



# wwPDB NMR Structure Validation Summary Report ⓘ

Apr 27, 2016 – 04:25 AM BST

PDB ID : 2PLD  
Title : NUCLEAR MAGNETIC RESONANCE STRUCTURE OF AN SH2 DOMAIN OF PHOSPHOLIPASE C-GAMMA1 COMPLEXED WITH A HIGH AFFINITY BINDING PEPTIDE  
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Deposited on : 1994-08-19

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 : 1.7.1 (RC1), CSD as537be (2016)  
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

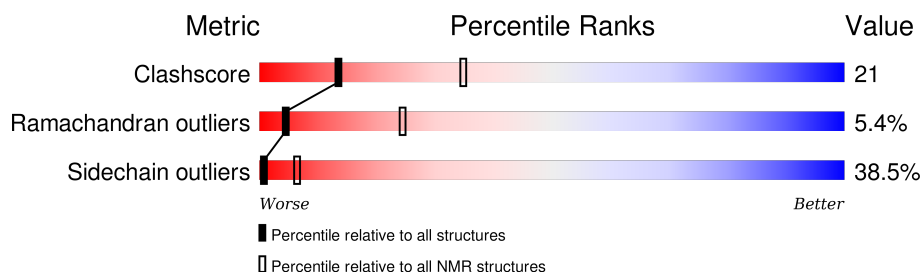
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 89%.

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	105	
2	B	12	

## 2 Ensemble composition and analysis ⓘ

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

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1906 atoms, of which 941 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PHOSPHOLIPASE C GAMMA-1, C-TERMINAL SH2 DOMAIN.

Mol	Chain	Residues	Atoms						Trace
1	A	105	Total	C	H	N	O	S	0
			1708	539	846	159	159	5	

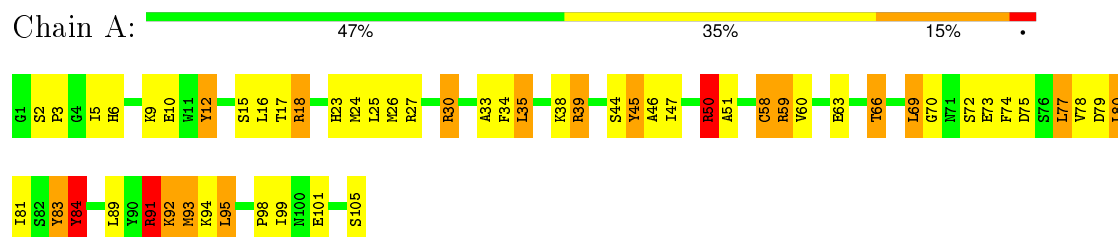
- Molecule 2 is a protein called PHOSPHOPEPTIDE FROM PDGF.

Mol	Chain	Residues	Atoms						Trace
2	B	12	Total	C	H	N	O	P	0
			198	64	95	14	24	1	

## 4 Residue-property plots

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: PHOSPHOLIPASE C GAMMA-1, C-TERMINAL SH2 DOMAIN



- Molecule 2: PHOSPHOPEPTIDE FROM PDGF



## 5 Refinement protocol and experimental data overview

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	

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 5310, BMRB entry 5318
Number of chemical shift lists	3
Total number of shifts	1570
Number of shifts mapped to atoms	1570
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

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

## 6 Model quality

### 6.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.10	0/882 (0.0%)	1.01	1/1183 (0.1%)
2	B	0.91	0/88 (0.0%)	0.95	0/118 (0.0%)
All	All	1.08	0/970 (0.0%)	1.01	1/1301 (0.1%)

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
1	A	0	7
All	All	0	7

There are no bond-length outliers.

All angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	TYR	CB-CG-CD2	-5.32	117.81	121.00

There are no chirality outliers.

5 of 7 planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	30	ARG	Sidechain
1	A	18	ARG	Sidechain
1	A	39	ARG	Sidechain
1	A	27	ARG	Sidechain
1	A	50	ARG	Sidechain

## 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	862	846	846	39
2	B	103	95	95	5
All	All	965	941	941	40

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 21.

5 of 40 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:84:TYR:CZ	1:A:89:LEU:HD13	0.84	2.08
1:A:25:LEU:HD21	1:A:35:LEU:HD11	0.78	1.52
1:A:25:LEU:HD21	1:A:35:LEU:CD1	0.71	2.16
1:A:25:LEU:HD22	1:A:50:ARG:HD2	0.70	1.62
1:A:69:LEU:HB2	1:A:80:LEU:HD11	0.67	1.65

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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	103/105 (98%)	78 (76%)	20 (19%)	5 (5%)	5	27
2	B	9/12 (75%)	6 (67%)	2 (22%)	1 (11%)	1	9
All	All	112/117 (96%)	84 (75%)	22 (20%)	6 (5%)	4	24

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

Mol	Chain	Res	Type
1	A	44	SER

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Mol	Chain	Res	Type
1	A	92	LYS
1	A	70	GLY
2	B	10	ASP
1	A	6	HIS

### 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	93/93 (100%)	57 (61%)	36 (39%)	1	6
2	B	11/11 (100%)	7 (64%)	4 (36%)	1	8
All	All	104/104 (100%)	64 (62%)	40 (38%)	1	6

5 of 40 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	69	LEU
1	A	105	SER
1	A	23	HIS
2	B	3	ASP
1	A	16	LEU

### 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	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	PTR	B	4	2	13,16,17	0.69	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	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	PTR	B	4	2	19,22,24	0.85	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	PTR	B	4	2	-	0,9,11,13	0,1,1,1

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

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 89% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 5310

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	1297
Number of shifts mapped to atoms	1297
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	103	$-0.07 \pm 0.19$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	98	$0.31 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	97	$0.35 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	98	$-0.20 \pm 0.26$	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 85%, i.e. 1279 atoms were assigned a chemical shift out of a possible 1509. 13 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	499/564 (88%)	201/224 (90%)	200/232 (86%)	98/108 (91%)
Sidechain	675/818 (83%)	415/488 (85%)	225/285 (79%)	35/45 (78%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	105/127 (83%)	52/65 (80%)	47/51 (92%)	6/11 (55%)
Overall	1279/1509 (85%)	668/777 (86%)	472/568 (83%)	139/164 (85%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

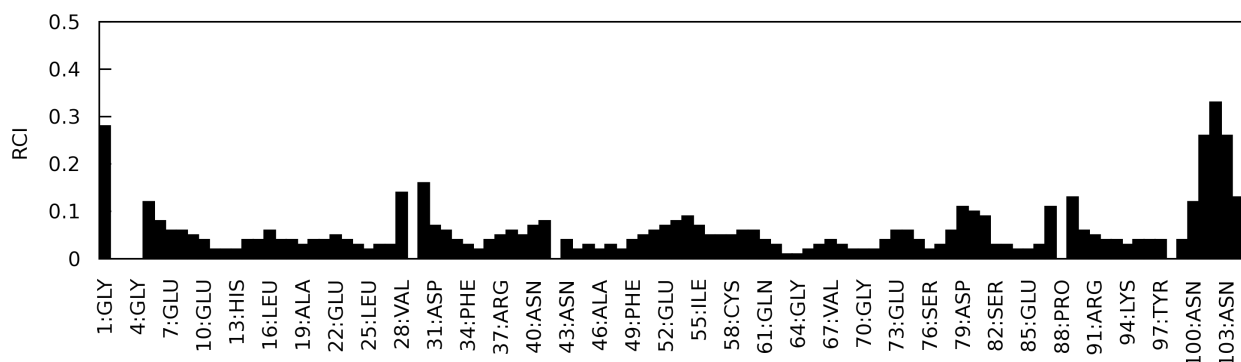
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	37	ARG	HH21	9.70	9.06 – 4.56	6.4
1	A	56	LYS	HB2	0.18	3.03 – 0.53	-6.4
1	A	37	ARG	HH11	9.45	9.21 – 4.61	5.5

#### 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 5318

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

### 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	196
Number of shifts mapped to atoms	196
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	—
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	0	—	—
$^{15}\text{N}$	98	$-0.58 \pm 0.29$	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 13%, i.e. 196 atoms were assigned a chemical shift out of a possible 1504. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	196/564 (35%)	98/224 (44%)	0/232 (0%)	98/108 (91%)
Sidechain	0/818 (0%)	0/488 (0%)	0/285 (0%)	0/45 (0%)
Aromatic	0/122 (0%)	0/65 (0%)	0/51 (0%)	0/6 (0%)
Overall	196/1504 (13%)	98/777 (13%)	0/568 (0%)	98/159 (62%)

### 7.2.4 Statistically unusual chemical shifts [i](#)

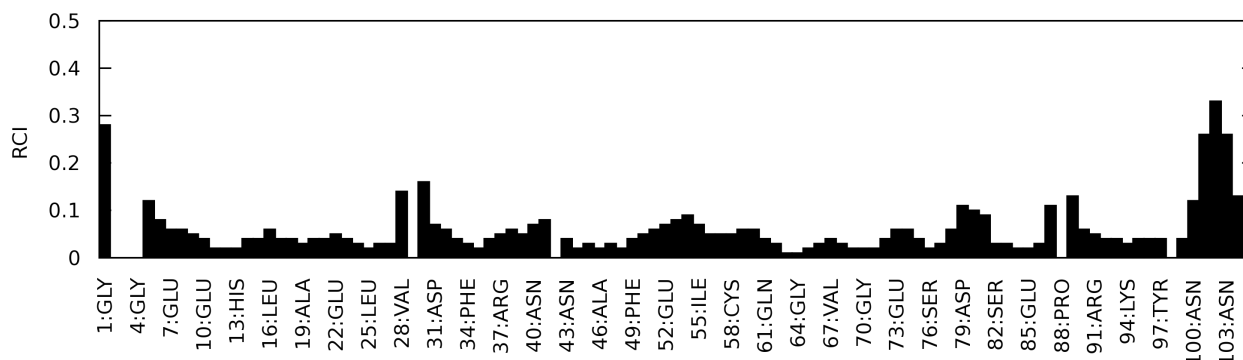
There are no statistically unusual chemical shifts.

### 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 A:



## 7.3 Chemical shift list 3

File name: BMRB entry 5310

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

### 7.3.1 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	77
Number of shifts mapped to atoms	77
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

No chemical shift referencing corrections were calculated (not enough data).

### 7.3.3 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 4%, i.e. 67 atoms were assigned a chemical shift out of a possible 1504. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	17/564 (3%)	17/224 (8%)	0/232 (0%)	0/108 (0%)
Sidechain	50/818 (6%)	50/488 (10%)	0/285 (0%)	0/45 (0%)
Aromatic	0/122 (0%)	0/65 (0%)	0/51 (0%)	0/6 (0%)
Overall	67/1504 (4%)	67/777 (9%)	0/568 (0%)	0/159 (0%)

### 7.3.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

### 7.3.5 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:

