

Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 10:52 pm BST

PDB ID	:	2L0I
Title	:	Solution structure of Rtt103 CTD-interacting domain bound to a Ser2 phos-
		phorylated CTD peptide
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Deposited on	:	2010-07-06

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 (1)) were used in the production of this report:

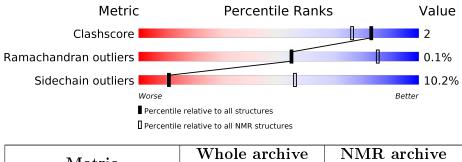
Cyrange	:	Kirchner and Güntert (2011)
$\operatorname{NmrClust}$:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as 541 be (2020)
Percentile statistics		
RCI	:	$v_1n_11_5_13_A$ (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
${ m ShiftChecker}$:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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	(#Entries)	(#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	142	80%	10% 6% •
2	В	14	64%	36%



2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 3 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 mod										
1	A:7-A:134 (128)	0.24	3							

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 2 clusters and 4 single-model clusters were found.

Cluster number	Models
1	3, 4, 8, 9
2	1, 2
Single-model clusters	5; 6; 7; 10



3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2378 atoms, of which 1202 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Regulator of Ty1 transposition protein 103.

Mol	Chain	Residues		Atoms									
1	Λ	136	Total	С	Η	Ν	0	S	0				
	A	190	2252	703	1145	199	202	3	0				

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference					
А	2	ALA	PRO	CLONING ARTIFACT	UNP Q05543					
A	132	ALA	-	EXPRESSION TAG	UNP Q05543					
А	133	ALA	-	EXPRESSION TAG	UNP Q05543					
A	134	ALA	-	EXPRESSION TAG	UNP Q05543					
А	135	LEU	-	EXPRESSION TAG	UNP Q05543					
А	136	GLU	-	EXPRESSION TAG	UNP Q05543					
A	137	HIS	-	EXPRESSION TAG	UNP Q05543					
А	138	HIS	-	EXPRESSION TAG	UNP Q05543					
А	139	HIS	-	EXPRESSION TAG	UNP Q05543					
А	140	HIS	-	EXPRESSION TAG	UNP Q05543					
А	141	HIS	-	EXPRESSION TAG	UNP Q05543					
А	142	HIS	-	EXPRESSION TAG	UNP Q05543					

• Molecule 2 is a protein called DNA-directed RNA polymerase.

Mol	Chain	Residues		Trace					
0	D	0	Total	С	Η	Ν	Ο	Р	0
	D	9	126	40	57	9	19	1	0

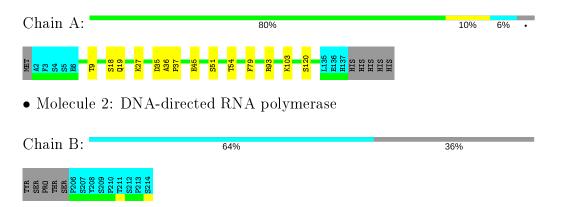


4 Residue-property plots (i)

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: Regulator of Ty1 transposition protein 103

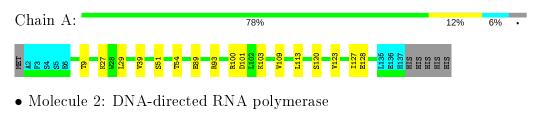


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Regulator of Ty1 transposition protein 103



Chain B: 64% 36%



4.2.2 Score per residue for model 2

• Molecule 1: Regulator of Ty1 transposition protein 103

Chain A:		74%					16%	6%	·
A B B B B B B B B B B B B B B B B B B B	T10 Q19 Q19 A36 A36 K38 K38 S51 S51 T54	H66 Q70 F79	E89 B93	D101 L102 K103	V109 V110 N111	N117 D126 1127 E128	R129 S130 L131 L135	E136 H137 HIS HIS	SIH SIH SIH
• Molecule	• Molecule 2: DNA-directed RNA polymerase								
Chain B:		64%					36%		_
TYR SER PRO THR SER P206 S207 Y207	5200 7210 7211 7213 7213 7213 7213								

4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: Regulator of Ty1 transposition protein 103

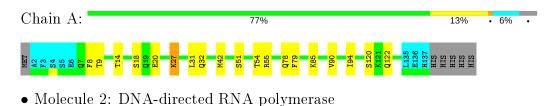
Chain A:								75	%										15%		•	• 6	%	•
MET A2 S5 E6 E6	T9	E16	019	 K27 W28	L31 Q32	D35	 K38	S51	T54	L61	078	F79	E89	R93	N111	<mark>\$120</mark>	V124	E128	L135 E136	ကျ	HIS		SIH	

• Molecule 2: DNA-directed RNA polymerase

Chain B:	64%	36%
TYR PRO PRO PRO PRO P206 P206 P210 P2111 P2113 P2113 P2113		

4.2.4 Score per residue for model 4

• Molecule 1: Regulator of Ty1 transposition protein 103

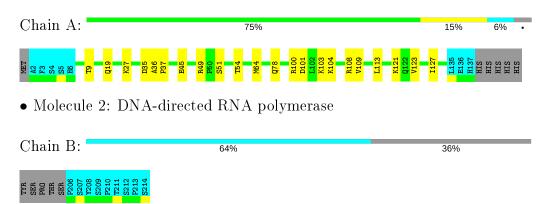


Chain B:	64%	36%
TYR SER PRO FRO FRO FRO F200 F200 F211 F211 F211 F213 F213 F213 F214 F213		



4.2.5 Score per residue for model 5

• Molecule 1: Regulator of Ty1 transposition protein 103



4.2.6 Score per residue for model 6

• Molecule 1: Regulator of Ty1 transposition protein 103

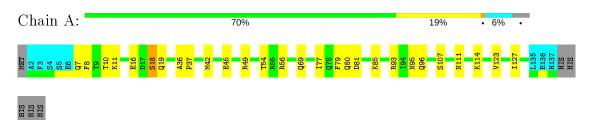
Chain A:									75%	6									15%		69	%	•
MET A 2 S 3 E 6 E 6	T9	L15	<mark>S18</mark> Q19	122	D35 A36	P37	E41	E45	R49 P50	S51	T54	N65	<mark>069</mark>	K85	R93	<mark>196</mark>	P99 R100	<mark>S107</mark>	L135 E136 H137	SIS	SIH	Η.	

• Molecule 2: DNA-directed RNA polymerase

Chain B:	64%	36%
TYR SER PRO THR SER SER SE0 Y208 S207 Y208 S209 P210 S212 S212 S214 S214		

4.2.7 Score per residue for model 7

• Molecule 1: Regulator of Ty1 transposition protein 103



• Molecule 2: DNA-directed RNA polymerase

Chain B: 64% 36%



TYR SER PRO THR SER SER 7206 S207 7208 S209 P210 T211 T211 T211 S212 S214 S214

4.2.8 Score per residue for model 8

• Molecule 1: Regulator of Ty1 transposition protein 103

Chain A: 79%	11%	• 6%	·
施士 113 114 114 114 114 114 114 114			
• Molecule 2: DNA-directed RNA polymerase			

Chain B:	64%	36%
TYR SER THR SER S200 S200 S200 S211 S211 S212 S212 S212		

4.2.9 Score per residue for model 9

 \bullet Molecule 1: Regulator of Ty1 transposition protein 103

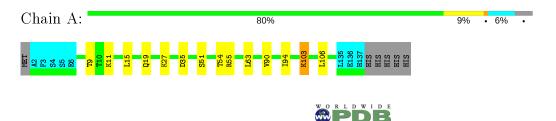
Chain A:	65%		24% •	6% •
MET 85 85 85 85 85 85 85 81 81 81 81 81 81 81 81 81 81 81 81 81	K2 K2 131 131 131 131 131 133 133 133 149 149 149 149 149 149 149 149 149 149	1154 1155 1161 1161 1161 1161 1172 1173 1173 1173 1173 1173 1173 117	K85 E89 V90 R93 194	L106 S120 K121 Q122 D125 D126
R129 5130 1131 1135 1135 1135 1135 1135 1135				

• Molecule 2: DNA-directed RNA polymerase

Chain B:	64%	36%
TYR SER FRO THR SER SER S207 S209 S209 S209 S212 S214 S213 S214 S213 S214		

4.2.10 Score per residue for model 10

• Molecule 1: Regulator of Ty1 transposition protein 103

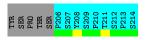


• Molecule 2: DNA-directed RNA polymerase

64%

Chain B:

36%





5 Refinement protocol and experimental data overview (i)

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

Of the 200 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	structure solution	1.2
CNS	structure solution	1.2
CNS	refinement	1.2

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 (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP

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	1043	1090	1090	5 ± 2
2	В	0	0	0	0 ± 0
All	All	10430	10900	10900	51

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.

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

Atom 1	Atom D	$Cleat (\lambda)$	Distance(Å)	Mod	lels
Atom-1	Atom-2	Clash(Å)	Distance(Å)	Worst	Total
1:A:89:GLU:O	1:A:93:ARG:HG2	0.53	2.04	1	4
1:A:27:LYS:O	1:A:31:LEU:HG	0.51	2.05	4	3
1:A:8:PHE:HB3	1:A:42:MET:SD	0.50	2.47	4	3
1:A:93:ARG:O	1:A:96:GLN:HG2	0.49	2.08	6	2
1:A:29:LEU:HD11	1:A:39:VAL:HG11	0.48	1.86	1	1
1:A:109:VAL:O	1:A:113:LEU:HG	0.47	2.09	5	2
1:A:37:PRO:O	1:A:41:GLU:HG2	0.47	2.09	6	1
1:A:7:GLN:O	1:A:11:LYS:HG2	0.47	2.09	9	2
1:A:45:GLU:O	1:A:49:ARG:HG2	0.47	2.09	7	1
1:A:107:SER:O	1:A:111:ASN:HB2	0.46	2.10	7	1
1:A:77:ILE:HA	1:A:80:GLN:OE1	0.45	2.11	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	\mathbf{Models}	
Atom-1	Atom-2		Distance(A)	Worst	Total
1:A:81:ASP:O	1:A:85:LYS:HE3	0.45	2.12	7	2
1:A:66:HIS:O	1:A:70:GLN:HG2	0.45	2.12	2	1
1:A:45:GLU:O	1:A:49:ARG:HG3	0.44	2.13	9	3
1:A:103:LYS:O	1:A:106:LEU:HG	0.44	2.13	10	1
1:A:36:ALA:N	1:A:37:PRO:HD2	0.43	2.28	5	5
1:A:104:LYS:O	1:A:108:ARG:HG3	0.43	2.13	5	1
1:A:18:SER:HB2	1:A:21:SER:OG	0.43	2.14	8	1
1:A:123:VAL:O	1:A:127:ILE:HG13	0.42	2.14	7	3
1:A:90:VAL:O	1:A:94:ILE:HG12	0.42	2.15	10	3
1:A:18:SER:O	1:A:22:ILE:HG12	0.42	2.14	6	1
1:A:126:ASP:O	1:A:129:ARG:HG2	0.42	2.14	2	2
1:A:65:ASN:O	1:A:69:GLN:HB2	0.41	2.15	6	1
1:A:11:LYS:O	1:A:15:LEU:HG	0.41	2.15	10	1
1:A:100:ARG:O	1:A:103:LYS:HG2	0.41	2.16	1	1
1:A:127:ILE:O	1:A:131:LEU:HG	0.41	2.15	2	1
1:A:28:TRP:O	1:A:32:GLN:HG2	0.41	2.16	3	1
1:A:44:LYS:O	1:A:48:LEU:HG	0.40	2.16	8	1
1:A:124:VAL:O	1:A:128:GLU:HG2	0.40	2.16	3	1

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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	128/142~(90%)	$126 \pm 1 \ (98 \pm 1\%)$	$2\pm1~(2\pm1\%)$	0±0 (0±0%)	54 85
2	В	0	-	-	-	-
All	All	1280/1560~(82%)	1255~(98%)	24~(2%)	$1 \ (0\%)$	54 85

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	А	99	PRO	1



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	А	115/128~(90%)	$103 \pm 4 \ (90 \pm 3\%)$	$12\pm4~(10\pm3\%)$	11 56	
2	В	0	-	-	-	
All	All	1150/1410~(82%)	1033~(90%)	117~(10%)	11 56	

All 43 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	А	54	THR	10
1	А	9	THR	9
1	А	51	SER	8
1	А	35	ASP	7
1	А	19	GLN	6
1	А	120	SER	5
1	А	79	PHE	5
1	А	10	THR	4
1	А	78	GLN	4
1	А	55	ARG	4
1	А	18	SER	4
1	А	27	LYS	4
1	А	38	LYS	3
1	А	61	LEU	3
1	А	103	LYS	3
1	А	101	ASP	3
1	А	100	ARG	2
1	А	121	LYS	2
1	А	85	LYS	2
1	А	122	GLN	2
1	А	125	ASN	2
1	А	16	GLU	2
1	А	111	ASN	2
1	А	14	THR	2
1	А	95	ASN	1
1	А	45	GLU	1
1	А	69	GLN	1
1	А	56	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	А	15	LEU	1
1	А	63	LEU	1
1	А	131	LEU	1
1	А	20	GLU	1
1	А	117	ASN	1
1	А	128	GLU	1
1	А	75	LYS	1
1	А	64	MET	1
1	А	109	VAL	1
1	А	107	SER	1
1	А	12	LEU	1
1	А	114	LYS	1
1	А	72	LYS	1
1	А	32	GLN	1
1	А	106	LEU	1

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6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Tune	Chain	Dec	Tink		gths	
	туре	Cham	nes		Counts	RMSZ	#Z>2
2	SEP	В	209	2	8,9,10	$0.99{\pm}0.02$	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of



the bond angles.

	Mol	Type	Chain	Dec	Link	Bond angles		
				nes		Counts	RMSZ	#Z>2
	2	SEP	В	209	2	8,12,14	2.11 ± 0.05	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	В	209	2	-	$0\pm 0,5,8,10$	-

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no carbohydrates 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

