



# wwPDB NMR Structure Validation Summary Report ⓘ

Apr 26, 2016 – 05:51 PM BST

PDB ID : 1WA7  
Title : SH3 DOMAIN OF HUMAN LYN TYROSINE KINASE IN COMPLEX WITH  
A HERPESVIRAL LIGAND  
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Deposited on : 2004-10-25

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

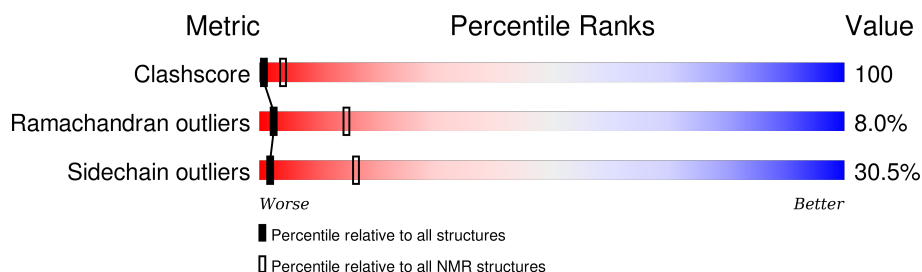
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 87%.

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	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	65	
2	B	22	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:11-A:65, B:179-B:187 (64)	0.18	8

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. No single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1306 atoms, of which 651 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TYROSINE-PROTEIN KINASE LYN.

Mol	Chain	Residues	Atoms						Trace
1	A	60	Total	C	H	N	O	S	0
			972	317	486	78	90	1	

- Molecule 2 is a protein called HYPOTHETICAL 28.7 KDA PROTEIN IN DHFR 3'REGION (ORF1).

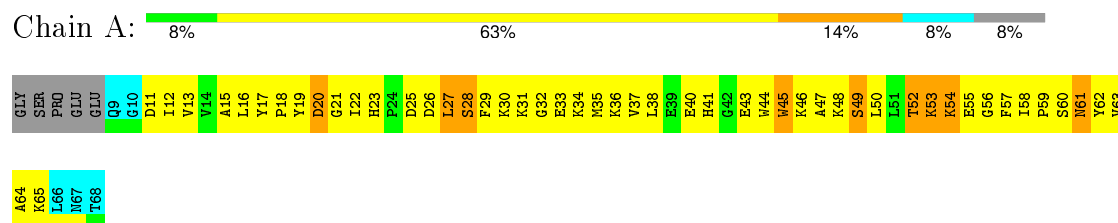
Mol	Chain	Residues	Atoms						Trace
2	B	22	Total	C	H	N	O	S	0
			334	107	165	31	30	1	

## 4 Residue-property plots [i](#)

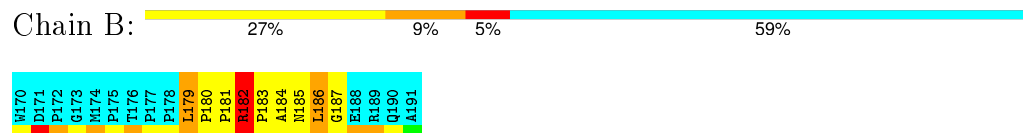
### 4.1 Average score per residue in the NMR ensemble

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: TYROSINE-PROTEIN KINASE LYN



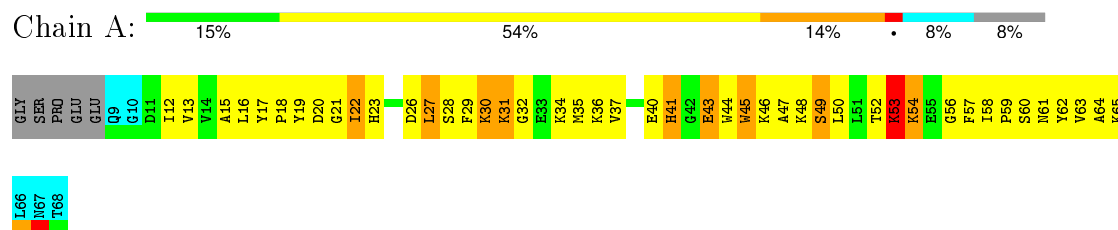
- Molecule 2: HYPOTHETICAL 28.7 KDA PROTEIN IN DHFR 3'REGION (ORF1)



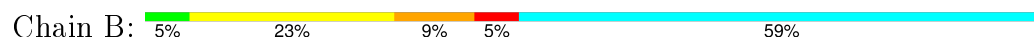
### 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 8. Colouring as in section 4.1 above.

- Molecule 1: TYROSINE-PROTEIN KINASE LYN



- Molecule 2: HYPOTHETICAL 28.7 KDA PROTEIN IN DHFR 3'REGION (ORF1)



H170	D171	P172	G173	M174	P175	T176	P177	P178	L179	P180	P181	R182	P183	A184	N185	L186	G187	F188	A189	Q190	A191
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## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *XPLOR*.

Of the 60 calculated structures, 20 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
X-PLOR 3.851	refinement	
NMRVIEW	structure solution	

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)	BMRB entry 6456
Number of chemical shift lists	2
Total number of shifts	1047
Number of shifts mapped to atoms	1008
Number of unparsed shifts	3
Number of shifts with mapping errors	36
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

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
2	B	0.0±0.0	0.9±0.3
All	All	0	18

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
2	B	182	ARG	Sidechain	18

### 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	A	449	451	451	92±7
2	B	65	70	70	42±3
All	All	10280	10420	10420	2069

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 100.

5 of 434 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LEU:HD11	1:A:64:ALA:HB2	1.09	1.13	17	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:TYR:CE2	2:B:179:LEU:HD21	1.07	1.84	13	6
1:A:62:TYR:CD2	2:B:179:LEU:HD21	0.99	1.92	13	6
2:B:186:LEU:HD23	2:B:187:GLY:N	0.98	1.73	20	1
1:A:16:LEU:HD11	1:A:64:ALA:CB	0.97	1.88	20	18

## 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	55/65 (85%)	47±1 (85±1%)	5±1 (9±1%)	3±1 (5±2%)	4	24
2	B	9/22 (41%)	4±1 (46±8%)	3±1 (31±9%)	2±1 (23±8%)	0	1
All	All	1280/1740 (74%)	1019 (80%)	159 (12%)	102 (8%)	2	15

5 of 12 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	53	LYS	20
2	B	182	ARG	19
1	A	21	GLY	18
2	B	186	LEU	17
1	A	41	HIS	9

### 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	48/56 (86%)	33±3 (69±6%)	15±3 (31±6%)	2	15
2	B	7/18 (39%)	5±1 (75±9%)	2±1 (25±9%)	3	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1100/1480 (74%)	764 (69%)	336 (31%)	<b>2</b> <b>16</b>

5 of 39 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	A	27	LEU	20
1	A	45	TRP	20
1	A	31	LYS	19
1	A	46	LYS	15
2	B	179	LEU	14

### 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 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

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 85% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 6456

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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	805
Number of shifts mapped to atoms	774
Number of unparsed shifts	3
Number of shifts with mapping errors	28
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 3 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
33	A	4	GLY	HA2	3.98	0.02	1
34	A	4	GLY	HA3	3.98	0.02	1
35	A	4	GLY	CA	45.12	0.2	1

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. First 5 (of 28) occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	3	LEU	CD1	25.52	0.2	1
A	2	PRO	HA	4.49	0.02	1
A	2	PRO	HB3	1.96	0.02	2
A	3	LEU	HD21	0.9	0.02	1
A	2	PRO	CB	32.38	0.2	1

### 7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	67	$-0.17 \pm 0.28$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	60	$-0.14 \pm 0.36$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	—
$^{15}\text{N}$	62	$0.24 \pm 0.50$	None needed ( $< 0.5$ ppm)

### 7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 75%, i.e. 613 atoms were assigned a chemical shift out of a possible 812. 1 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	214/308 (69%)	107/122 (88%)	55/128 (43%)	52/58 (90%)
Sidechain	325/424 (77%)	203/252 (81%)	121/158 (77%)	1/14 (7%)
Aromatic	74/80 (92%)	38/42 (90%)	34/34 (100%)	2/4 (50%)
Overall	613/812 (75%)	348/416 (84%)	210/320 (66%)	55/76 (72%)

### 7.1.4 Statistically unusual chemical shifts ⓘ

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.

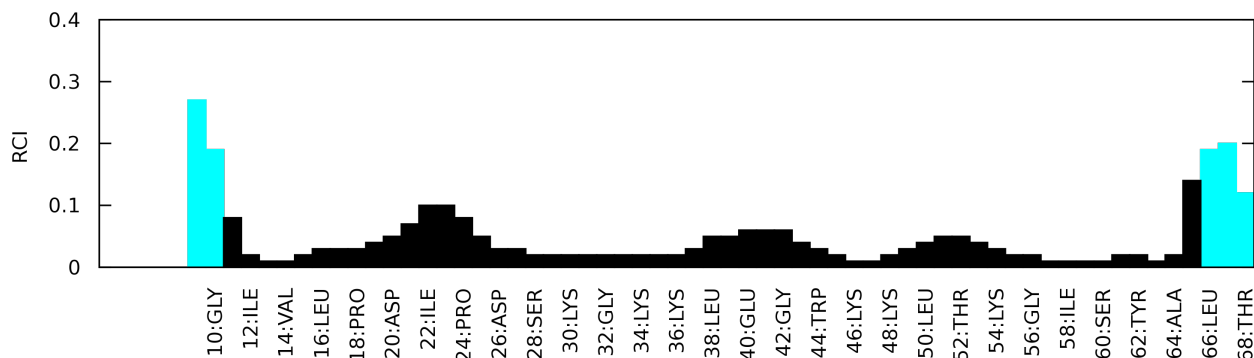
Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	60	SER	HB3	1.49	5.25 – 2.45	-8.4
1	A	40	GLU	HG3	0.74	3.31 – 1.21	-7.2
1	A	60	SER	HB2	2.06	5.18 – 2.58	-7.0
1	A	59	PRO	HG3	0.06	3.56 – 0.26	-5.6
1	A	59	PRO	HB2	0.15	3.82 – 0.32	-5.5
1	A	19	TYR	HB3	0.85	4.75 – 0.95	-5.3

### 7.1.5 Random Coil Index (RCI) plots ⓘ

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 A:



## 7.2 Chemical shift list 2

File name: BMRB entry 6456

Chemical shift list name: *assigned\_chem\_shift\_list\_2*

### 7.2.1 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	242
Number of shifts mapped to atoms	234
Number of unparsed shifts	0
Number of shifts with mapping errors	8
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. First 5 (of 8) occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	1	THR	HG21	1.21	0.02	1
B	1	THR	HG22	1.21	0.02	1
B	1	THR	CG2	21.74	0.2	1
B	1	THR	CA	62.45	0.2	1
B	1	THR	HB	4.15	0.02	1

### 7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, <i>ppm</i>	Suggested action
$^{13}\text{C}_\alpha$	23	$0.76 \pm 0.21$	Should be applied
$^{13}\text{C}_\beta$	21	$0.52 \pm 0.23$	Should be applied
$^{13}\text{C}'$	0	—	—
$^{15}\text{N}$	15	$-2.05 \pm 0.65$	Should be applied

### 7.2.3 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 11%, i.e. 92 atoms were assigned a chemical shift out of a possible 812. 1 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	30/308 (10%)	15/122 (12%)	9/128 (7%)	6/58 (10%)
Sidechain	62/424 (15%)	39/252 (15%)	22/158 (14%)	1/14 (7%)
Aromatic	0/80 (0%)	0/42 (0%)	0/34 (0%)	0/4 (0%)
Overall	92/812 (11%)	54/416 (13%)	31/320 (10%)	7/76 (9%)

### 7.2.4 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, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
2	B	182	ARG	HD2	1.76	4.27 – 1.97	-5.9
2	B	182	ARG	HD3	1.76	4.36 – 1.86	-5.4
2	B	177	PRO	HD2	1.76	5.45 – 1.85	-5.2

### 7.2.5 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 B:

