



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2OII
Title : Structure of EMILIN-1 C1q-like domain
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Deposited on : 2007-01-11

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

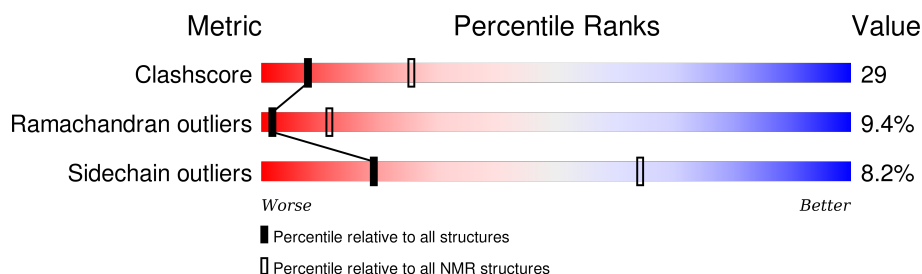
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 42%.

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	162	
1	B	162	
1	C	162	

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 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:846-A:926, A:946-A:995, B:846-B:926, B:946-B:995, C:846-C:926, C:946-C:995 (393)	0.17	8

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5793 atoms, of which 2877 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called EMILIN-1.

Mol	Chain	Residues	Atoms						Trace
1	A	131	Total	C	H	N	O	S	0
			1931	619	959	164	187	2	
1	B	131	Total	C	H	N	O	S	0
			1931	619	959	164	187	2	
1	C	131	Total	C	H	N	O	S	0
			1931	619	959	164	187	2	

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	834	MET	-	CLONING ARTIFACT	UNP Q9Y6C2
A	835	ARG	-	CLONING ARTIFACT	UNP Q9Y6C2
A	836	GLY	-	CLONING ARTIFACT	UNP Q9Y6C2
A	837	SER	-	CLONING ARTIFACT	UNP Q9Y6C2
A	838	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
A	839	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
A	840	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
A	841	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
A	842	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
A	843	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
A	844	GLY	-	CLONING ARTIFACT	UNP Q9Y6C2
A	845	SER	-	CLONING ARTIFACT	UNP Q9Y6C2
B	834	MET	-	CLONING ARTIFACT	UNP Q9Y6C2
B	835	ARG	-	CLONING ARTIFACT	UNP Q9Y6C2
B	836	GLY	-	CLONING ARTIFACT	UNP Q9Y6C2
B	837	SER	-	CLONING ARTIFACT	UNP Q9Y6C2
B	838	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
B	839	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
B	840	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
B	841	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
B	842	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
B	843	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
B	844	GLY	-	CLONING ARTIFACT	UNP Q9Y6C2
B	845	SER	-	CLONING ARTIFACT	UNP Q9Y6C2
C	834	MET	-	CLONING ARTIFACT	UNP Q9Y6C2
C	835	ARG	-	CLONING ARTIFACT	UNP Q9Y6C2
C	836	GLY	-	CLONING ARTIFACT	UNP Q9Y6C2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	837	SER	-	CLONING ARTIFACT	UNP Q9Y6C2
C	838	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
C	839	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
C	840	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
C	841	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
C	842	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
C	843	HIS	-	EXPRESSION TAG	UNP Q9Y6C2
C	844	GLY	-	CLONING ARTIFACT	UNP Q9Y6C2
C	845	SER	-	CLONING ARTIFACT	UNP Q9Y6C2

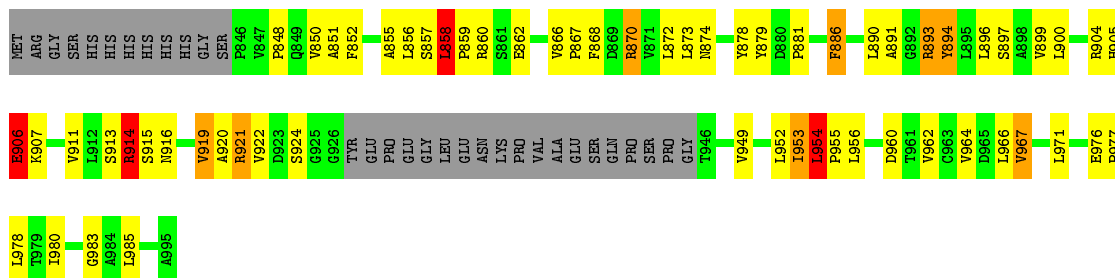


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 8. Colouring as in section 4.1 above.

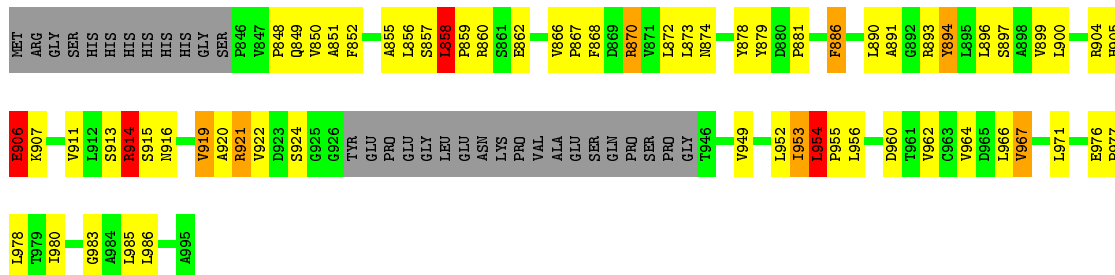
- Molecule 1: EMILIN-1

Chain A: 43% 31% 5% 19%



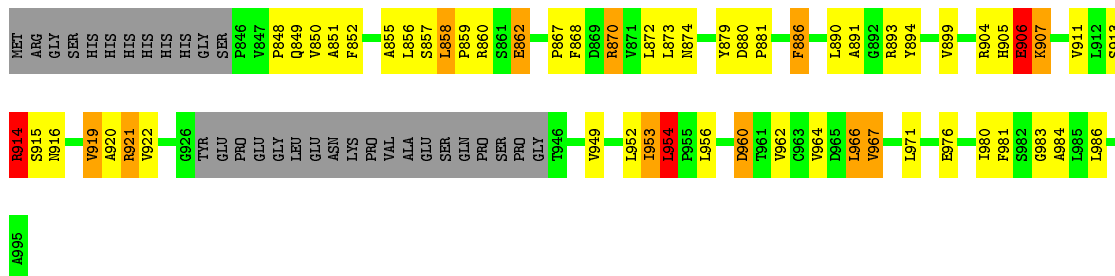
- Molecule 1: EMILIN-1

Chain B: 41% 33% 19%



- Molecule 1: EMILIN-1

Chain C: 46% 27% 7% 19%



5 Refinement protocol and experimental data overview

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

Of the 100 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
X-PLOR	refinement	2.9.9

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 5882
Number of chemical shift lists	1
Total number of shifts	2151
Number of shifts mapped to atoms	2151
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	42%

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](#)

There are no covalent bond-length or bond-angle outliers.

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	1.0±0.0	6.0±0.0
1	B	1.0±0.0	6.0±0.0
1	C	1.0±0.0	6.0±0.0
All	All	30	180

There are no bond-length outliers.

There are no bond-angle outliers.

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

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	995	ALA	CA	10
1	B	995	ALA	CA	10
1	C	995	ALA	CA	10

5 of 18 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	B	921	ARG	Sidechain	10
1	A	914	ARG	Sidechain	10
1	A	893	ARG	Sidechain	10
1	C	904	ARG	Sidechain	10
1	A	904	ARG	Sidechain	10

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	972	959	961	58±3
1	B	972	959	961	58±2
1	C	972	959	961	55±4
All	All	29160	28770	28830	1690

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 29.

5 of 389 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:856:LEU:HD11	1:C:858:LEU:HD23	0.99	1.29	6	7
1:C:920:ALA:HB3	1:C:949:VAL:HG12	0.90	1.44	9	10
1:C:890:LEU:HD22	1:C:985:LEU:HD13	0.88	1.44	5	4
1:B:920:ALA:HB3	1:B:949:VAL:HG12	0.87	1.46	1	10
1:A:890:LEU:HD22	1:A:985:LEU:HD13	0.86	1.46	4	8

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	127/162 (78%)	86±1 (68±1%)	29±1 (23±1%)	12±1 (9±1%)	2	12
1	B	127/162 (78%)	86±1 (68±1%)	30±1 (23±1%)	12±1 (9±1%)	2	12
1	C	127/162 (78%)	85±1 (67±1%)	29±1 (23±1%)	13±1 (10±1%)	2	11
All	All	3810/4860 (78%)	2575 (68%)	878 (23%)	357 (9%)	2	11

5 of 44 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	967	VAL	10
1	C	953	ILE	10
1	B	954	LEU	10
1	C	867	PRO	10
1	A	859	PRO	10

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	105/131 (80%)	97±1 (92±1%)	9±1 (8±1%)	19	64
1	B	105/131 (80%)	97±1 (92±1%)	9±1 (8±1%)	19	64
1	C	105/131 (80%)	96±1 (92±1%)	9±1 (8±1%)	18	63
All	All	3150/3930 (80%)	2891 (92%)	259 (8%)	19	64

5 of 46 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	B	894	TYR	10
1	B	954	LEU	10
1	A	954	LEU	10
1	B	906	GLU	10
1	C	914	ARG	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 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 42% for the well-defined parts and 42% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5882

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	2151
Number of shifts mapped to atoms	2151
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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
$^{13}\text{C}_\alpha$	450	0.57 ± 0.11	Should be applied
$^{13}\text{C}_\beta$	402	0.98 ± 0.09	Should be applied
$^{13}\text{C}'$	441	0.67 ± 0.08	Should be applied
^{15}N	396	-0.47 ± 0.29	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 42%, i.e. 1890 atoms were assigned a chemical shift out of a possible 4479. 0 out of 99 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1497/1905 (79%)	357/756 (47%)	783/786 (100%)	357/363 (98%)
Sidechain	393/2262 (17%)	18/1314 (1%)	366/873 (42%)	9/75 (12%)

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	Total	^1H	^{13}C	^{15}N
Aromatic	0/312 (0%)	0/171 (0%)	0/132 (0%)	0/9 (0%)
Overall	1890/4479 (42%)	375/2241 (17%)	1149/1791 (64%)	366/447 (82%)

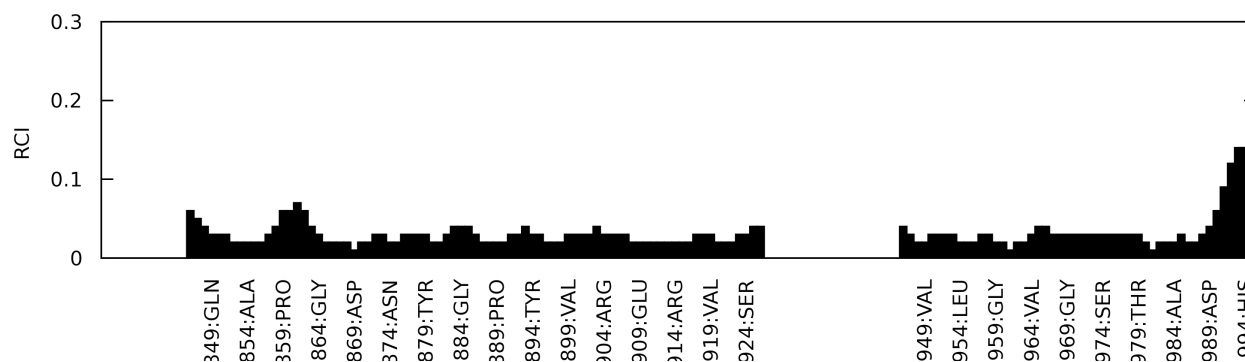
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

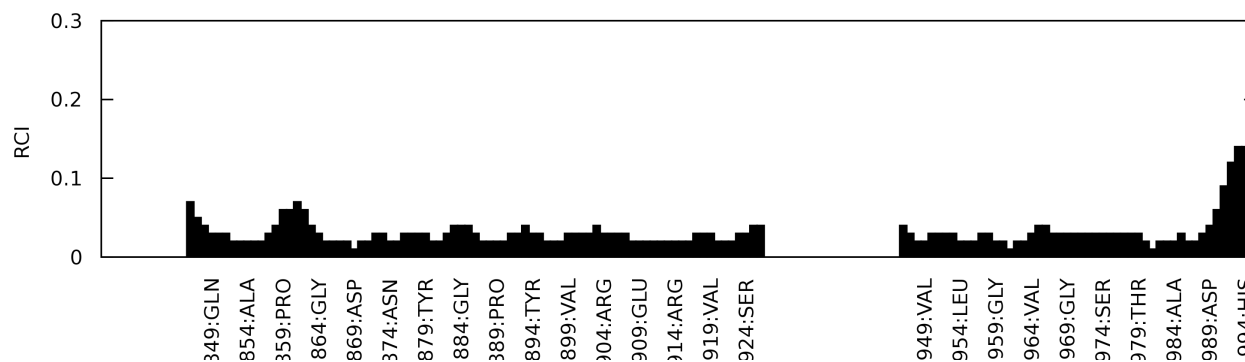
7.1.5 Random Coil Index (RCI) plots [i](#)

The images below report *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:



Random coil index (RCI) for chain B:



Random coil index (RCI) for chain C:

