

wwPDB NMR Structure Validation Summary Report (i)

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PDB ID : 1RQU

Title : NMR structure of L7 dimer from E.coli

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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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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 : 2.29

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.29

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.

There are no overall percentile quality scores available for this entry.

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	120	100%
1	В	120	100%



2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3476 atoms, of which 1776 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues		Atoms							
1	Λ	120	Total	С	Н	N	О	S	0		
1	А	120	1738	534	888	138	175	3	U		
1	1 B	120	Total	С	Н	N	О	S	0		
1		120	1738	534	888	138	175	3	U		



4 Residue-property plots (i)

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: 50S ribosomal protein L7/L12

Chain	A:													10	0%																			
12 12 13 K4	10 17 18	E9 A10 V11	A12 A13	M14 S15	V16 M17	D18	V20	122	123 S24	A25	M26 E27	E28	K29	G31	V32	A34	A35	A37	V38	V40	A41	A42 G43	P44	v45 E46	A47	A48	E50	K51	152 E53	F54	V56	157	L50 K59	A60
A61 G62 A63 N64	V66 A67 V68	I69 K70 A71	V72 R73	G74 A75	T76 G77	L78	L80	E82	A83 K84	D85	L86 V87	E88	289	P91	A92 A93	1.94	K95	Z65	867	X100	D101	A103	E104	A105 L106	K107	K108	A109 L110	E111	E112 A113	G114	A115 E116	V117	V119	K120
• Mol	ecule	1:	50S	i ri	bo	SOI	na	lр	ro	te	in	L	7	/L	12																			
Chain	В:													10	0%																			
S1 12 13 K4	06 17 18	E9 A10 V11	A12 A13	M14 S15	V16 M17	D18	V20	1.22	123 S24	A25	M26 F.27	E28	K29	G31	V32	A34	A35	A37	V38	V40	A41	A42 G43	P44	v45 E46	A47	A48	E50	K51	152 E53	F54	V56	157	L50 K59	A60
A61 G62 A63 N64	V66 A67 V68	I69 K70	N72 V72 R73	G74 A75	T76 G77	L78	180	E82	A83 K84	D85	L86 V87	E88	889	A30 P91	A92 A93	L94	K95 F96	265 CB7	V98	X100	D101	D102 A103	E104	A105 L106	K107	K108	A109 L110	E111	E112 A113	G114	A115 E116	V117	V119	K120



Refinement protocol and experimental data overview (i) 5



The models were refined using the following method: simulated annealing combined with molecular dynamics in torsion angle space.

Of the 100 calculated structures, 1 were deposited, based on the following criterion: structures with the least restraint violations, target function.

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

Software name	Classification	Version
CYANA	structure solution	1.01
FANTOM	refinement	4

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	0	0	0	0
1	В	0	0	0	0
All	All	0	0	0	-

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 -.

There are no clashes.

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	0	-	-	-	-
1	В	0	-	=	-	-
All	All	0	-	=	-	-

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	0	-	-	-
1	В	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

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

