



wwPDB NMR Structure Validation Summary Report ⓘ

May 29, 2020 – 08:40 am BST

PDB ID : 5VZM
Title : Solution NMR structure of human Rev1 (932-1039) in complex with ubiquitin
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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 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
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

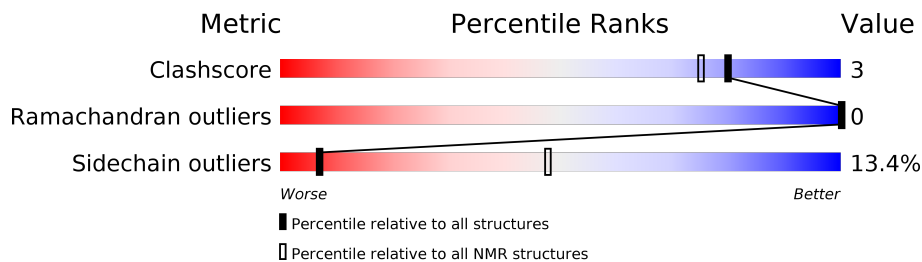
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	76	 79% 16% 5%
2	B	111	 15% .. 82%

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 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 model
1	A:1-A:72, B:1015-B:1034 (92)	0.09	13

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 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2898 atoms, of which 1455 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	76	1231	378	629	105	118	1	0

- Molecule 2 is a protein called DNA repair protein REV1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	111	1667	522	826	145	171	3	0

There are 3 discrepancies between the modelled and reference sequences:

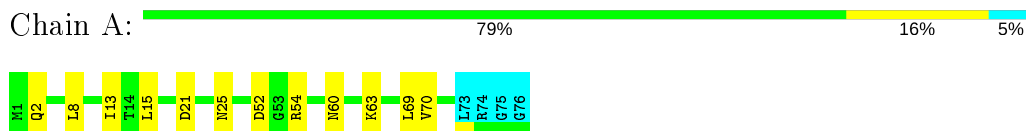
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q9UBZ9
B	-2	HIS	-	expression tag	UNP Q9UBZ9
B	-1	MET	-	expression tag	UNP Q9UBZ9

4 Residue-property plots

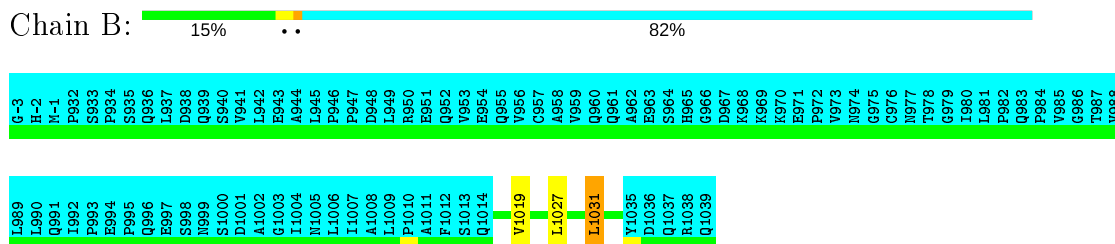
4.1 Average score per residue in the NMR ensemble

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: Ubiquitin



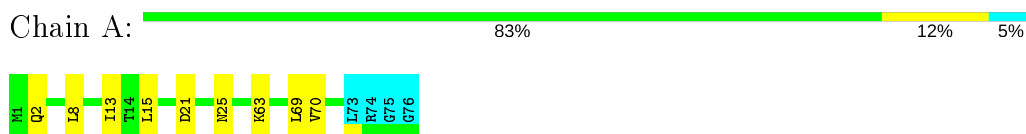
- Molecule 2: DNA repair protein REV1



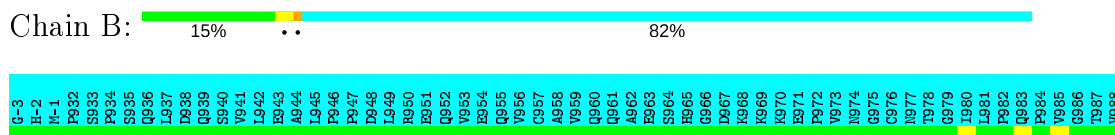
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 13. Colouring as in section 4.1 above.

- Molecule 1: Ubiquitin



- Molecule 2: DNA repair protein REV1



L989	V1019	Y1035
L990	L1027	D1036
Q991	L1081	Q1037
I992		R1038
P993		Q1039
E994		
P995		
Q996		
E997		
S998		
N999		
S1000		
D1001		
A1002		
G1003		
I1004		
N1005		
L1006		
I1007		
A1008		
L1009		
P1010		
A1011		
F1012		
S1013		
Q1014		

5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 20 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
CYANA	structure calculation	
Amber	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	2268
Number of shifts mapped to atoms	2268
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	574	599	599	4±1
2	B	152	155	155	2±1
All	All	14520	15080	15080	79

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 3.

5 of 9 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:1023:LEU:HD22	2:B:1024:PRO:HD2	0.71	1.62	16	3
2:B:1023:LEU:HD21	2:B:1027:LEU:HD12	0.56	1.76	16	2
1:A:8:LEU:HD11	2:B:1031:LEU:HD21	0.55	1.77	8	18
1:A:70:VAL:HG21	2:B:1027:LEU:CD1	0.51	2.35	16	16
1:A:8:LEU:HD21	1:A:70:VAL:HG22	0.48	1.86	9	13

5.2 Torsion angles [i](#)

5.2.1 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	71/76 (93%)	68±0 (96±0%)	3±0 (4±0%)	0±0 (0±0%)	100	100
2	B	20/111 (18%)	20±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	1820/3740 (49%)	1760 (97%)	60 (3%)	0 (0%)	100	100

There are no Ramachandran outliers.

5.2.2 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	66/68 (97%)	57±1 (87±2%)	9±1 (13±2%)	7	48
2	B	15/94 (16%)	13±1 (86±4%)	2±1 (14±4%)	6	46
All	All	1620/3240 (50%)	1403 (87%)	217 (13%)	7	48

5 of 24 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	2	GLN	20

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Mol	Chain	Res	Type	Models (Total)
1	A	69	LEU	20
2	B	1019	VAL	20
1	A	13	ILE	20
1	A	15	LEU	20

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

There are no ligands in this entry.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 88% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *Ub-Rev1_Complex_31.str*

6.1.1 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	2268
Number of shifts mapped to atoms	2268
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

6.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	183	-0.27 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	172	0.25 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	176	-0.28 ± 0.13	None needed (< 0.5 ppm)
^{15}N	165	-0.13 ± 0.17	None needed (< 0.5 ppm)

6.1.3 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 92%, i.e. 1059 atoms were assigned a chemical shift out of a possible 1156. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	439/450 (98%)	176/179 (98%)	179/184 (97%)	84/87 (97%)
Sidechain	582/664 (88%)	358/386 (93%)	214/249 (86%)	10/29 (34%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	38/42 (90%)	20/23 (87%)	18/18 (100%)	0/1 (0%)
Overall	1059/1156 (92%)	554/588 (94%)	411/451 (91%)	94/117 (80%)

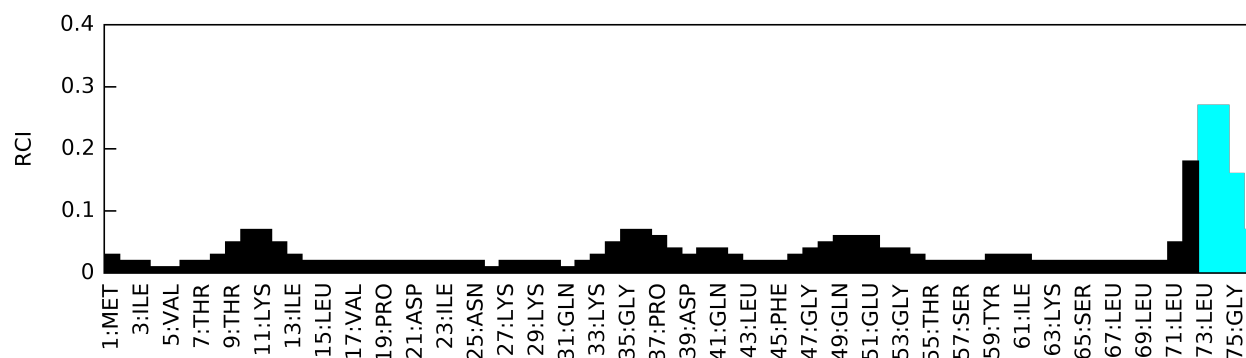
6.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

6.1.5 Random Coil Index (RCI) plots [i](#)

The images below report *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:



Random coil index (RCI) for chain B:

