wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2MP2
BMRB ID	:	19961
Title	:	Solution structure of SUMO dimer in complex with SIM2-3 from RNF4
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Deposited on	:	2014-05-09

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:

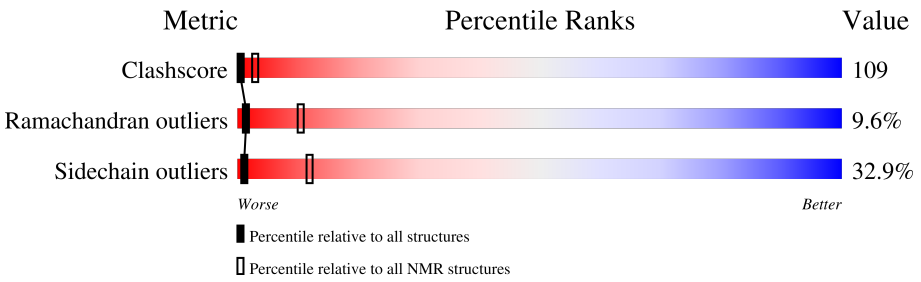
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 is 65%.

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	82	10% 50% 22% 18%
2	B	90	8% 47% 28% • 17%
3	C	25	100%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 7 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:4-A:13, A:17-A:37, A:43-A:78 (67)	0.35	2
2	B:14-B:88 (75)	0.55	7

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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3097 atoms, of which 1531 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Small ubiquitin-related modifier 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	82	1292	401	639	118	130	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P55854

- Molecule 2 is a protein called Small ubiquitin-related modifier 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	90	1436	445	712	129	146	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP P55854

- Molecule 3 is a protein called E3 ubiquitin-protein ligase RNF4.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
3	C	25	369	115	180	28	45	1	0

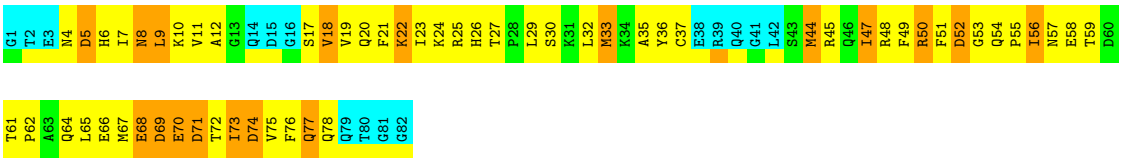
4 Residue-property plots (i)

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.

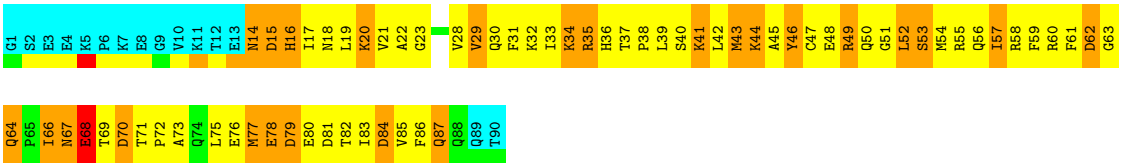
• Molecule 1: Small ubiquitin-related modifier 3

Chain A: 10% 50% 22% 18%



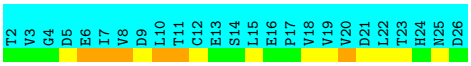
• Molecule 2: Small ubiquitin-related modifier 3

Chain B: 8% 47% 28% • 17%



• Molecule 3: E3 ubiquitin-protein ligase RNF4

Chain C: 100%



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

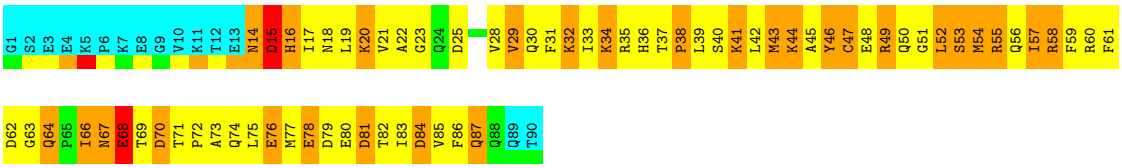
The representative model is number 7. Colouring as in section 4.1 above.

• Molecule 1: Small ubiquitin-related modifier 3

Chain A: 15% 46% 20% • 18%

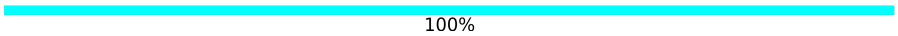
- Molecule 2: Small ubiquitin-related modifier 3

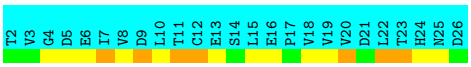
Chain B:



- Molecule 3: E3 ubiquitin-protein ligase RNF4

Chain C:





5 Refinement protocol and experimental data overview (i)

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

Of the 60 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
CNS	structure solution	
ARIA	structure solution	
CNS	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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1516
Number of shifts mapped to atoms	1516
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	65%

6 Model quality (i)

6.1 Standard geometry (i)

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 (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	547	544	542	115±8
2	B	609	600	598	135±12
3	C	0	0	0	0±0
All	All	11560	11440	11400	2504

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 109.

5 of 746 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:PHE:O	1:A:56:ILE:HB	1.21	1.33	1	10
1:A:56:ILE:HD11	1:A:73:ILE:HD12	1.01	1.27	9	8
2:B:20:LYS:HG2	2:B:28:VAL:CG2	0.98	1.87	8	10
1:A:47:ILE:HD12	1:A:49:PHE:CD1	0.96	1.95	4	6
2:B:16:HIS:HA	2:B:34:LYS:HA	0.95	1.38	4	10

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	67/82 (82%)	54±1 (81±2%)	8±2 (12±2%)	4±2 (7±3%)	2 18
2	B	75/90 (83%)	53±2 (71±3%)	13±3 (17±3%)	9±2 (12±3%)	1 6
3	C	0	-	-	-	-
All	All	1420/1970 (72%)	1073 (76%)	210 (15%)	137 (10%)	1 10

5 of 37 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	52	ASP	10
2	B	16	HIS	10
2	B	68	GLU	10
2	B	62	ASP	8
2	B	34	LYS	7

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	62/72 (86%)	42±2 (67±4%)	20±2 (33±4%)	1 12
2	B	68/81 (84%)	46±3 (67±4%)	22±3 (33±4%)	1 12
3	C	0	-	-	-
All	All	1300/1770 (73%)	872 (67%)	428 (33%)	1 12

5 of 78 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	9	LEU	10
1	A	18	VAL	10
1	A	33	MET	10
1	A	45	ARG	10
1	A	47	ILE	10

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)

The completeness of assignment taking into account all chemical shift lists is 65% for the well-defined parts and 57% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

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	1516
Number of shifts mapped to atoms	1516
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	17

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	90	-0.29 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	89	-0.28 ± 0.24	None needed (< 0.5 ppm)
$^{13}C'$	89	-0.01 ± 0.11	None needed (< 0.5 ppm)
^{15}N	88	0.68 ± 0.29	Should be applied

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 65%, i.e. 1309 atoms were assigned a chemical shift out of a possible 2002. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	388/704 (55%)	163/284 (57%)	150/284 (53%)	75/136 (55%)
Sidechain	853/1168 (73%)	599/748 (80%)	233/363 (64%)	21/57 (37%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	68/130 (52%)	34/64 (53%)	34/58 (59%)	0/8 (0%)
Overall	1309/2002 (65%)	796/1096 (73%)	417/705 (59%)	96/201 (48%)

7.1.4 Statistically unusual chemical shifts (i)

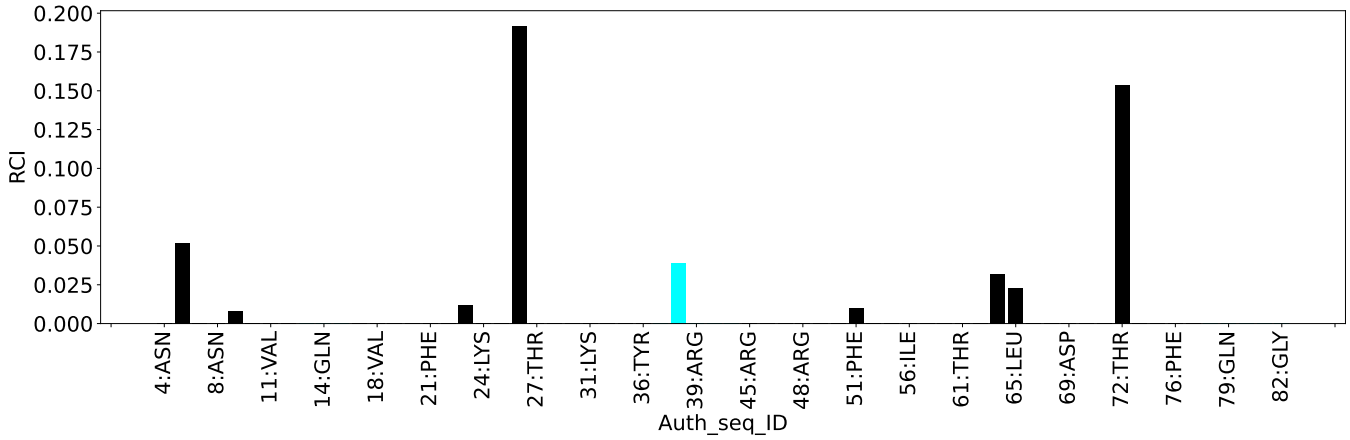
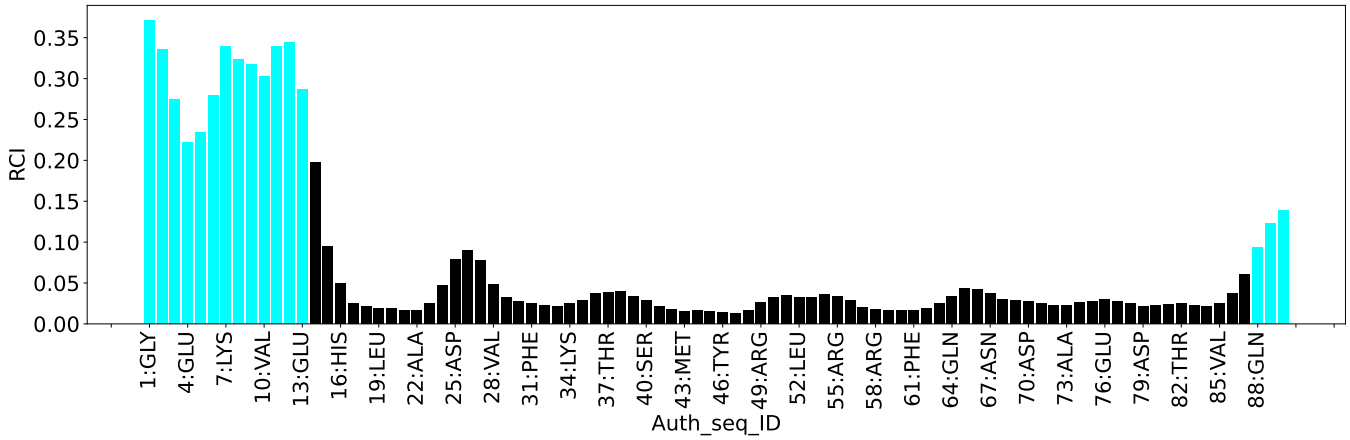
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	76	PHE	CE2	61.40	124.80 – 136.72	-58.2
1	A	76	PHE	CE1	61.40	124.17 – 137.29	-52.8
1	A	67	MET	CE	88.20	8.39 – 25.85	40.7
1	A	33	MET	CE	87.60	8.39 – 25.85	40.4
1	A	45	ARG	NE	108.37	76.53 – 92.65	14.8
1	A	25	ARG	NE	107.11	76.53 – 92.65	14.0
1	B	56	GLN	HE21	2.39	5.02 – 9.43	-11.0
1	B	87	GLN	HE21	2.39	5.02 – 9.43	-11.0
1	B	89	GLN	HE21	2.39	5.02 – 9.43	-11.0
1	B	87	GLN	HE22	2.31	4.88 – 9.19	-11.0
1	B	56	GLN	HE22	2.48	4.88 – 9.19	-10.6
1	B	89	GLN	HE22	2.48	4.88 – 9.19	-10.6
1	B	46	TYR	CE2	130.84	111.68 – 124.17	10.3
1	A	8	ASN	HD21	2.57	4.94 – 9.72	-10.0
1	B	46	TYR	CE1	130.84	111.24 – 124.66	9.6
1	A	8	ASN	HD22	2.76	4.69 – 9.61	-8.9
1	A	33	MET	HG3	0.35	0.54 – 4.26	-5.5

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B: