



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2QMV / pdb_00002qmv
Title : High Resolution Structure of Peroxisome Proliferation-Activated Receptor gamma and Characterisation of its Interaction with the Co-activator Transcriptional 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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

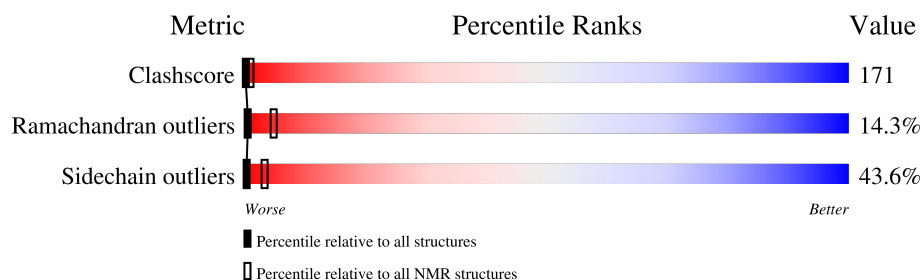
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	

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)	1.04	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.

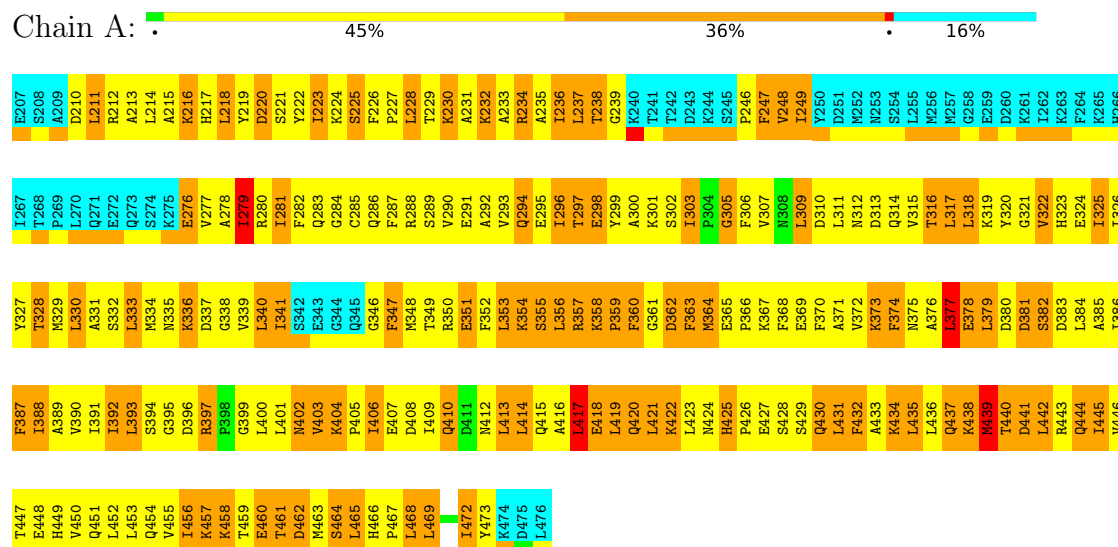
Mol	Chain	Residues	Atoms						Trace
1	A	270	Total	C	H	N	O	S	0
			4441	1397	2276	354	404	10	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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.

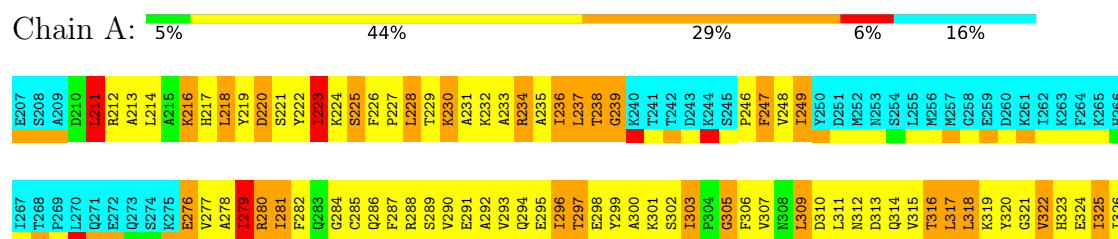
- Molecule 1: Peroxisome proliferator-activated receptor gamma



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



Y327	F387	T447
T328	I388	E448
K329	A389	H449
L330	V390	V450
A331	I391	Q451
S332	I392	L452
L333	L393	L453
K334	S394	Q454
N335	G395	V455
K336	D396	L456
D337	R397	K457
G338	P398	K458
V339	G399	T459
L340	L400	E460
I341	L401	T461
S342	N402	D462
E343	V403	N463
K344	K404	S464
I345	P405	L465
G346	I406	H466
F347	E407	P467
K348	D408	L468
T349	I409	L469
R350	Q410	I472
E351	D411	Y473
F352	N412	K474
L353	L413	D475
K354	L414	L476
S355	Q415	
L356	A416	
R357	L417	
K358	E418	
F359	L419	
F360	Q420	
G361	L421	
D362	K422	
F363	L423	
N364	N424	
E365	H425	
P366	P426	
K367	E427	
F368	S428	
E369	S429	
F370	Q430	
A371	L431	
K372	F432	
K373	A433	
F374	K434	
N375	L435	
A376	L436	
L377	Q437	
E378	K438	
L379	M439	
D380	T440	
D381	D441	
S382	L442	
D383	R443	
L384	Q444	
A385	I445	
I386	V446	

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

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	0.72±0.00	0±0/1865 (0.0± 0.0%)	1.07±0.01	1±1/2520 (0.0± 0.0%)
All	All	0.72	0/16785 (0.0%)	1.07	6/22680 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	404	LYS	O-C-N	5.26	124.54	120.38	3	5
1	A	247	PHE	CB-CA-C	-5.12	109.01	116.53	9	1

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	636±39
All	All	16479	17415	17109	5727

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 171.

5 of 2498 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%)	0	5
All	All	2052/2430 (84%)	1230 (60%)	528 (26%)	294 (14%)	0	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	301	LYS	9
1	A	360	PHE	9
1	A	417	LEU	9
1	A	439	MET	9
1	A	440	THR	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	204/243 (84%)	115±6 (56±3%)	89±6 (44±3%)	0	3
All	All	1836/2187 (84%)	1035 (56%)	801 (44%)	0	3

5 of 166 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	211	LEU	9
1	A	216	LYS	9
1	A	228	LEU	9
1	A	234	ARG	9
1	A	249	ILE	9

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 oligosaccharides 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

No chemical shift data were provided