HA	1:A:26:LEU:HD12	0.61	1.72	11	20
1:A:23:LEU:HD22	1:A:34:ILE:HG12	0.61	1.73	20	11
1:A:19:LYS:HD3	1:A:38:ILE:HG23	0.59	1.74	15	10
1:A:31:TRP:CB	1:A:42:ALA:HB1	0.57	2.29	19	1
1:A:35:ALA:HB3	1:A:36:PRO:CD	0.56	2.31	1	20
1:A:22:HIS:NE2	1:A:26:LEU:HD11	0.56	2.16	15	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:TRP:HB3	1:A:42:ALA:HB1	0.55	1.78	19	1
1:A:49:TYR:CE1	1:A:53:LEU:HD21	0.53	2.38	1	19
1:A:21:LEU:CD2	1:A:52:LEU:HD13	0.53	2.33	7	1
1:A:21:LEU:CD2	1:A:21:LEU:N	0.53	2.72	5	20
1:A:35:ALA:N	1:A:36:PRO:HD2	0.52	2.20	20	20
1:A:17:GLU:O	1:A:20:LEU:N	0.51	2.44	13	20
1:A:33:THR:HG22	1:A:37:ILE:HD12	0.50	1.84	17	2
1:A:20:LEU:HD23	1:A:52:LEU:HD11	0.50	1.83	7	1
1:A:29:THR:O	1:A:30:GLN:NE2	0.49	2.45	3	8
1:A:23:LEU:O	1:A:26:LEU:N	0.49	2.45	11	3
1:A:27:MET:O	1:A:34:ILE:HD11	0.49	2.06	12	1
1:A:51:PHE:CE2	1:A:55:LYS:HD3	0.48	2.43	8	2
1:A:35:ALA:HB1	1:A:40:ARG:O	0.47	2.09	8	1
1:A:28:PRO:O	1:A:31:TRP:NE1	0.47	2.47	6	4
1:A:41:THR:O	1:A:44:GLN:N	0.47	2.47	8	1
1:A:17:GLU:OE1	1:A:52:LEU:HD22	0.47	2.08	19	1
1:A:31:TRP:CE2	1:A:46:LEU:HD13	0.46	2.44	20	2
1:A:31:TRP:CZ2	1:A:46:LEU:CD1	0.46	2.95	14	3
1:A:51:PHE:CD1	1:A:51:PHE:C	0.45	2.89	19	2
1:A:41:THR:O	1:A:42:ALA:C	0.45	2.55	8	1
1:A:33:THR:HG22	1:A:37:ILE:HD11	0.45	1.85	1	2
1:A:23:LEU:HD13	1:A:34:ILE:CG2	0.45	2.37	3	1
1:A:17:GLU:O	1:A:18:GLU:C	0.44	2.56	13	16
1:A:49:TYR:O	1:A:52:LEU:N	0.43	2.51	5	1
1:A:23:LEU:O	1:A:24:ALA:C	0.43	2.56	7	4
1:A:15:GLU:O	1:A:16:GLU:C	0.43	2.55	10	2
1:A:35:ALA:N	1:A:36:PRO:CD	0.42	2.82	20	1
1:A:19:LYS:HG2	1:A:20:LEU:N	0.42	2.30	3	18
1:A:53:LEU:HD22	1:A:53:LEU:N	0.42	2.29	7	4
1:A:35:ALA:CB	1:A:36:PRO:CD	0.42	2.97	1	7
1:A:19:LYS:CD	1:A:38:ILE:HG23	0.42	2.45	12	1
1:A:40:ARG:CG	1:A:44:GLN:OE1	0.41	2.68	4	1
1:A:28:PRO:O	1:A:31:TRP:CE2	0.41	2.74	19	1
1:A:20:LEU:HD23	1:A:52:LEU:CD1	0.41	2.45	7	1
1:A:23:LEU:HB3	1:A:34:ILE:HD13	0.41	1.91	3	1
1:A:53:LEU:N	1:A:53:LEU:HD22	0.41	2.31	10	1
1:A:21:LEU:HD21	1:A:52:LEU:CD1	0.40	2.47	3	1
1:A:44:GLN:N	1:A:44:GLN:CD	0.40	2.71	20	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	Percentiles	
1	A	42/66 (64%)	37±1 (89±3%)	5±1 (11±3%)	0±0 (0±0%)	100	100
All	All	840/1320 (64%)	744 (89%)	96 (11%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	36/54 (67%)	33±1 (92±2%)	3±1 (8±2%)	17	65
All	All	720/1080 (67%)	666 (92%)	54 (8%)	17	65

All 8 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	21	LEU	20
1	A	40	ARG	14
1	A	25	LYS	9
1	A	19	LYS	5
1	A	15	GLU	3
1	A	32	ARG	1
1	A	16	GLU	1
1	A	51	PHE	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