wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2N1A
BMRB ID	:	25553
Title	:	Docked structure between SUMO1 and ZZ-domain from CBP
Authors	:	Diehl, C.
Deposited on	:	2015-03-26

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:

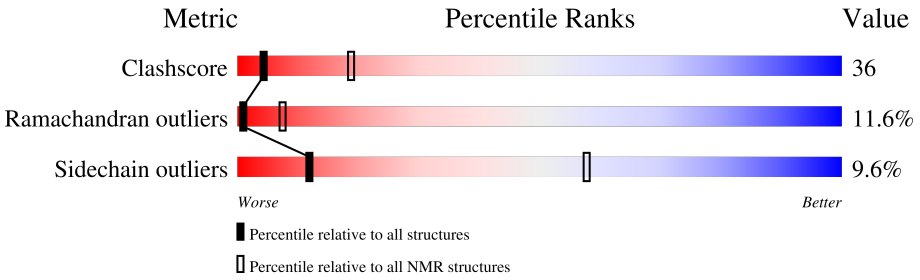
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 9%.

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	103	60% 34% 6%
2	B	53	36% 38% 25% .

2 Ensemble composition and analysis

This entry contains 6 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:-1-A:101 (103)	0.00	3
2	B:201-B:253 (53)	0.00	2

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. No single-model clusters were found.

Cluster number	Models
1	2, 3, 4, 5
2	1, 6

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2453 atoms, of which 1195 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	103	1621	506	803	140	167	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P63165
A	0	SER	-	expression tag	UNP P63165

- Molecule 2 is a protein called CREB-binding protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	53	830	271	392	79	81	7	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
3	B	2	2	2

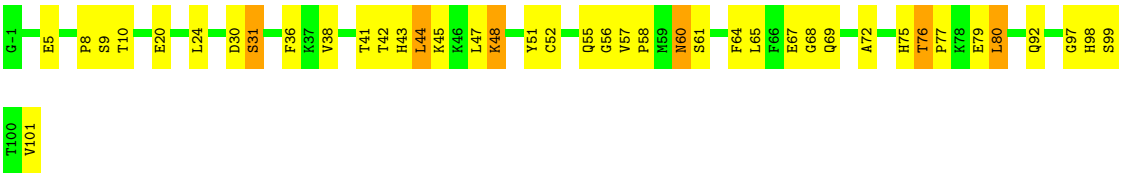
4 Residue-property plots (i)

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.

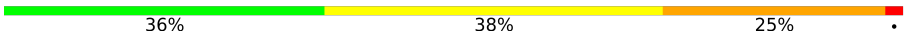
• Molecule 1: Small ubiquitin-related modifier 1

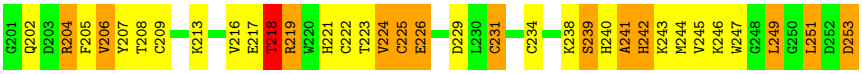
Chain A:



• Molecule 2: CREB-binding protein

Chain B:



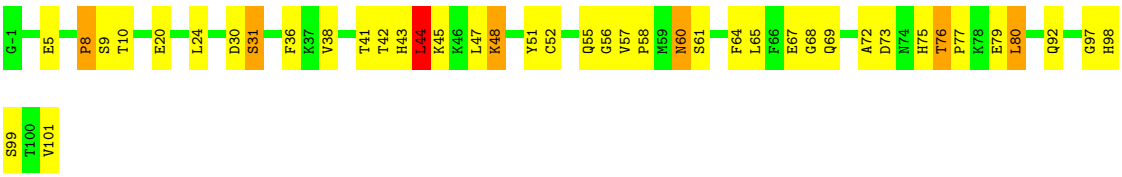


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

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

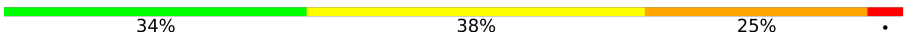
• Molecule 1: Small ubiquitin-related modifier 1

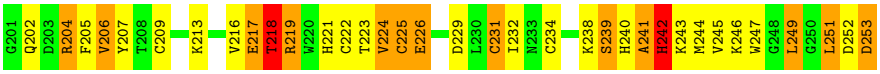
Chain A:



• Molecule 2: CREB-binding protein

Chain B:




G201
Q202
D203
R204
F205
V206
Y207
T208
C209
K213
V216
E217
T218
R219
W220
H221
C222
T223
V224
C225
E226
D229
L230
C231
T232
N233
C234
K238
S239
H240
A241
H242
K243
M244
V245
K246
W247
G248
L249
G250
L251
D252
D253

5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 6 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 calculation	
HADDOCK	structure calculation	
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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	198
Number of shifts mapped to atoms	198
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	9%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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±0.71	0±0/830 (0.0± 0.1%)	0.98±0.15	2±1/1109 (0.2± 0.1%)
2	B	2.05±0.46	4±1/450 (0.8± 0.2%)	1.14±0.08	3±1/608 (0.5± 0.2%)
All	All	1.63	24/7680 (0.3%)	1.05	29/10302 (0.3%)

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	0.5±0.5	0.0±0.0
All	All	3	0

5 of 6 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	77	PRO	CA-CB	73.88	3.01	1.53	6	1
2	B	240	HIS	CA-CB	45.35	2.53	1.53	6	5
2	B	231	CYS	CA-CB	29.39	2.18	1.53	2	5
2	B	225	CYS	CA-CB	-14.34	1.22	1.53	3	6
2	B	234	CYS	CA-CB	-12.76	1.25	1.53	1	6

5 of 12 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	77	PRO	N-CA-CB	-21.55	77.44	103.30	6	1
1	A	77	PRO	CB-CA-C	-19.78	62.54	112.00	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	101	VAL	CA-C-O	-16.17	86.14	120.10	2	6
2	B	240	HIS	CB-CA-C	15.59	141.57	110.40	4	3
2	B	231	CYS	CA-CB-SG	-14.99	87.01	114.00	2	4

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	240	HIS	CA	3

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	818	803	803	51±4
2	B	438	392	392	37±3
All	All	7548	7170	7170	523

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 36.

5 of 132 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:231:CYS:CA	2:B:231:CYS:CB	1.60	1.75	4	4
2:B:240:HIS:CA	2:B:240:HIS:CB	1.59	1.79	2	4
2:B:216:VAL:O	2:B:218:THR:N	0.95	2.00	3	6
2:B:240:HIS:CA	2:B:240:HIS:CG	0.88	2.56	2	1
1:A:44:LEU:O	1:A:44:LEU:HD23	0.84	1.72	5	1

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	101/103 (98%)	81±0 (80±0%)	12±0 (12±0%)	8±0 (8±0%)	2 14
2	B	51/53 (96%)	36±0 (71±0%)	5±0 (10±1%)	10±0 (19±1%)	0 2
All	All	912/936 (97%)	702 (77%)	104 (11%)	106 (12%)	1 7

5 of 18 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	5	GLU	6
1	A	9	SER	6
1	A	31	SER	6
1	A	44	LEU	6
1	A	60	ASN	6

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	92/92 (100%)	89±1 (97±1%)	3±1 (3±1%)	45 89
2	B	49/49 (100%)	38±0 (78±1%)	11±0 (22±1%)	3 30
All	All	846/846 (100%)	765 (90%)	81 (10%)	12 58

5 of 17 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	48	LYS	6
2	B	202	GLN	6

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Mol	Chain	Res	Type	Models (Total)
2	B	209	CYS	6
2	B	213	LYS	6
2	B	218	THR	6

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers

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 9% for the well-defined parts and 9% 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

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	198
Number of shifts mapped to atoms	198
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	8	—	None (insufficient data)
$^{13}C_{\beta}$	6	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	92	0.40 ± 0.56	None needed (< 0.5 ppm)

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 9%, i.e. 198 atoms were assigned a chemical shift out of a possible 2091. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	192/786 (24%)	92/321 (29%)	8/312 (3%)	92/153 (60%)
Sidechain	6/1124 (1%)	0/719 (0%)	6/362 (2%)	0/43 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/181 (0%)	0/92 (0%)	0/78 (0%)	0/11 (0%)
Overall	198/2091 (9%)	92/1132 (8%)	14/752 (2%)	92/207 (44%)

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	7	LYS	CB	69.57	24.03 – 41.47	21.1
1	A	68	GLY	N	133.45	91.59 – 127.52	6.7
1	A	72	ALA	H	11.08	5.31 – 11.08	5.0

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: