



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 27, 2016 – 04:45 AM BST

PDB ID : 2QMV
Title : High Resolution Structure of Peroxisome Proliferation-Activated Receptor
gamma and Characterisation of its Interaction with the Co-activator Tran-
scriptional Intermediary Factor 2
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Deposited on : 2007-07-17

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at 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.

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

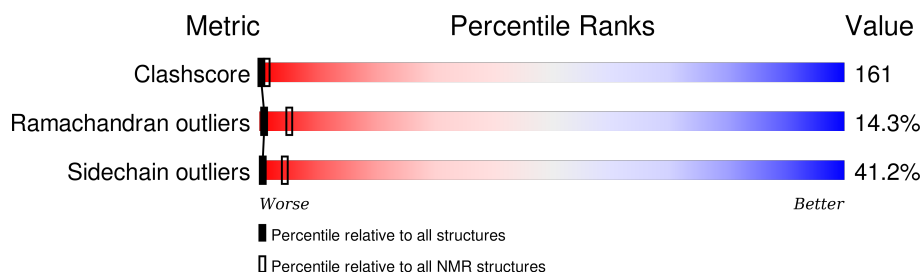
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 35%.

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 ≥ 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	270	<p>47% 33% 16%</p>

2 Ensemble composition and analysis ⓘ

This entry contains 9 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:210-A:239, A:246-A:249, A:276-A:341, A:346-A:473 (228)	0.60	7

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 5 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 4441 atoms, of which 2276 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

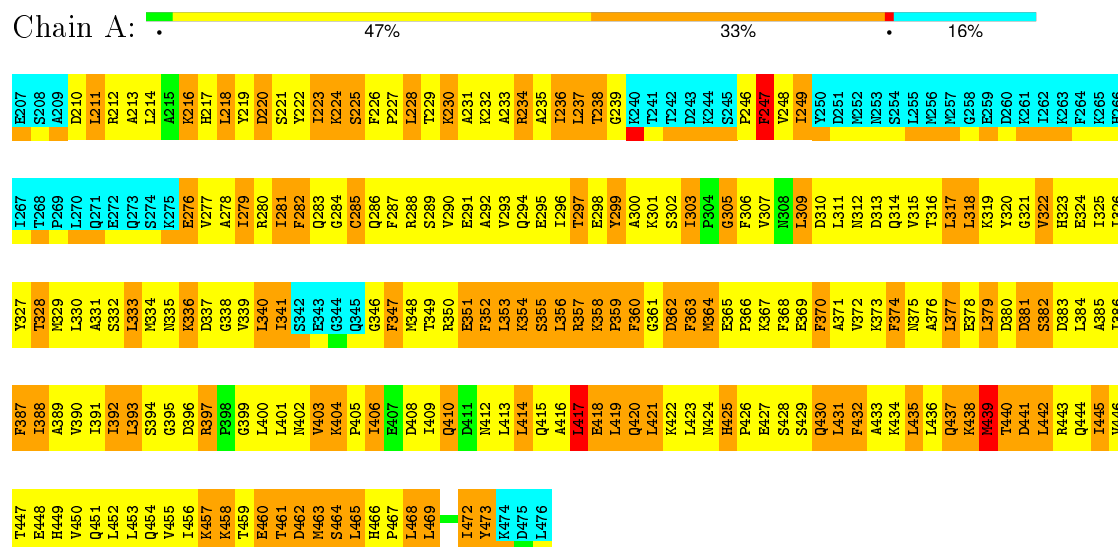
Mol	Chain	Residues	Atoms						Trace
1	A	270	Total	C	H	N	O	S	0
			4441	1397	2276	354	404	10	

4 Residue-property plots

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.

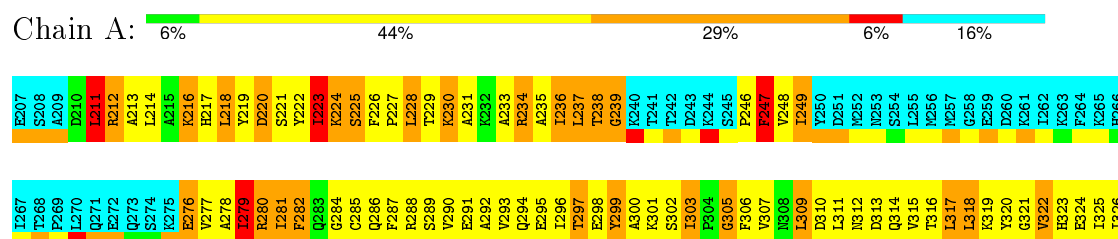
- Molecule 1: Peroxisome proliferator-activated receptor gamma



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

The representative model is number 7. Colouring as in section 4.1 above.

- Molecule 1: Peroxisome proliferator-activated receptor gamma



T447	F387	Y327
E448	I388	I328
H449	A389	I329
V450	V390	I330
Q451	I391	A331
L452	I392	S332
L453	I393	I333
Q454	S394	I334
V455	G395	I335
I456	D396	I336
K457	R397	D337
K458	P398	G338
T459	G399	V339
E460	L400	I340
T461	L401	I341
D462	N402	S342
N463	V403	E343
S464	K404	E344
L465	P405	I345
H466	I406	G346
P467	E407	F347
L468	D408	I348
L469	I409	T349
	Q410	R350
I472	D411	E351
Y473	N412	F352
K474	L413	I353
D475	L414	K354
L476	Q415	S355
	A416	L356
	L417	R357
	E418	K358
	L419	F359
	Q420	F360
	L421	G361
	K422	D362
	L423	F363
	N424	I364
	H425	E365
	P426	P366
	E427	K367
	S428	F368
	S429	E369
	Q430	F370
	L431	A371
	F432	V372
	A433	K373
	K434	F374
	L435	I375
	L436	A376
	Q437	L377
	K438	E378
	M439	L379
	T440	D380
	D441	D381
	L442	S382
	R443	D383
	Q444	I384
	I445	A385
	V446	I386

5 Refinement protocol and experimental data overview

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

Of the 1024 calculated structures, 9 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
DYANA	structure solution	1.5
DYANA	refinement	1.5

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 6549
Number of chemical shift lists	1
Total number of shifts	1142
Number of shifts mapped to atoms	1142
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	35%

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](#)

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	A	1831	1935	1901	603±40
All	All	16479	17415	17109	5423

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 161.

5 of 2447 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:402:ASN:O	1:A:406:ILE:CD1	1.28	1.80	4	8
1:A:221:SER:O	1:A:299:TYR:CD2	1.26	1.88	5	1
1:A:402:ASN:O	1:A:405:PRO:HD2	1.26	1.24	4	8
1:A:402:ASN:O	1:A:406:ILE:HD13	1.22	1.34	2	3
1:A:359:PRO:O	1:A:361:GLY:N	1.16	1.78	2	9

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	228/270 (84%)	137±2 (60±1%)	59±3 (26±1%)	33±3 (14±1%)	1	5
All	All	2052/2430 (84%)	1230 (60%)	528 (26%)	294 (14%)	1	5

5 of 73 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	462	ASP	9
1	A	439	MET	9
1	A	463	MET	9
1	A	360	PHE	9
1	A	301	LYS	9

6.3.2 Protein sidechains ⓘ

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	204/243 (84%)	120±7 (59±4%)	84±7 (41±4%)	0	4
All	All	1836/2187 (84%)	1080 (59%)	756 (41%)	0	4

5 of 157 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	336	LYS	9
1	A	353	LEU	9
1	A	420	GLN	9
1	A	435	LEU	9
1	A	461	THR	9

6.3.3 RNA ⓘ

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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 35% for the well-defined parts and 33% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6549

Chemical shift list name: *assigned_chem_shift_list_1*

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	1142
Number of shifts mapped to atoms	1142
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 [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	245	0.48 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	233	1.77 ± 0.11	Should be applied
$^{13}\text{C}'$	214	-0.40 ± 0.10	None needed (< 0.5 ppm)
^{15}N	225	-0.26 ± 0.18	None needed (< 0.5 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 35%, i.e. 1036 atoms were assigned a chemical shift out of a possible 2921. 0 out of 49 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	828/1122 (74%)	206/447 (46%)	416/456 (91%)	206/219 (94%)
Sidechain	208/1585 (13%)	0/923 (0%)	208/601 (35%)	0/61 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/214 (0%)	0/114 (0%)	0/90 (0%)	0/10 (0%)
Overall	1036/2921 (35%)	206/1484 (14%)	624/1147 (54%)	206/290 (71%)

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	A	221	SER	CB	38.68	71.24 – 56.34	-16.9
1	A	346	GLY	N	136.67	129.07 – 90.27	7.0
1	A	401	LEU	H	11.54	11.47 – 4.97	5.1

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 A:

