

Full wwPDB NMR Structure Validation Report (i)

Feb 27, 2022 – 05:41 PM EST

PDB ID	:	2D9P
Title	:	Solution structure of RNA binding domain 4 in Polyadenylation binding pro-
		tein 3
Authors	:	Tsuda, K.; Muto, Y.; Inoue, M.; Kigawa, T.; Terada, T.; Shirouzu, M.;
		Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-12-12

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.



Motria	Whole archive	NMR archive
wietric	$(\# {\rm Entries})$	$(\# {\rm Entries})$
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	А	103	50%	18%	•	31%								



2 Ensemble composition and analysis (i)

This entry contains 20 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 mode													
1	A:293-A:326, A:332-A:368	0.21	14										
	(71)												

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 1 single-model cluster was found.

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



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1554 atoms, of which 775 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Polyadenylate-binding protein 3.

Mol	Chain	Residues		Trace					
1	٨	102	Total	С	Η	Ν	0	\mathbf{S}	0
	A	105	1554	481	775	140	154	4	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	279	GLY	-	cloning artifact	UNP Q9H361
А	280	SER	-	cloning artifact	UNP Q9H361
А	281	SER	-	cloning artifact	UNP Q9H361
А	282	GLY	-	cloning artifact	UNP Q9H361
А	283	SER	-	cloning artifact	UNP Q9H361
А	284	SER	-	cloning artifact	UNP Q9H361
А	285	GLY	-	cloning artifact	UNP Q9H361
А	376	SER	-	cloning artifact	UNP Q9H361
А	377	GLY	-	cloning artifact	UNP Q9H361
А	378	PRO	-	cloning artifact	UNP Q9H361
А	379	SER	-	cloning artifact	UNP Q9H361
А	380	SER	-	cloning artifact	UNP Q9H361
А	381	GLY	-	cloning artifact	UNP Q9H361



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: Polyadenylate-binding protein 3



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

• Molecule 1: Polyadenylate-binding protein 3



4.2.2 Score per residue for model 2



4.2.3 Score per residue for model 3

• Molecule 1: Polyadenylate-binding protein 3



4.2.4 Score per residue for model 4

• Molecule 1: Polyadenylate-binding protein 3



4.2.5 Score per residue for model 5

• Molecule 1: Polyadenylate-binding protein 3



4.2.6 Score per residue for model 6





4.2.7 Score per residue for model 7

• Molecule 1: Polyadenylate-binding protein 3



4.2.8 Score per residue for model 8

 \bullet Molecule 1: Polyadenylate-binding protein 3



4.2.9 Score per residue for model 9



4.2.10 Score per residue for model 10

• Molecule 1: Polyadenylate-binding protein 3



- 4.2.11 Score per residue for model 11
- Molecule 1: Polyadenylate-binding protein 3



4.2.12 Score per residue for model 12

• Molecule 1: Polyadenylate-binding protein 3



4.2.13 Score per residue for model 13





4.2.14 Score per residue for model 14 (medoid)

• Molecule 1: Polyadenylate-binding protein 3



4.2.15 Score per residue for model 15

• Molecule 1: Polyadenylate-binding protein 3

С	h	ai	n	1	A	:									Z	4	%														23	3%					•							31	%	_								
G279	S280	S281	G 282	S 283	S 284	G 285	D286	T 288	T289	Doc a	1001	14 29 Z	V293	V294	N295	L296		K299	N300	L301	D302	D303	G304	1 305	D306	E314	F014	0100	P316	1320		M326	M327	E328	G329	G330	R331	S332	K333	G334	1 330	P343	E344	E345	A346		V350	M353	N354	G355	R356	6961	L303	V365
_	Q369	R370	K371	E372	E373	R374	Q375	0.00	P378	2370 2370	0000 0000	1221																																										

4.2.16 Score per residue for model 16

• Molecule 1: Polyadenylate-binding protein 3



4.2.17 Score per residue for model 17





4.2.18 Score per residue for model 18

• Molecule 1: Polyadenylate-binding protein 3



4.2.19 Score per residue for model 19

• Molecule 1: Polyadenylate-binding protein 3

Chain A:	47%	19%	•	31%	
6279 5280 5281 6282 5283 5283 5284 5285 5284 6285 7285 7286 7286 7286 7286 7286	Y291 Y293 V293 V295 L296 L296 K299 K299 K299 K299 K299 K299 K299 K	L310 F314 F314 S315 F315 F317 F317 F317 E328 G329 G330 G330 G331	S332 K333 G334 F335 P343	A346 V350 V350 E352 M363 N354	1357 1360 1360 1361 1361 1361 1367 1368
q369 K371 E372 E373 R374 q375 g375 g375 g377 P378 S379 S380	6 381				

4.2.20 Score per residue for model 20





5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: torsion angle dynamics, restrainted molecular dynamics.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: target function, structures with the lowest energy, 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
CYANA	refinement	2.0

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	А	541	552	552	18 ± 3				
All	All	10820	11040	11040	352				

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 16.

Atom 1	Atom 2	$Clach(\lambda)$	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:296:LEU:HD21	1:A:346:ALA:HB1	0.78	1.56	9	16
1:A:314:PHE:HB3	1:A:320:ILE:HD11	0.74	1.56	2	7
1:A:320:ILE:HG23	1:A:339:CYS:O	0.73	1.83	4	8
1:A:302:ASP:OD2	1:A:359:ALA:HB3	0.72	1.82	16	3
1:A:314:PHE:CB	1:A:320:ILE:HD11	0.72	2.15	2	11
1:A:310:LEU:HD21	1:A:338:VAL:HG22	0.70	1.61	17	1
1:A:296:LEU:HD22	1:A:350:VAL:CG2	0.69	2.17	12	7
1:A:340:PHE:HB2	1:A:346:ALA:HB2	0.67	1.67	7	1
1:A:296:LEU:HD12	1:A:340:PHE:CE1	0.64	2.26	10	5
1:A:315:SER:N	1:A:316:PRO:CD	0.64	2.61	12	20
1:A:346:ALA:O	1:A:350:VAL:HG23	0.62	1.94	15	13
1:A:296:LEU:HD22	1:A:350:VAL:HG22	0.60	1.73	12	11
1:A:314:PHE:CZ	1:A:353:MET:SD	0.60	2.94	18	1
1:A:297:TYR:HB2	1:A:368:ALA:HB2	0.59	1.73	8	6

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

Continued on next page...



2D9P

	ious puge		D . (8)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:310:LEU:HD11	1:A:338:VAL:HG21	0.59	1.74	18	2
1:A:310:LEU:HD21	1:A:310:LEU:HD21 1:A:338:VAL:CG2		2.28	4	3
1:A:311:ARG:HD2	1:A:323:ALA:HB3	0.56	1.77	17	1
1:A:350:VAL:HG21	1:A:367:LEU:CD2	0.56	2.31	19	2
1:A:315:SER:N	1:A:316:PRO:HD2	0.56	2.16	12	20
1:A:360:THR:CG2	1:A:361:LYS:N	0.56	2.69	19	1
1:A:299:LYS:CG	1:A:300:ASN:N	0.55	2.70	1	18
1:A:294:VAL:HG12	1:A:343:PRO:N	0.53	2.17	20	4
1:A:296:LEU:CD2	1:A:367:LEU:HD23	0.53	2.32	1	2
1:A:305:ILE:HG22	1:A:306:ASP:N	0.53	2.18	15	1
1:A:311:ARG:HG3	1:A:320:ILE:HG21	0.53	1.80	11	1
1:A:298:VAL:HG21	1:A:310:LEU:HD11	0.52	1.81	4	1
1:A:320:ILE:HG21	1:A:323:ALA:HB2	0.52	1.80	16	3
1:A:326:MET:HB2	1:A:335:PHE:CZ	0.51	2.39	3	1
1:A:295:ASN:O	1:A:296:LEU:HD23	0.51	2.05	16	1
1:A:314:PHE:CE1	1:A:353:MET:SD	0.51	3.04	18	1
1:A:310:LEU:HD12	1:A:314:PHE:CE1	0.51	2.41	4	13
1:A:311:ARG:HG3	1:A:320:ILE:HD12	0.51	1.83	10	1
1:A:314:PHE:CD2	1:A:338:VAL:HG11	0.51	2.40	1	1
1:A:301:LEU:HD12	1:A:335:PHE:C	0.51	2.26	14	4
1:A:310:LEU:HD11	1:A:338:VAL:CG2	0.51	2.35	18	1
1:A:353:MET:O	1:A:356:ARG:N	0.51	2.44	3	7
1:A:317:PHE:CE1	1:A:352:GLU:HB3	0.51	2.41	5	10
1:A:350:VAL:O	1:A:354:ASN:CB	0.50	2.60	6	16
1:A:297:TYR:CB	1:A:368:ALA:HB2	0.50	2.36	8	1
1:A:326:MET:HB2	1:A:335:PHE:CE2	0.50	2.42	18	1
1:A:326:MET:SD	1:A:326:MET:N	0.49	2.85	18	1
1:A:360:THR:HG23	1:A:361:LYS:CD	0.48	2.38	1	1
1:A:353:MET:O	1:A:356:ARG:CB	0.48	2.62	6	2
1:A:353:MET:HB3	1:A:365:VAL:HG21	0.48	1.85	20	1
1:A:301:LEU:HD21	1:A:310:LEU:HD13	0.48	1.84	6	1
1:A:296:LEU:HD23	1:A:367:LEU:HD23	0.48	1.86	1	1
1:A:353:MET:CB	1:A:365:VAL:HG21	0.48	2.39	20	1
1:A:299:LYS:HE3	1:A:364:TYR:CD1	0.47	2.45	13	1
1:A:299:LYS:HE2	1:A:364:TYR:CD1	0.47	2.44	12	1
1:A:293:VAL:O	1:A:293:VAL:HG13	0.47	2.09	17	2
1:A:351:THR:O	1:A:353:MET:N	0.47	2.48	9	3
1:A:363:LEU:O	1:A:365:VAL:HG23	0.47	2.10	14	5
1:A:301:LEU:HD23	1:A:363:LEU:CD2	0.47	2.40	6	1
1:A:333:LYS:HB3	1:A:335:PHE:CE2	0.46	2.45	6	2
1:A:300:ASN:N	1:A:334:GLY:O	0.46	2.48	8	1

Continued from previous page...

Continued on next page...



2D9P

	ious puge			Models	
Atom-1	Atom-2	$\operatorname{Clash}(A)$	Distance(A)	Worst	Total
1:A:343:PRO:O	1:A:346:ALA:N	0.46	2.47	9	2
1:A:333:LYS:HD3 1:A:335:PHE:C		0.46	2.46	15	2
1:A:354:ASN:C	1:A:354:ASN:OD1	0.46	2.54	16	1
1:A:299:LYS:HG2	1:A:300:ASN:N	0.46	2.26	1	4
1:A:311:ARG:HG3	1:A:320:ILE:HD13	0.46	1.87	7	1
1:A:296:LEU:CD1	1:A:340:PHE:CE1	0.46	2.98	10	1
1:A:326:MET:CB	1:A:335:PHE:CZ	0.46	2.99	3	1
1:A:310:LEU:CD1	1:A:314:PHE:CE1	0.46	2.99	19	4
1:A:326:MET:HG3	1:A:335:PHE:CE2	0.45	2.46	15	3
1:A:332:SER:O	1:A:333:LYS:C	0.45	2.55	18	4
1:A:353:MET:O	1:A:354:ASN:C	0.45	2.55	3	9
1:A:308:GLU:O	1:A:309:ARG:C	0.45	2.55	4	3
1:A:314:PHE:CE2	1:A:353:MET:SD	0.45	3.09	18	1
1:A:307:ASP:C	1:A:307:ASP:OD1	0.45	2.55	20	1
1:A:333:LYS:HB3	1:A:335:PHE:CE1	0.44	2.47	19	2
1:A:348:LYS:O	1:A:349:ALA:C	0.44	2.56	1	12
1:A:301:LEU:HD23	1:A:363:LEU:HD21	0.44	1.90	6	1
1:A:347:THR:O	1:A:348:LYS:C	0.44	2.56	13	2
1:A:317:PHE:CZ	1:A:352:GLU:HB3	0.43	2.47	19	2
1:A:299:LYS:HE2	1:A:364:TYR:CG	0.43	2.47	12	1
1:A:305:ILE:CG2	1:A:306:ASP:N	0.43	2.81	15	1
1:A:335:PHE:CD1	1:A:335:PHE:N	0.43	2.86	20	1
1:A:301:LEU:O	1:A:302:ASP:C	0.43	2.57	16	2
1:A:357:ILE:HD13	1:A:362:PRO:CA	0.43	2.43	19	3
1:A:343:PRO:O	1:A:344:GLU:C	0.43	2.57	12	10
1:A:357:ILE:HD13	1:A:362:PRO:N	0.43	2.28	14	3
1:A:351:THR:C	1:A:353:MET:N	0.43	2.72	12	3
1:A:326:MET:HG3	1:A:335:PHE:CD2	0.42	2.49	15	1
1:A:317:PHE:CE2	1:A:353:MET:HG2	0.42	2.49	2	3
1:A:314:PHE:CB	1:A:320:ILE:CD1	0.42	2.95	2	1
1:A:326:MET:CB	1:A:335:PHE:CE2	0.42	3.02	18	1
1:A:349:ALA:O	1:A:350:VAL:C	0.42	2.58	2	1
1:A:302:ASP:O	1:A:303:ASP:C	0.42	2.57	10	1
1:A:311:ARG:HG3	1:A:323:ALA:CB	0.42	2.45	17	1
1:A:314:PHE:HB2	1:A:320:ILE:HD11	0.41	1.88	11	2
1:A:360:THR:HG23	1:A:361:LYS:N	0.41	2.29	19	1
1:A:345:GLU:CD	1:A:345:GLU:N	0.41	2.73	3	1
1:A:301:LEU:HD12	1:A:335:PHE:CA	0.41	2.45	19	1
1:A:308:GLU:O	1:A:310:LEU:N	0.41	2.54	3	1
1:A:326:MET:O	1:A:335:PHE:CE1	0.41	2.74	3	1
1:A:351:THR:O	1:A:352:GLU:C	0.41	2.59	9	1

Continued from previous page...

Continued on next page...



Atom 1	Atom 2	$Clack(\hat{\lambda})$	$\operatorname{Distance}(\operatorname{\AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:326:MET:HG3	1:A:335:PHE:CZ	0.40	2.51	13	1
1:A:360:THR:HG23	1:A:361:LYS:HD2	0.40	1.93	1	1
1:A:301:LEU:HD13	1:A:325:VAL:HG22	0.40	1.93	5	1
1:A:311:ARG:HG3	1:A:320:ILE:CD1	0.40	2.46	14	1

Continued from previous page...

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	А	71/103~(69%)	54 ± 3 (76 $\pm4\%$)	$16\pm3~(22\pm4\%)$	1±1 (1±1%)	14 59
All	All	1420/2060~(69%)	1086 (76%)	313 (22%)	21 (1%)	14 59

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	310	LEU	6
1	А	354	ASN	6
1	А	352	GLU	3
1	А	302	ASP	3
1	А	334	GLY	2
1	А	347	THR	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	59/84~(70%)	$56\pm1 (95\pm2\%)$	$3\pm1~(5\pm2\%)$	26 75
All	All	1180/1680 (70%)	1118 (95%)	62 (5%)	26 75



Mol	Chain	Res	Type	Models (Total)
1	А	315	SER	15
1	А	361	LYS	10
1	А	360	THR	7
1	А	306	ASP	6
1	А	356	ARG	4
1	А	345	GLU	3
1	А	307	ASP	3
1	А	324	LYS	2
1	А	342	SER	2
1	А	302	ASP	2
1	А	303	ASP	2
1	А	295	ASN	2
1	А	309	ARG	1
1	А	333	LYS	1
1	А	308	GLU	1
1	А	299	LYS	1

All 16 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

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

