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wwPDB
PROTEIN DATA BANK

wwPDB NMR Structure Validation Summary Report (i)

Feb 12, 2017 – 05:48 pm GMT

PDB ID	:	1D6K
Title	:	NMR SOLUTION STRUCTURE OF THE 5S RRNA E-LOOP/L25 COMPLEX
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Deposited on	:	1999-10-14

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

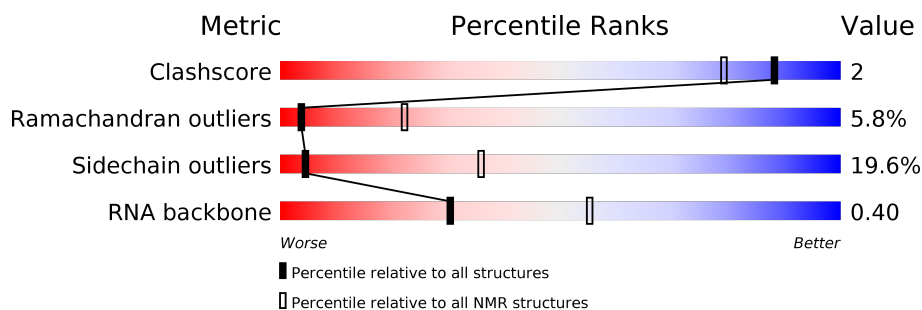|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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		2
Ramachandran outliers		5.8%
Sidechain outliers		19.6%
RNA backbone		0.40

Worse   *Better*

■ Percentile relative to all structures
▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367
RNA backbone	3398	623

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	B	37	30% 54% 14% •
2	A	94	66% 27% • 6%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 2 as representative, based on the following criterion: *closest to the average*.

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:31, A:37-A:94 (88)	0.20	5

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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2729 atoms, of which 1180 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 5S RRNA E-LOOP (5SE).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	B	37	1196	355	400	146	259	36	0

- Molecule 2 is a protein called RIBOSOMAL PROTEIN L25.

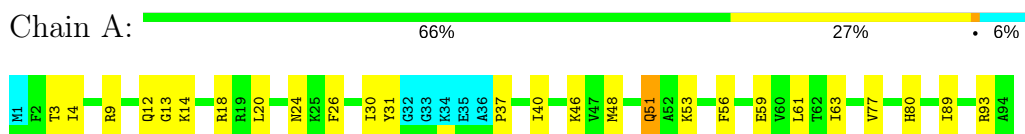| Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	A	94	1533	479	780	137	134	3	0

4 Residue-property plots ⓘ

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.

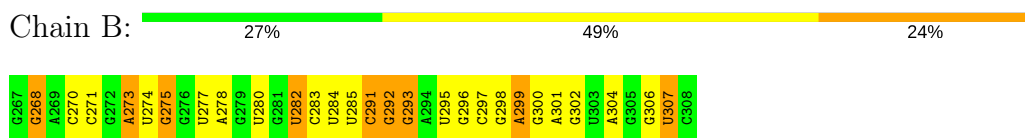• Molecule 1: 5S RRNA E-LOOP (5SE)
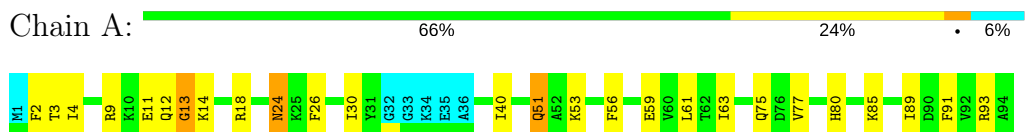
Chain B:

• Molecule 2: RIBOSOMAL PROTEIN L25

Chain A:

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

The representative model is number 5. Colouring as in section 4.1 above.

• Molecule 1: 5S RRNA E-LOOP (5SE)

Chain B:

• Molecule 2: RIBOSOMAL PROTEIN L25

Chain A:

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *HYBRID DISTANCE GEOMETRY/SIMULATED ANNEALING*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *TARGET FUNCTION*.

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

Software name	Classification	Version
DYANA	structure solution	1.5
OPAL/AMBER94	refinement	2.6

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 ⓘ

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	B	1.21±0.01	0±0/891 (0.0±0.0%)	1.77±0.03	21±3/1390 (1.5±0.2%)
2	A	0.61±0.01	0±0/727 (0.0±0.0%)	1.13±0.03	2±1/974 (0.2±0.1%)
All	All	0.99	0/32360 (0.0%)	1.54	466/47280 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	B	0.1±0.2	9.0±2.4
2	A	0.0±0.0	1.4±0.7
All	All	1	207

There are no bond-length outliers.

5 of 69 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	B	271	C	O4'-C1'-N1	10.07	116.25	108.20	20	20
1	B	295	U	O4'-C1'-N1	9.17	115.54	108.20	10	20
1	B	280	U	O4'-C1'-N1	9.13	115.51	108.20	14	20
1	B	291	C	O4'-C1'-N1	9.05	115.44	108.20	14	5
2	A	31	TYR	CB-CG-CD2	-8.98	115.61	121.00	17	11

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	B	300	G	C4'	1

5 of 33 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	B	273	A	Sidechain	20
1	B	299	A	Sidechain	19
2	A	26	PHE	Sidechain	17
1	B	276	G	Sidechain	16
1	B	284	U	Sidechain	16

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
1	B	796	400	400	1±1
2	A	714	739	739	5±2
All	All	30200	22780	22780	114

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 2.

5 of 31 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
2:A:30:ILE:HD11	2:A:63:ILE:HG13	0.71	1.61	18	11
2:A:77:VAL:HG12	2:A:89:ILE:HG23	0.60	1.71	13	18
2:A:29:ILE:HD11	2:A:37:PRO:HB2	0.56	1.77	8	9
2:A:86:LEU:HD13	2:A:89:ILE:HD11	0.55	1.78	3	9
2:A:64:VAL:HG22	2:A:69:GLU:HG2	0.55	1.77	17	1

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	
2	A	87/94 (93%)	68±2 (78±2%)	14±2 (16±2%)	5±1 (6±1%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1740/1880 (93%)	1361 (78%)	278 (16%)	101 (6%)	4 22

5 of 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	A	3	THR	18
2	A	93	ARG	18
2	A	14	LYS	16
2	A	13	GLY	16
2	A	46	LYS	14

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
2	A	75/78 (96%)	60±2 (80±3%)	15±2 (20±3%)	4 36
All	All	1500/1560 (96%)	1206 (80%)	294 (20%)	4 36

5 of 41 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)
2	A	12	GLN	20
2	A	80	HIS	20
2	A	53	LYS	20
2	A	40	ILE	20
2	A	4	ILE	20

6.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	B	36/37 (97%)	7±2 (18±5%)	0±0 (0±0%)	0.40±0.05
All	All	720/740 (97%)	132 (18%)	0 (0%)	0.40

The overall RNA backbone suiteness is 0.40.

5 of 20 unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	292	G	19
1	B	268	G	19
1	B	291	C	16
1	B	299	A	10
1	B	293	G	9

There are no RNA pucker outliers to report.

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 carbohydrates 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 (i)

No chemical shift data were provided