wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1W6V
Title	:	Solution structure of the DUSP domain of hUSP15
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Deposited on	:	2004-08-24

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 (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:

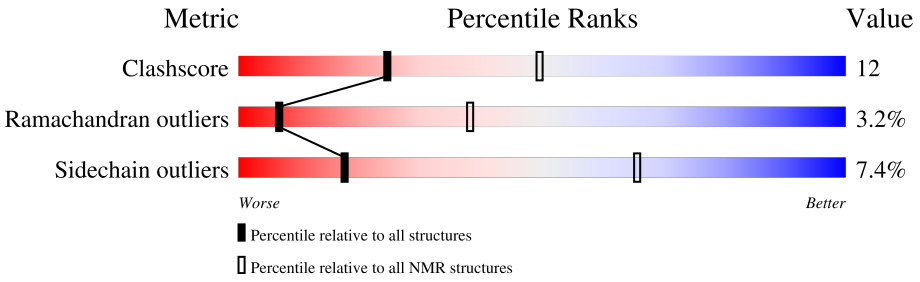
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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.



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 <=5%

Mol	Chain	Length	Quality of chain
1	A	141	53% 21% • 9% 15%

2 Ensemble composition and analysis (i)

This entry contains 13 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:7-A:72, A:76-A:117 (108)	0.71	3

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 2 single-model clusters were found.

Cluster number	Models
1	1, 3, 5, 7, 8, 9, 10, 11, 13
2	2, 4
Single-model clusters	6; 12

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1924 atoms, of which 947 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 15.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	120	1924	624	947	160	190	3	0

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 CARBOXYL-TERMINAL HYDROLASE 15

Chain A: 53% 21% • 9% 15%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET M1 A2 E3 G4 G5 A6 A7 D8 T11 Q12 R13 I16 L20 K21 L24 R25 W30 Y31 L32 K39 Y44 V45 G46 K52 V60 Y61 L71 K72 D73

G74 D75 I84 D85 E86 L87 D88 Y89 I90 G96 L100 W103 Y104 T105 L106 M107 R115 K116 V117 V118 E119 Q120

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

The representative model is number 3. Colouring as in section 4.1 above.

• Molecule 1: UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 15

Chain A: 49% 23% • • 9% 15%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET M1 A2 E3 G4 G5 A6 A7 D8 Q12 I16 L20 K21 L24 W30 Y31 L32 W37 Q40 W41 K42 K43 Y44 V45 G46 F47 D48 D51 K52 Y53 Q54

V60 Y61 D66 D73 G74 D75 E81 I84 D85 E86 L87 D88 Y89 I90 L91 G96 L100 T105 L106 M107 I113 A114 R115 K116 V117 V118 E119 Q120

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *CANDID IN CYANA AND CNS FOR WATER REFINEMENT*.

Of the 20 calculated structures, 13 were deposited, based on the following criterion: *SMALLEST MAXIMUM RESTRAINT VIOLATION*.

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

Software name	Classification	Version
CNS	refinement	
Sparky	structure solution	

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	1.09±0.03	0±1/921 (0.1± 0.1%)	0.85±0.01	0±0/1251 (0.0± 0.0%)
All	All	1.09	6/11973 (0.1%)	0.85	2/16263 (0.0%)

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
1	A	0.0±0.0	0.5±0.6
All	All	0	6

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	60	VAL	CB-CG1	-5.85	1.40	1.52	6	2
1	A	108	GLU	N-CA	-5.62	1.35	1.46	6	1
1	A	107	MET	N-CA	-5.62	1.35	1.46	13	1
1	A	45	VAL	CB-CG2	-5.35	1.41	1.52	9	1
1	A	19	LEU	N-CA	-5.14	1.36	1.46	13	1

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	52	LYS	N-CA-CB	-7.03	97.95	110.60	13	1
1	A	108	GLU	N-CA-CB	-5.07	101.48	110.60	6	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the

ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	13	ARG	Sidechain	4
1	A	115	ARG	Sidechain	1
1	A	36	ARG	Sidechain	1

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	896	880	879	21±4
All	All	11648	11440	11427	272

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 12.

5 of 121 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ARG:HD3	1:A:45:VAL:HG21	0.76	1.54	11	2
1:A:32:LEU:HD11	1:A:89:TYR:CG	0.69	2.22	7	4
1:A:32:LEU:HD11	1:A:89:TYR:CD1	0.67	2.24	2	4
1:A:46:GLY:HA2	1:A:52:LYS:HB2	0.64	1.67	9	4
1:A:86:GLU:HA	1:A:89:TYR:O	0.63	1.94	5	11

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	108/141 (77%)	97±2 (90±2%)	7±2 (7±2%)	3±1 (3±1%)	7 38
All	All	1404/1833 (77%)	1264 (90%)	95 (7%)	45 (3%)	7 38

5 of 10 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	85	ASP	13
1	A	105	THR	13
1	A	86	GLU	11
1	A	117	VAL	2
1	A	25	ARG	1

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	97/122 (80%)	90±2 (93±2%)	7±2 (7±2%)	17	65
All	All	1261/1586 (80%)	1168 (93%)	93 (7%)	17	65

5 of 29 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	24	LEU	11
1	A	44	TYR	9
1	A	86	GLU	7
1	A	100	LEU	7
1	A	21	LYS	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 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