



# wwPDB NMR Structure Validation Summary Report ⓘ

Feb 13, 2017 – 01:31 am GMT

PDB ID : 2N13  
Title : Complex structure of MyUb (1080-1122) of human Myosin VI with K63-diUb  
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Deposited on : 2015-03-20

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  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

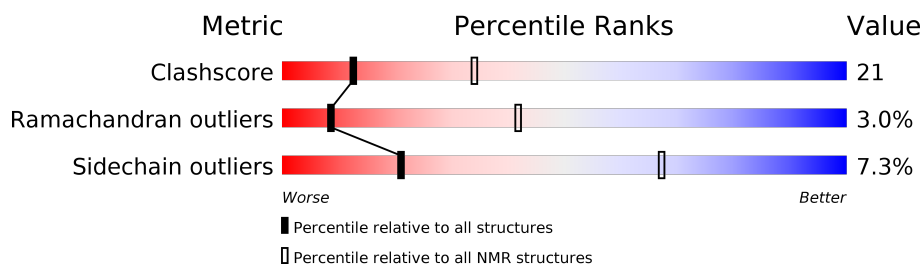
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 60%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	43	
1	D	43	
2	B	76	
3	C	76	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:13-A:51, B:101-B:176, C:201-C:274, D:313-D:346 (223)	0.68	1

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 4 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3925 atoms, of which 1986 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Unconventional myosin-VI.

Mol	Chain	Residues	Atoms						Trace
1	A	43	Total	C	H	N	O	S	0
			730	231	364	66	67	2	
1	D	43	Total	C	H	N	O	S	0
			730	231	364	66	67	2	

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms						Trace
2	B	76	Total	C	H	N	O	S	0
			1232	378	629	107	117	1	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	163	ARG	LYS	ENGINEERED MUTATION	UNP P0CG47

- Molecule 3 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms						Trace
3	C	76	Total	C	H	N	O	S	0
			1233	379	629	105	118	2	

There is a discrepancy between the modelled and reference sequences:

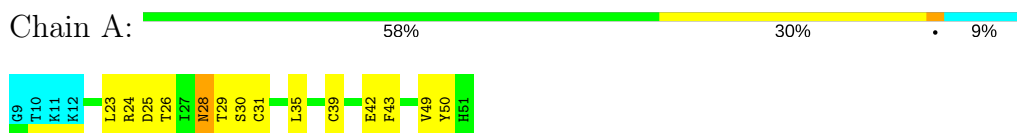
Chain	Residue	Modelled	Actual	Comment	Reference
C	276	CYS	GLY	ENGINEERED MUTATION	UNP P0CG47

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

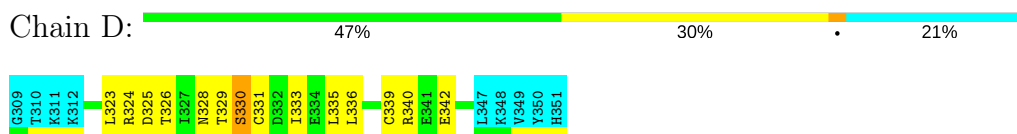
### 4.1 Average score per residue in the NMR ensemble

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.

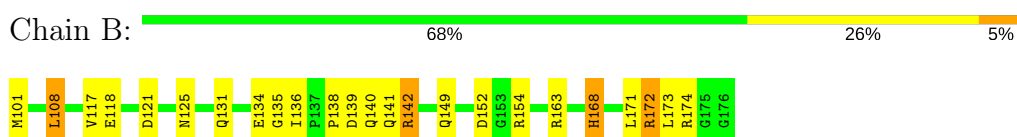
- Molecule 1: Unconventional myosin-VI



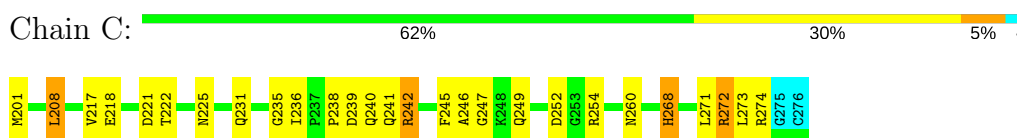
- Molecule 1: Unconventional myosin-VI



- Molecule 2: Ubiquitin



- Molecule 3: Ubiquitin



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

The representative model is number 1. Colouring as in section 4.1 above.

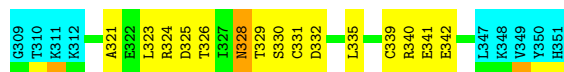
- Molecule 1: Unconventional myosin-VI

Chain A:  53% 37% 9%



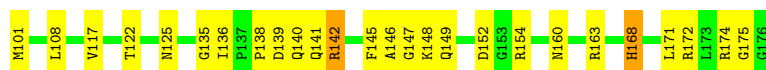
- Molecule 1: Unconventional myosin-VI

Chain D:  44% 33% 21%



- Molecule 2: Ubiquitin

Chain B:  66% 32%



- Molecule 3: Ubiquitin

Chain C:  59% 34%



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	
X-PLOR NIH	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)	2n13_cs.str
Number of chemical shift lists	2
Total number of shifts	1999
Number of shifts mapped to atoms	1999
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	60%

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.

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	4.6±0.7
3	C	0.0±0.0	3.4±0.7
All	All	0	159

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

5 of 9 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	B	174	ARG	Sidechain	20
2	B	163	ARG	Sidechain	19
2	B	172	ARG	Sidechain	19
3	C	274	ARG	Sidechain	18
2	B	154	ARG	Sidechain	18

### 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	337	328	328	19±3
1	D	290	279	279	15±4
2	B	603	629	626	27±4
3	C	593	621	618	27±7
All	All	36460	37140	37018	1550



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 600 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:208:LEU:H	3:C:208:LEU:HD22	0.96	1.20	20	9
2:B:108:LEU:H	2:B:108:LEU:HD22	0.94	1.21	18	9
3:C:208:LEU:HD22	3:C:208:LEU:H	0.87	1.29	4	7
3:C:271:LEU:HD22	3:C:271:LEU:N	0.84	1.88	10	2
2:B:108:LEU:HD22	2:B:108:LEU:H	0.82	1.35	17	8

## 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	38/43 (88%)	32±1 (83±3%)	6±1 (16±4%)	1±1 (1±2%)	19	65
1	D	34/43 (79%)	29±1 (86±4%)	5±1 (14±4%)	0±0 (0±0%)	100	100
2	B	74/76 (97%)	60±2 (81±3%)	10±3 (14±4%)	3±1 (5±2%)	5	28
3	C	73/76 (96%)	59±3 (80±4%)	12±3 (16±4%)	3±1 (4±2%)	7	36
All	All	4380/4760 (92%)	3594 (82%)	655 (15%)	131 (3%)	9	42

5 of 24 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	135	GLY	19
3	C	235	GLY	19
2	B	134	GLU	12
2	B	139	ASP	10
3	C	239	ASP	8

### 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	36/39 (92%)	34±1 (94±3%)	2±1 (6±3%)	29	75
1	D	31/39 (79%)	29±1 (93±4%)	2±1 (7±4%)	24	70
2	B	68/68 (100%)	63±2 (92±2%)	5±2 (8±2%)	19	65
3	C	68/69 (99%)	63±2 (92±2%)	5±2 (8±2%)	18	64
All	All	4060/4300 (94%)	3765 (93%)	295 (7%)	21	67

5 of 69 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)
2	B	168	HIS	19
3	C	252	ASP	18
3	C	268	HIS	17
2	B	108	LEU	16
2	B	152	ASP	16

### 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 ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 60% for the well-defined parts and 57% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2n13\_cs.str

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	997
Number of shifts mapped to atoms	997
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

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	76	$-0.16 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	70	$0.09 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	75	$-0.14 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	70	$0.59 \pm 0.65$	None needed (imprecise)

#### 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 30%, i.e. 875 atoms were assigned a chemical shift out of a possible 2901. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	369/1103 (33%)	148/440 (34%)	151/446 (34%)	70/217 (32%)
Sidechain	476/1629 (29%)	294/951 (31%)	174/591 (29%)	8/87 (9%)

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	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Aromatic	30/169 (18%)	16/90 (18%)	14/72 (19%)	0/7 (0%)
Overall	875/2901 (30%)	458/1481 (31%)	339/1109 (31%)	78/311 (25%)

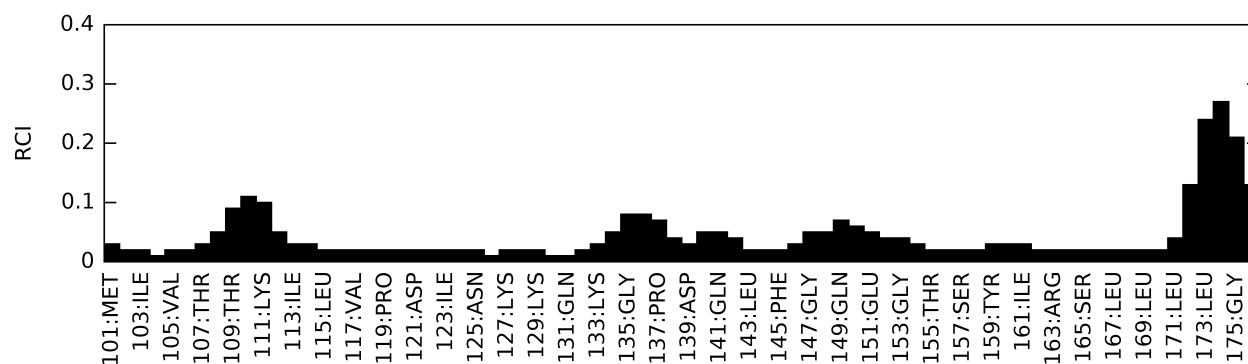
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 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 B:



## 7.2 Chemical shift list 2

File name: 2n13\_cs.str

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	1002
Number of shifts mapped to atoms	1002
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
$^{13}\text{C}_\alpha$	76	$-0.10 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	71	$0.13 \pm 0.22$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	75	$-0.14 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	70	$0.74 \pm 0.64$	None needed (imprecise)

### 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 30%, i.e. 868 atoms were assigned a chemical shift out of a possible 2901. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	359/1103 (33%)	144/440 (33%)	147/446 (33%)	68/217 (31%)
Sidechain	479/1629 (29%)	296/951 (31%)	175/591 (30%)	8/87 (9%)
Aromatic	30/169 (18%)	16/90 (18%)	14/72 (19%)	0/7 (0%)
Overall	868/2901 (30%)	456/1481 (31%)	336/1109 (30%)	76/311 (24%)

### 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 C:

