



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2DEN
Title : Solution Structure of the Ubiquitin-Associated Domain of Human BMSC-UbP
and its 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
<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

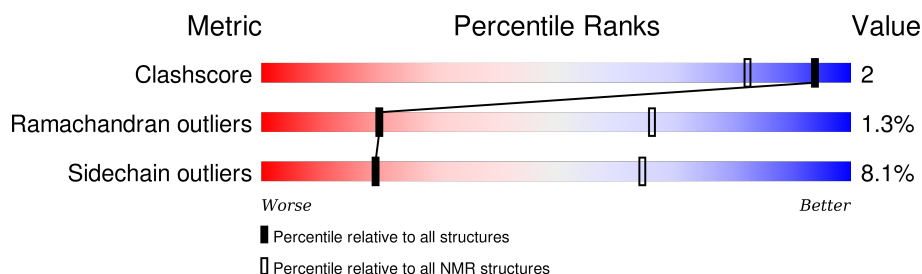
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 30%.

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	108	
2	B	76	

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 10 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:64-A:108, B:1-B:76 (121)	0.63	10

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, 3, 4, 5, 9, 10
2	2, 7, 8
Single-model clusters	6

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1912 atoms, of which 965 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called chimera of Immunoglobulin G binding protein G and Ubiquitin-like protein 7.

Mol	Chain	Residues	Atoms						Trace
1	A	46	Total	C	H	N	O	S	0
			680	213	335	61	70	1	

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP P06654
A	2	HIS	-	EXPRESSION TAG	UNP P06654
A	3	HIS	-	EXPRESSION TAG	UNP P06654
A	4	HIS	-	EXPRESSION TAG	UNP P06654
A	5	HIS	-	EXPRESSION TAG	UNP P06654
A	6	HIS	-	EXPRESSION TAG	UNP P06654
A	7	HIS	-	EXPRESSION TAG	UNP P06654
A	8	GLN	-	EXPRESSION TAG	UNP P06654
A	12	ALA	ILE	ENGINEERED	UNP P06654
A	63	GLY	-	LINKER	UNP Q96S82

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms						Trace
2	B	76	Total	C	H	N	O	S	0
			1232	378	630	105	118	1	

M1	T14	S20	D21	T22	R42	R54	V70	R74	G75	G76
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5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 200 calculated structures, 10 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
HADDOCK	refinement	1.3
HADDOCK	structure solution	1.3

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 6988
Number of chemical shift lists	1
Total number of shifts	1139
Number of shifts mapped to atoms	1139
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	30%

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

6 Model quality

6.1 Standard geometry

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

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	341	332	332	2±1
2	B	602	630	629	2±1
All	All	9430	9620	9610	31

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 2.

5 of 22 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:TRP:O	1:A:70:LEU:HG	0.59	1.98	9	4
1:A:69:GLN:HB3	1:A:95:ILE:HD11	0.57	1.77	8	3
1:A:73:LEU:O	1:A:76:MET:HG2	0.53	2.04	4	1
1:A:95:ILE:O	1:A:99:LEU:HG	0.52	2.03	10	1
1:A:73:LEU:O	1:A:76:MET:HG3	0.52	2.04	9	1

6.3 Torsion angles

6.3.1 Protein backbone

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	44/108 (41%)	41±1 (93±3%)	2±1 (5±2%)	1±1 (2±1%)	14	55
2	B	74/76 (97%)	71±2 (96±3%)	3±2 (4±2%)	1±1 (1±1%)	29	74
All	All	1180/1840 (64%)	1114 (94%)	51 (4%)	15 (1%)	20	66

All 5 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	93	GLY	7
2	B	7	THR	3
2	B	10	GLY	2
1	A	77	GLY	2
2	B	46	ALA	1

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	34/85 (40%)	31±1 (92±3%)	3±1 (8±3%)	20	65
2	B	68/68 (100%)	62±1 (92±1%)	6±1 (8±1%)	19	64
All	All	1020/1530 (67%)	937 (92%)	83 (8%)	19	64

5 of 28 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	20	SER	9
2	B	14	THR	7
2	B	57	SER	7
2	B	9	THR	6
2	B	22	THR	6

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 [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 30% for the well-defined parts and 31% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6988

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	1139
Number of shifts mapped to atoms	1139
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
$^{13}\text{C}_\alpha$	103	-0.42 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	93	0.48 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	102	1.06 ± 0.13	Should be applied
^{15}N	101	0.02 ± 0.48	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 30%, i.e. 453 atoms were assigned a chemical shift out of a possible 1495. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	220/595 (37%)	88/237 (37%)	89/242 (37%)	43/116 (37%)
Sidechain	230/845 (27%)	141/492 (29%)	89/312 (29%)	0/41 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	3/55 (5%)	3/29 (10%)	0/23 (0%)	0/3 (0%)
Overall	453/1495 (30%)	232/758 (31%)	178/577 (31%)	43/160 (27%)

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	37	LYS	HE2	1.60	3.87 – 1.97	-6.9
1	A	60	VAL	HB	0.10	3.59 – 0.39	-5.9
1	A	37	LYS	HE3	1.89	3.86 – 1.96	-5.4

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:

