

Full wwPDB NMR Structure Validation Report (i)

Sep 18, 2023 – 10:06 PM EDT

PDB ID	:	1WR1
Title	:	The complex structure of Dsk2p UBA with ubiquitin
Authors	:	Ohno, A.; Jee, J.G.; Fujiwara, K.; Tenno, T.; Goda, N.; Tochio, H.; Hiroaki,
		H.; kobayashi, H.; Shirakawa, M.
Deposited on	:	2004-10-08

This is a Full wwPDB NMR Structure Validation 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 (i) 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 (i)) were used in the production of this report:

MolProbity Percentile statistics wwPDB-RCI PANAV wwPDB-ShiftChecker Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	::	4.02b-467 20191225.v01 (using entries in the PDB archive December 25th 2019) v_1n_11_5_13_A (Berjanski et al., 2005) Wang et al. (2010) v1.2 Engh & Huber (2001) Parkinson et al. (1996) 2.35.1
---	----	--

1 Overall quality at a glance (i)

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.



Matria	Whole archive	NMR archive
Metric	$(\# { m Entries})$	$(\# {\rm Entries})$
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 <=5%

Mol	Chain	Length	Quality of chain			
1	А	76	86%		9%	5%
2	В	58	71%	9%	21%	



2 Ensemble composition and analysis (i)

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. The authors have identified model 16 as representative, based on the following criterion: *closest to the average*. No medoid model was calculated.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues							
Well-defined core	Residue ra	nge (total)	Backbone RMSD (Å)	Medoid model			
1	A:1-A:72,	B:328-B:373	Not calculated	Not calculated			
	(118)						

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models in file



3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2072 atoms, of which 1036 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Ubiquitin.

Mol	Chain	Residues		Atoms					
1	٨	76	Total	С	Н	Ν	0	S	0
	А	A (0	1226	375	625	105	120	1	

• Molecule 2 is a protein called Ubiquitin-like protein DSK2.

Mol	Chain	Residues	Atoms						Trace
0	D	59	Total	С	Η	Ν	0	S	0
2	Б	58	846	265	411	81	88	1	

I here are 12 discrepancies between the modelled and reference sequence	There are	12 discrepancie	s between	the modelled	and	reference	sequences
---	-----------	-----------------	-----------	--------------	-----	-----------	-----------

Chain	Residue	Modelled	Actual	Comment	Reference
В	316	PRO	-	cloning artifact	UNP P48510
В	317	GLY	-	cloning artifact	UNP P48510
В	318	ILE	-	cloning artifact	UNP P48510
В	319	SER	-	cloning artifact	UNP P48510
В	320	GLY	-	cloning artifact	UNP P48510
В	321	GLY	-	cloning artifact	UNP P48510
В	322	GLY	-	cloning artifact	UNP P48510
В	323	GLY	-	cloning artifact	UNP P48510
В	324	GLY	-	cloning artifact	UNP P48510
В	325	ILE	-	cloning artifact	UNP P48510
В	326	LEU	-	cloning artifact	UNP P48510
В	327	ASP	-	cloning artifact	UNP P48510



4 Residue-property plots (i)

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: Ubiquitin



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1





4.2.2 Score per residue for model 2

Chain	A: 86%	9%	5%
M1 V5 D49	R 24 R 26 R 26		
• Mole	ecule 2: Ubiquitin-like protein DSK2		
Chain	B: 78% .	21%	
P316 G317 I318 S319 C320	6321 6323 6323 1325 1325 1325 1327 734 7373		
4.2.3	Score per residue for model 3		
• Mole	ecule 1: Ubiquitin		
Chain	A: 84%	11%	5%
M1 V5 K6	Q49 N60 Q76 Q76 Q76 Q76 Q76		
• Mole	ecule 2: Ubiquitin-like protein DSK2		
Chain	B: 71% 9%	21%	
P316 6317 1318 5319 6320	(332) (332) (3324) (3325) (3325) (3321) (3321) (3321) (3321) (3322) (3323) (3322) (3325) (3321) (3325) (3321) (3321) (3325) (3321) (3321) (3321) (3322) (332) (33		
4.2.4	Score per residue for model 4		
• Mole	ecule 1: Ubiquitin		
Chain	A: 82%	13%	5%
M1 V5 K6	L15 K37 K37 <td></td> <td></td>		
• Mole	ecule 2: Ubiquitin-like protein DSK2		
Chain	B: 71% 9%	21%	
P316 G317 I318 S319 C320	C C C C C C C C C C C C C C C C C C C		



4.2.5 Score per residue for model 5

Chain	A: 87%	8%	5%
M1 V5 B42	R54 K63 H68 G75 G75 G75 G76		
• Mole	ecule 2: Ubiquitin-like protein DSK2		
Chain	B: 76% ·	21%	
P316 G317 I318 S319 G320	G321 G322 G323 G322 C323 C322 C322 C322 C322		
4.2.6	Score per residue for model 6		
• Mole	ecule 1: Ubiquitin		
Chain	A: 84%	11%	5%
M1 V5 K6	R4 2 R5 4 R5 4 R5 4 R5 4 R5 4 C7 0 G7 5 G7 5 G7 5		
• Mole	ecule 2: Ubiquitin-like protein DSK2		
Chain	B: 72% 7%	21%	
P316 6317 1318 5319 6320	G321 G322 G322 C3223 G322 C322 C322 C322 C32		
4.2.7	Score per residue for model 7		
• Mole	ecule 1: Ubiquitin		
Chain	A: 84%	9%	5%
M1 V5 K6	R4 2 R5 4 R6 3 K6 3 C7 5 G7 5 G7 5 G7 5		
• Mole	ecule 2: Ubiquitin-like protein DSK2		
Chain	B: 71% 5% ·	21%	
P316 G317 I318 S319 G320	G321 G322 G322 C322 C322 C326 L326 C326 R326 R326 R326 R372 V373		



4.2.8 Score per residue for model 8

Chain A	A: 89%	5%	5%
M1 V5 K6	K63 874 676 676		
• Molec	cule 2: Ubiquitin-like protein DSK2		
Chain I	B: 76% ·	21%	
P316 G317 I318 S319 G320	6322 1322 1325 1325 1325 1325 1325 1325 1		
4.2.9	Score per residue for model 9		
• Molec	cule 1: Ubiquitin		
Chain A	A: 83%	12%	5%
M1 V5 V26 V26	156 158 158 158 158 158 158 158 158 158 158		
• Molec	cule 2: Ubiquitin-like protein DSK2		
Chain I	3: 72% 7%	21%	
F316 G317 I318 S319 G320	G 322 G 322 G 322 G 322 C 322		
4.2.10	Score per residue for model 10		
• Moleo	cule 1: Ubiquitin		
Chain A	A: 86%	9%	5%
M1 V5 R42	R5 K <thk< th=""> K K K</thk<>		
• Moleo	cule 2: Ubiquitin-like protein DSK2		
Chain I	3: 76% ·	21%	
P316 G317 I318 S319 G320	6322 (5323 (5323 (5323 (5323 (5323) (532)		



4.2.11 Score per residue for model 11





4.2.14 Score per residue for model 14

Chain A:	87%		7% • 5%
M1 V5 K6 R54 R54 K63 K63 K63 K63 L17 C67 C75 C75 C75 C75 C75 C75 C75 C75 C75 C7			
• Molecule 2: Ubiquitin	n-like protein DSK2		
Chain B:	71%	7% •	21%
P316 6317 1318 1318 5320 6322 6322 6322 1325 1325 1325 1325 1325 1325 1325 1	R349 R355 V373		
4.2.15 Score per re	sidue for model 15		
• Molecule 1: Ubiquitin	1		
Chain A:	89%		5% 5%
M1 K6 K6 K6 K6 K7 K7 K7 G7 G75 G75			
• Molecule 2: Ubiquitin	n-like protein DSK2		
Chain B:	72%	5% •	21%
P316 3317 1318 3319 5320 6322 6322 6322 1325 1325 1325 1325 1325 1325 1325 1	1365 1365 1365 1365 1365 1365 1365 1365		
4.2.16 Score per re	sidue for model 16		
• Molecule 1: Ubiquitin	1		
Chain A:	86%		9% 5%
M1 VG VG KG R54 R63 KG3 L67 L68 L68 R74 R74	675 676		
• Molecule 2: Ubiquitin	n-like protein DSK2		
Chain B:	74%	5%	21%
P316 0317 1318 1318 1318 1328 0322 1328 1324 1326 1326 1326 1326 1326 1326 1326 1326	1355 1373		



4.2.17 Score per residue for model 17

Chain A:	88%		7% 5%					
M1 V5 R64 K63 K63 L67	R74 G75 G76							
• Molecule 2: Ubiquitin-like protein DSK2								
Chain B:	71%	7% •	21%					
P316 0317 1318 1318 1318 0321 0321 0323 0323 1326 1326 1326	R331 R337 C343 R349 R356 V373							
4.2.18 Score p	per residue for model 18							
• Molecule 1: Ub	iquitin							
Chain A:	83%		11% • 5%					
M1 V5 K27 K27 K27 L50 L50 R54	K63 L67 R72 R72 R73 R73 G75 G75							
• Molecule 2: Ub	iquitin-like protein DSK2							
Chain B:	71%	7% •	21%					
P316 1317 1318 1318 1328 1328 1328 1328 1326 1326 1326	R331 R337 R349 R346 L366 V373							
4.2.19 Score p	per residue for model 19							
• Molecule 1: Ub	iquitin							
Chain A:	84%		11% 5%					
M1 V5 R42 R54 R54 D58 K63	L67 V70 G75 G75							
• Molecule 2: Ub	iquitin-like protein DSK2							
Chain B:	74%	•••	21%					
P316 G317 1318 S319 G320 G321 G322 G324 G324 C324 C324 C324 C324 C324 C324 C324 C	R349 D372 V373							



4.2.20 Score per residue for model 20





5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: torsion angle dynamics, simulated annealing, molecular dynamics, energy minimization.

Of the 100 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 solution	2.0.17
Amber	refinement	7

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	Chain	Bond lengths		Bond angles		
	RMSZ	$\#Z{>}5$	RMSZ	$\#Z{>}5$		
1	А	$0.64{\pm}0.00$	$0{\pm}0/579~(~0.0{\pm}~0.0\%)$	$0.98 {\pm} 0.03$	$2{\pm}1/780~(~0.2{\pm}~0.2\%)$	
2	В	$0.74{\pm}0.01$	$0{\pm}0/371~(~0.0{\pm}~0.0\%)$	1.08 ± 0.03	$3{\pm}1/495$ ($0.5{\pm}$ $0.2\%)$	
All	All	0.68	0/18999 ($0.0%$)	1.02	92/25498~(~0.4%)	

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.

Mal	Iol Chain		Turne	Atoma	7	Observed(0)	Ideal(?)	Models	
	Unam	nes	туре	Atoms		Observed(*)	Ideal(*)	Worst	Total
2	В	356	ARG	NE-CZ-NH1	7.45	124.02	120.30	9	11
1	А	42	ARG	NE-CZ-NH1	7.15	123.87	120.30	11	10
1	А	54	ARG	NE-CZ-NH1	7.13	123.86	120.30	14	12
2	В	337	ARG	NE-CZ-NH1	7.10	123.85	120.30	16	8
2	В	349	ARG	NE-CZ-NH1	6.98	123.79	120.30	6	19
2	В	331	ARG	NE-CZ-NH1	6.32	123.46	120.30	14	9
1	А	54	ARG	NE-CZ-NH2	-6.10	117.25	120.30	12	13
1	А	72	ARG	NE-CZ-NH1	5.88	123.24	120.30	7	4
2	В	356	ARG	CD-NE-CZ	5.37	131.12	123.60	4	1
2	В	349	ARG	NE-CZ-NH2	-5.22	117.69	120.30	11	2
2	В	355	ARG	NE-CZ-NH1	5.13	122.86	120.30	16	2
2	В	349	ARG	CD-NE-CZ	5.00	130.61	123.60	2	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	А	573	595	595	0±1
2	В	366	342	342	0±0
All	All	18779	18740	18736	7

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 0.

Atom 1	Atom 2	$Clack(\lambda)$	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:26:VAL:HG21	1:A:56:LEU:HD21	0.48	1.84	12	3
1:A:15:LEU:HD22	1:A:29:LYS:HB3	0.45	1.88	4	2
2:B:362:GLN:HE21	2:B:365:LEU:HD13	0.41	1.75	15	1
2:B:362:GLN:HE21	2:B:365:LEU:HD21	0.41	1.75	12	1

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

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	Perce	ntiles
1	А	71/76~(93%)	$69 \pm 1 (97 \pm 2\%)$	$2\pm1 (3\pm2\%)$	0±0 (0±0%)	100	100
2	В	45/58~(78%)	$43 \pm 1 (96 \pm 3\%)$	2 ± 1 (4±3%)	0±0 (0±1%)	50	82
All	All	2320/2680~(87%)	2241 (97%)	77 (3%)	2 (0%)	54	85

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
2	В	343	GLY	2

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed and the total number of residues.



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	67/69~(97%)	$61 \pm 1 (91 \pm 2\%)$	$6\pm1 (9\pm2\%)$	13	60
2	В	38/44~(86%)	$37 \pm 1 (96 \pm 3\%)$	$1\pm1 (4\pm3\%)$	37	85
All	All	2099/2260~(93%)	1952 (93%)	147 (7%)	19	67

All 27 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	А	5	VAL	20
1	А	63	LYS	20
1	А	67	LEU	15
1	А	69	LEU	15
1	А	6	LYS	13
2	В	365	LEU	11
1	А	58	ASP	9
1	А	70	VAL	6
2	В	337	ARG	5
1	А	49	GLN	5
1	А	27	LYS	5
2	В	356	ARG	3
1	А	42	ARG	3
2	В	333	GLU	2
2	В	331	ARG	2
2	В	372	ASP	2
1	А	21	ASP	1
1	А	40	GLN	1
1	А	60	ASN	1
2	В	334	HIS	1
2	В	373	VAL	1
1	А	72	ARG	1
1	А	39	ASP	1
1	А	68	HIS	1
1	А	1	MET	1
2	В	342	MET	1
1	А	50	LEU	1

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 monosaccharides 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)

No chemical shift data were provided

