wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1G7E
Title	:	NMR STRUCTURE OF N-DOMAIN OF ERP29 PROTEIN
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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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

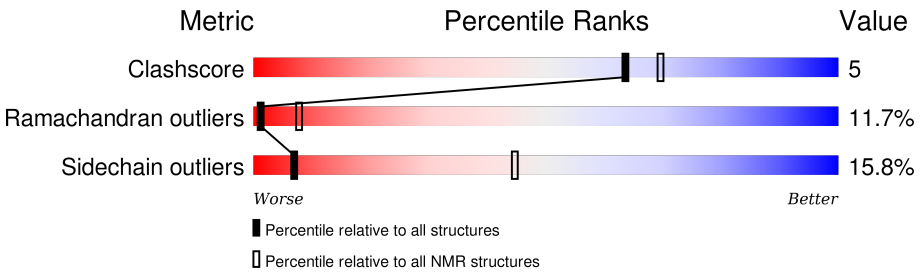
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 71%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	122	57% 35% 6% •

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models). The authors have identified model 17 as representative, based on the following criterion: *lowest energy. model #1 was best after dyana calculations, model #17 was best after opal refinement.*

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:33-A:152 (120)	0.62	1

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 5 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 5, 6, 15, 16
2	10, 12, 18
3	4, 8, 19
4	14, 20
5	7, 11
Single-model clusters	9; 13; 17

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1951 atoms, of which 971 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ENDOPLASMIC RETICULUM PROTEIN ERP29.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	122	1951	638	971	154	186	2	0

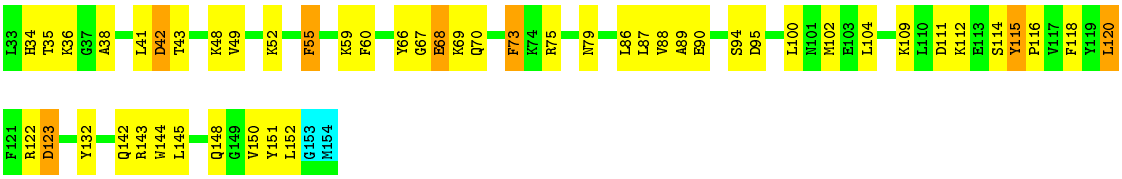
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: ENDOPLASMIC RETICULUM PROTEIN ERP29

Chain A: 57% 35% 6%

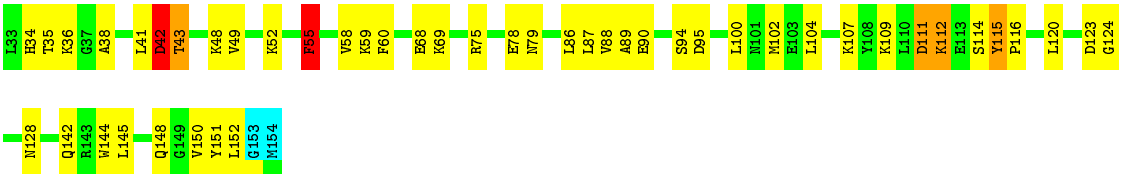


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29

Chain A: 60% 34%



5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy,target function.*

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

Software name	Classification	Version
DYANA	structure solution	1.5
OPAL	refinement	2.6

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 4919
Number of chemical shift lists	1
Total number of shifts	1290
Number of shifts mapped to atoms	1226
Number of unparsed shifts	0
Number of shifts with mapping errors	64
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	71%

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

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	0.74±0.01	0±0/993 (0.0±0.0%)	1.46±0.05	9±3/1343 (0.7±0.2%)
All	All	0.74	0/19860 (0.0%)	1.46	187/26860 (0.7%)

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	4.8±1.4
All	All	0	95

There are no bond-length outliers.

5 of 58 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	73	PHE	CB-CG-CD1	-10.61	113.38	120.80	10	11
1	A	151	TYR	CB-CG-CD2	-9.37	115.38	121.00	7	7
1	A	73	PHE	CB-CG-CD2	-9.35	114.25	120.80	2	11
1	A	151	TYR	CB-CG-CD1	-9.12	115.53	121.00	16	5
1	A	67	GLY	C-N-CA	8.19	142.18	121.70	15	7

There are no chirality outliers.

5 of 19 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	73	PHE	Sidechain	13
1	A	115	TYR	Sidechain	13
1	A	75	ARG	Sidechain	12

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	66	TYR	Sidechain	11
1	A	132	TYR	Sidechain	9

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	968	959	957	10±2
All	All	19360	19180	19140	203

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 5.

5 of 82 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:THR:HG21	1:A:38:ALA:HB3	0.80	1.51	3	2
1:A:38:ALA:HB1	1:A:89:ALA:HA	0.69	1.65	7	12
1:A:120:LEU:HD22	1:A:145:LEU:HD23	0.68	1.64	2	5
1:A:41:LEU:HD12	1:A:42:ASP:H	0.68	1.47	9	13
1:A:86:LEU:HD13	1:A:152:LEU:CD1	0.65	2.21	6	6

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	119/122 (98%)	80±4 (67±3%)	25±4 (21±3%)	14±2 (12±1%)	1 8
All	All	2380/2440 (98%)	1599 (67%)	502 (21%)	279 (12%)	1 8

5 of 32 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	109	LYS	20
1	A	42	ASP	20
1	A	68	GLU	20
1	A	123	ASP	19
1	A	111	ASP	19

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	105/106 (99%)	88±3 (84±3%)	17±3 (16±3%)	7 45
All	All	2100/2120 (99%)	1769 (84%)	331 (16%)	7 45

5 of 44 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	19
1	A	36	LYS	19
1	A	115	TYR	18
1	A	69	LYS	17
1	A	79	ASN	16

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 71% for the well-defined parts and 71% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4919

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	1290
Number of shifts mapped to atoms	1226
Number of unparsed shifts	0
Number of shifts with mapping errors	64
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. First 5 (of 64) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1	MET	HA	4.047	0.02	1
A	1	MET	HE1	2.014	0.02	1
A	4	SER	HB2	3.721	0.02	2
A	135	PRO	CA	63.5	0.1	1
A	12	SER	C	176.7	0.1	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	129	0.32 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	0	—	—
$^{13}C'$	122	0.08 ± 0.06	None needed (< 0.5 ppm)

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
^{15}N	121	0.04 ± 0.40	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 71%, i.e. 1064 atoms were assigned a chemical shift out of a possible 1501. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	580/588 (99%)	234/234 (100%)	233/240 (97%)	113/114 (99%)
Sidechain	408/758 (54%)	401/445 (90%)	0/284 (0%)	7/29 (24%)
Aromatic	76/155 (49%)	75/81 (93%)	0/71 (0%)	1/3 (33%)
Overall	1064/1501 (71%)	710/760 (93%)	233/595 (39%)	121/146 (83%)

7.1.4 Statistically unusual chemical shifts (i)

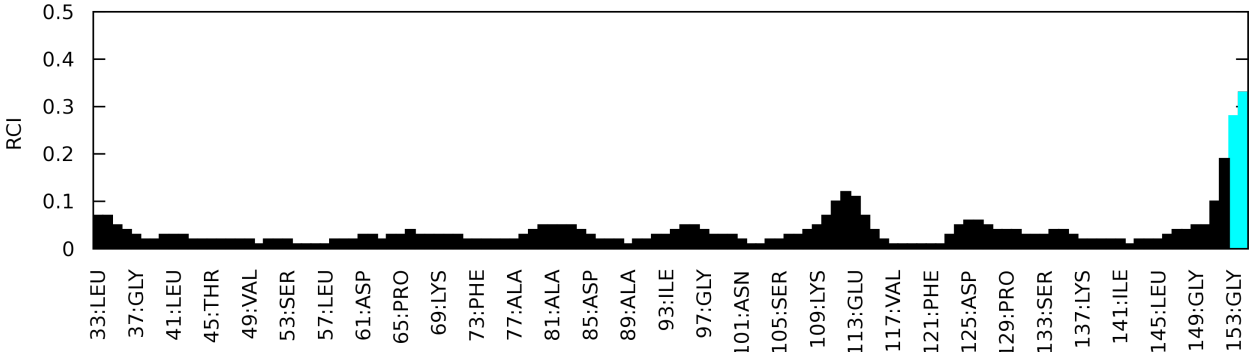
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	150	VAL	HG11	-0.48	2.13 – -0.47	-5.0
1	A	150	VAL	HG12	-0.48	2.13 – -0.47	-5.0
1	A	150	VAL	HG13	-0.48	2.13 – -0.47	-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.

Random coil index (RCI) for chain A:


RCI
0.5
0.4
0.3
0.2
0.1
0
33:LEU
37:GLY
41:LEU
45:THR
49:VAL
53:SER
57:LEU
61:ASP
65:PRO
69:LYS
73:PHE
77:ALA
81:ALA
85:ASP
89:ALA
93:ILE
97:GLY
101:ASN
105:SER
109:LYS
113:GLU
117:VAL
121:PHE
125:ASP
129:PRO
133:SER
137:LYS
141:ILE
145:LEU
149:GLY
153:GLY