

Full wwPDB NMR Structure Validation Report (i)

Mar 16, 2022 – 04:13 PM EDT

PDB ID : 6C8U

Title: Solution structure of Musashi2 RRM1

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Deposited on : 2018-01-25

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.

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	1	115	100%



2 Ensemble composition and analysis (i)

This entry contains 10 models. The authors have identified model 1 as representative, based on the following criterion: *lowest energy*. No medoid model was calculated.

The following residues are included in the computation of the global validation metrics.

	Well-defined (core) p	protein residues	
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1834 atoms, of which 910 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called RNA-binding protein Musashi homolog 2.

Mol	Chain	Residues			Aton	ns			Trace
1	1	115	Total	С	Н	N	О	S	0
1	1	115	1834	580	910	171	167	6	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-3	MET	-	expression tag	UNP Q96DH6
1	-2	HIS	-	expression tag	UNP Q96DH6
1	-1	HIS	-	expression tag	UNP Q96DH6
1	0	HIS	-	expression tag	UNP Q96DH6
1	1	HIS	-	expression tag	UNP Q96DH6
1	2	HIS	-	expression tag	UNP Q96DH6
1	3	HIS	-	expression tag	UNP Q96DH6
1	4	SER	-	expression tag	UNP Q96DH6
1	5	THR	-	expression tag	UNP Q96DH6
1	6	SER	-	expression tag	UNP Q96DH6
1	7	VAL	-	expression tag	UNP Q96DH6
1	8	ASP	-	expression tag	UNP Q96DH6
1	9	LEU	-	expression tag	UNP Q96DH6
1	10	GLY	-	expression tag	UNP Q96DH6
1	11	THR	-	expression tag	UNP Q96DH6
1	12	GLU	-	expression tag	UNP Q96DH6
1	13	ASN	-	expression tag	UNP Q96DH6
1	14	LEU	-	expression tag	UNP Q96DH6
1	15	TYR	-	expression tag	UNP Q96DH6
1	16	PHE	-	expression tag	UNP Q96DH6
1	17	GLN	-	expression tag	UNP Q96DH6
1	18	SER	-	expression tag	UNP Q96DH6
1	19	ASN	-	expression tag	UNP Q96DH6
1	20	ALA	-	expression tag	UNP Q96DH6



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.

C	h	ai	in	١.	1:																						10	00°	%																							
M-3	H-2	H-1	НО	H	H2	S4 S4	TS	36	77	D8	J 6	0 F	1 1	E12	N I S	4 17	F16	0.17	S18	N19	A20	G21	K22	M23	F 24	125	G27	801	S29	W30	Q31	T32	S33	D35	236	L37	R38	V40	F41	S42	K43	F44	G45	E46	147 R48	E49	C20	M51	V52	M53	D55	P56
T57	T58	K59	R60	S61	R62	F64	G65	F66	797	T68	100	A7.0	170	P72	A1.0	V7.5	D76	K77	V78	L79	089	1 81	P82	H83	104 100	E85	D87	0 00	K89		191		P93		~	F97	P98	R100	A101	\overline{a}	÷	K104	M105	Ξ,	T107	T109	K110	K111				

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: RNA-binding protein Musashi homolog 2

• Molecule 1: RNA-binding protein Musashi homolog 2

C	Ch.	ıa	iı	1	1	:																								1	00)%)																					1			
M-3	- 1	- 1	ОН	H1	H2	H3	S4	TS	36	2.0	D8	L9	610	T11	E12	N13	L14	Y15	F16	0.17	\$18	N19	A 20	100	KOO	MOS	MZ3	F24 T0F	971	G26	G27				က	က ၊	833	P.34	236		R38	D39	Y40	F41	S42	K43	F44	G45 745	E46	147 R48	E49	C20	M51	V52	M53	ĿΩ	P56
T57	T58	K59	R60	S61	R62	G63	F64	G65	F66	767	T68	F69	A70	D71	P72	A73	S74	V75	D76	K77	V78	L79	080	183	D83	102	103	H84	Egg	L86	D87	288	K89	T90	191	D92	P93	N94 Vor	904	F97	P98	R99		10		9	K104	ဌဒ	V106	1107	T109	Ξ	K111				

4.2.2 Score per residue for model 2

• Molecule 1: RNA-binding protein Musashi homolog 2

Chain 1: 100%



157 158
4.2.3 Score per residue for model 3
• Molecule 1: RNA-binding protein Musashi homolog 2
Chain 1: 100%
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157 158 158 158 158 169 160 160 160 160 160 160 160 160 160 160
4.2.4 Score per residue for model 4
• Molecule 1: RNA-binding protein Musashi homolog 2
Chain 1: 100%
H-3 H-1 H-1 H-1 H-1 H-1 H-2 H-2 H-2 H-3 H-1 H-1 H-1 H-1 H-1 H-2 H-1 H-1 H-2 H-2 H-2 H-3 H-3 H-3 H-3 H-3 H-1 H-1 H-1 H-2 H-2 H-3
157 N - 3 K59 N - 1 K59 N - 1 K60 S61 K62 H0 K62 H0 K64 S4 G65 H5 K65 H5 K66 K6 K70 G10 K77 G10 K77 G11 K77 G11 K77 G11 K78 K72 K78 K72 K78 K72 K79 K72 K79 K72 K79 K72 K79 K79 K89 K29 K89 K89 K89 K94 K100 K40 K110 K41 K111 K15 K111 K111
157 K59 K69 R60 R60 R60 R67 R67 R67 R67 R67 R77 R100 R111 R183 R184 R29 R89 R99 R99 R99 R100 R110 R111
4.2.5 Score per residue for model 5
4.2.5 Score per residue for model 5 • Molecule 1: RNA-binding protein Musashi homolog 2
4.2.5 Score per residue for model 5 • Molecule 1: RNA-binding protein Musashi homolog 2 Chain 1: 100%

 \bullet Molecule 1: RNA-binding protein Musashi homolog2



Chain	1: 100%	
M-3 H-2 H-1 H0	H2 H3 H3 H3 H3 H3 H3 H3 H3 H3 H3	M5.3 R5.4 D5.5 P5.6
T57 T58 K59 R60 S61	R62 G63 G64 G65 F66 V67 V67 T68 A70 A70 A71 B71 B71 B72 B73 B74 B73 B74 B74 B75 B76 B77 B76 B77 B77 B77 B77 B77 B77 B77	
4.2.7	Score per residue for model 7	
• Mole	ecule 1: RNA-binding protein Musashi homolog 2	
Chain	1: 100%	
M-3 H-2 H-1 H1	H2 H2 H3 H43 H43 H43 H43 H43 H43 H43 H43 H43	R54 D55 P56
T57 T58 K59 R60 S61	R62 663 663 764 764 765 766 770 771 773 774 775 777 777 777 777 777 777 777 777	
4.2.8	Score per residue for model 8	
• Mole	ecule 1: RNA-binding protein Musashi homolog 2	
Chain	1: 100%	
M-3 H-1 H0 H1	H2 H3 H4 H5 H5 H6 H6 H7 H7 H7 H7 H7 H7 H7 H7	R54 D55 P56
T57 T58 K59 R60 S61	R62 663 664 665 766 766 770 773 773 773 774 774 777 777 777 777 777	
4.2.9	Score per residue for model 9	
• Mole	ecule 1: RNA-binding protein Musashi homolog 2	
Chain	1: 100%	
M-3 H-2 H0 H1	H2 H	M5.3 R5.4 D5.5 P5.6
57 58 59 60 61	R62 F64 F65 F66 F66 F66 F66 F69 F70 D71 F69 F73 F74 V78 V78 V77 V78 V78 V78 V78 V78 F82 B83 E88 E88 E88 E88 E88 E88 F89 F97 F97 F97 F97 F97 F97 F97 F97 F97 F9	



4.2.10 Score per residue for model 10

 \bullet Molecule 1: RNA-binding protein Musashi homolog2

Chain 1: 100%

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5 Refinement protocol and experimental data overview (i)



The models were refined using the following method: simulated annealing.

Of the 100 calculated structures, 10 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	refinement	1.3
CNS	structure calculation	1.3

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1326
Number of shifts mapped to atoms	1326
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	



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	1	0	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	1	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	1	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)

The completeness of assignment taking into account all chemical shift lists is undefined for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: working cs.cif

Chemical shift list name: MSI2-RRM1_assignments_unassigned_deleted_180125.txt

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1326
Number of shifts mapped to atoms	1326
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\mathrm{C}_{\alpha}$	108	-0.40 ± 0.10	None needed ($< 0.5 \text{ ppm}$)
$^{13}C_{\beta}$	100	0.18 ± 0.05	None needed ($< 0.5 \text{ ppm}$)
¹³ C′	108	0.05 ± 0.15	None needed (< 0.5 ppm)
^{15}N	98	0.13 ± 0.42	None needed ($< 0.5 \text{ ppm}$)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is —%, i.e. 0 atoms were assigned a chemical shift out of a possible 0. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathbf{C}$	$^{15}\mathbf{N}$
Backbone	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Sidechain	0/0 (%)	0/0 (—%)	0/0 (%)	0/0 (%)

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	Total	$^{1}{ m H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Aromatic	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Overall	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1199 atoms were assigned a chemical shift out of a possible 1462. 8 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}{ m H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Backbone	520/561 (93%)	$206/223 \ (92\%)$	$216/230 \ (94\%)$	98/108 (91%)
Sidechain	601/737 (82%)	374/440 (85%)	$219/258 \ (85\%)$	8/39 (21%)
Aromatic	78/164 (48%)	45/86 (52%)	32/61 (52%)	1/17 (6%)
Overall	1199/1462 (82%)	625/749 (83%)	467/549 (85%)	107/164 (65%)

7.1.4 Statistically unusual chemical shifts (i)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
???	1	74	SER	HB3	2.39	5.25 - 2.45	-5.2

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports random coil index values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain 1:



