



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2022 – 03:42 PM EST

PDB ID : 2OII  
Title : Structure of EMILIN-1 C1q-like domain  
Authors : Verdone, G.; Colebrooke, S.A.; Corazza, A.; Cicero, D.O.; Eliseo, T.; Viglino, P.; Campbell, I.D.; Colombatti, A.; Esposito, G.  
Deposited on : 2007-01-11

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.27  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

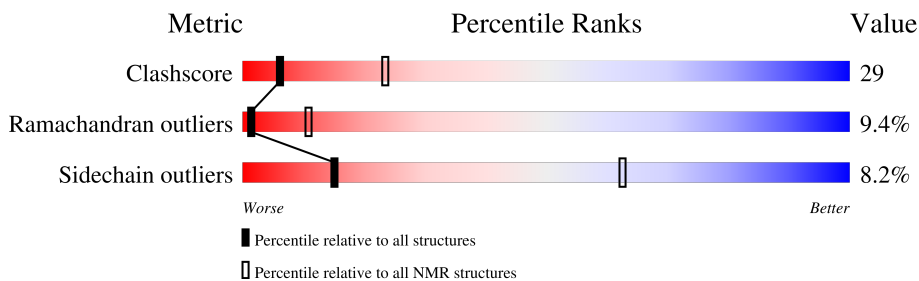
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment 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  $\geq 3$ , 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	46% 27% 6% • 19%
1	B	162	46% 27% 6% • 19%
1	C	162	47% 26% 6% • 19%

## 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 i

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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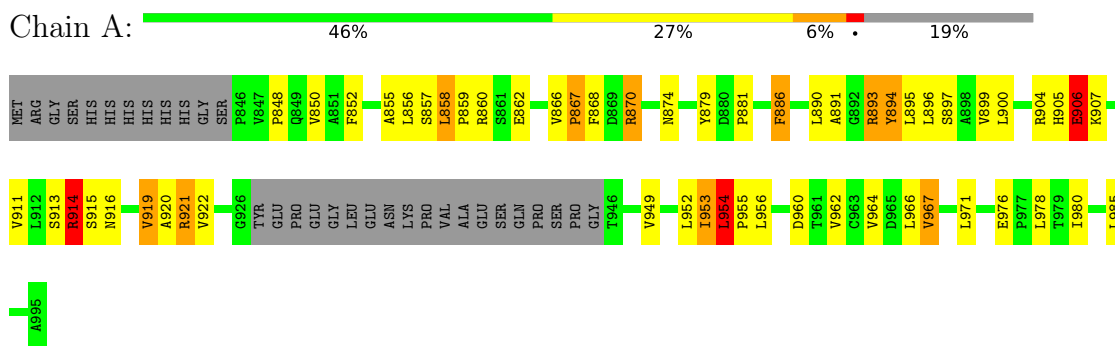
Chain	Residue	Modelled	Actual	Comment	Reference
C	837	SER	-	cloning artifact	UNP Q9Y6C2
C	838	HIS	-	expression tag	UNP Q9Y6C2
C	839	HIS	-	expression tag	UNP Q9Y6C2
C	840	HIS	-	expression tag	UNP Q9Y6C2
C	841	HIS	-	expression tag	UNP Q9Y6C2
C	842	HIS	-	expression tag	UNP Q9Y6C2
C	843	HIS	-	expression tag	UNP Q9Y6C2
C	844	GLY	-	cloning artifact	UNP Q9Y6C2
C	845	SER	-	cloning artifact	UNP Q9Y6C2

## 4 Residue-property plots [i](#)

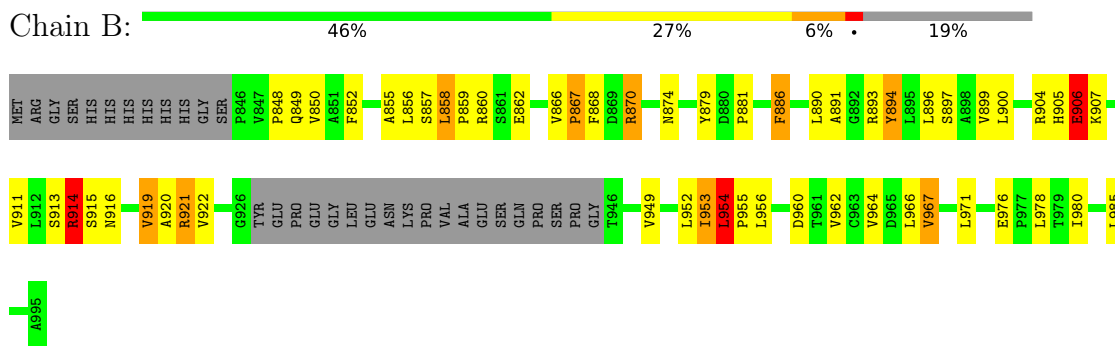
### 4.1 Average score per residue in the NMR ensemble

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.

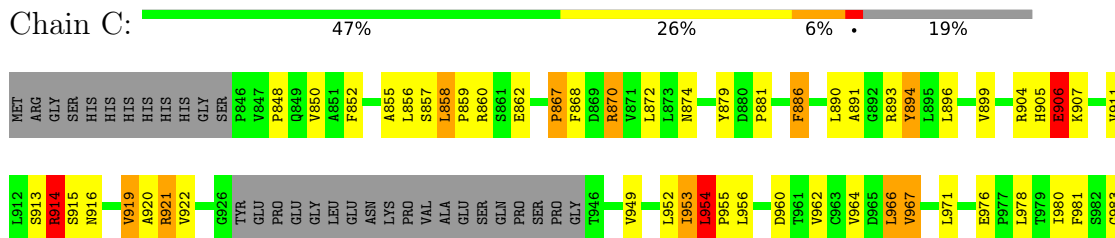
- Molecule 1: EMILIN-1



- Molecule 1: EMILIN-1



- Molecule 1: EMILIN-1



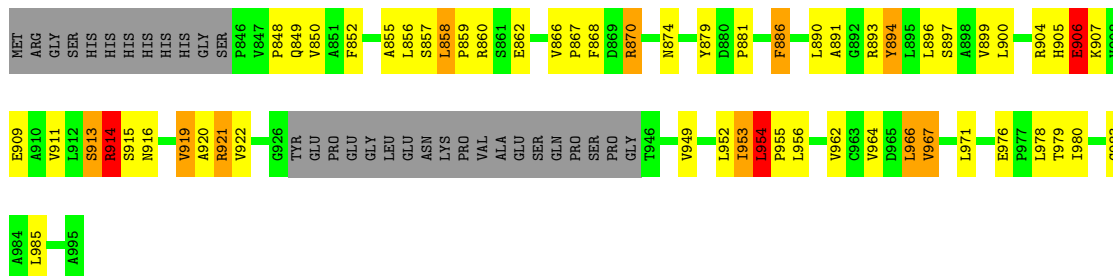






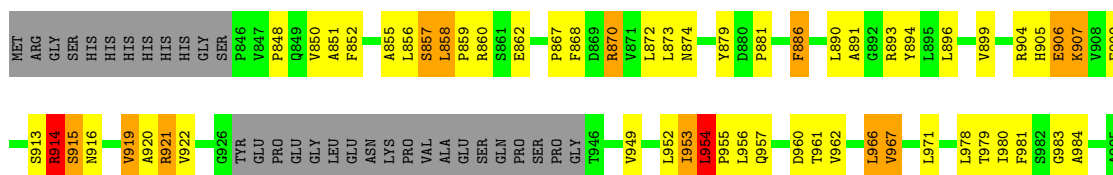
- Molecule 1: EMILIN-1

Chain B: 



- Molecule 1: EMILIN-1

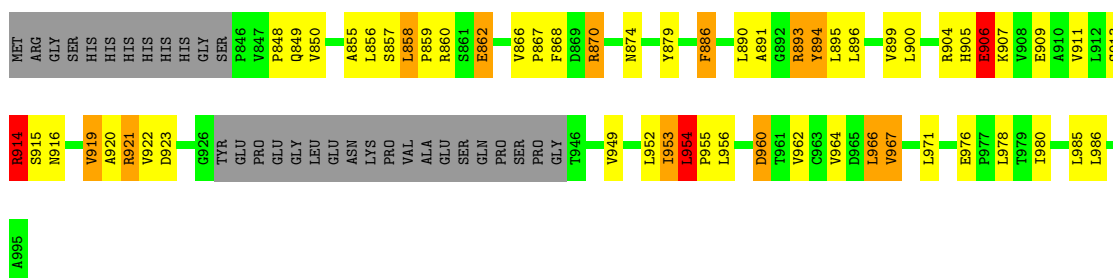
Chain C: 



#### 4.2.4 Score per residue for model 4

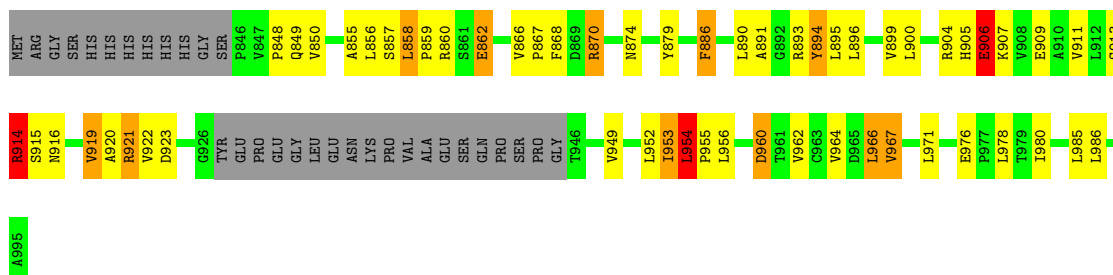
- Molecule 1: EMILIN-1

Chain A: 



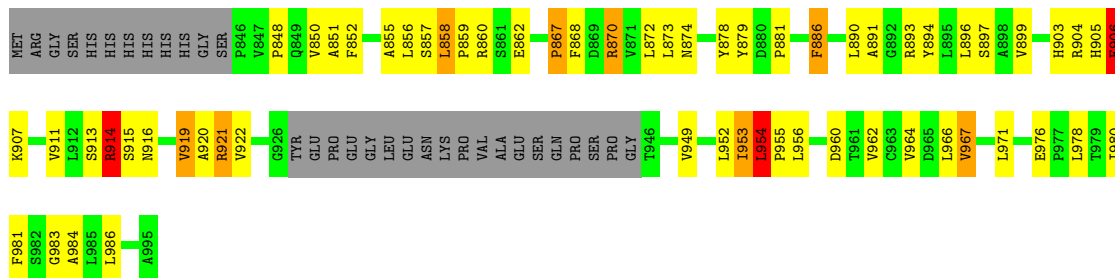
- Molecule 1: EMILIN-1

Chain B: 



- Molecule 1: EMILIN-1

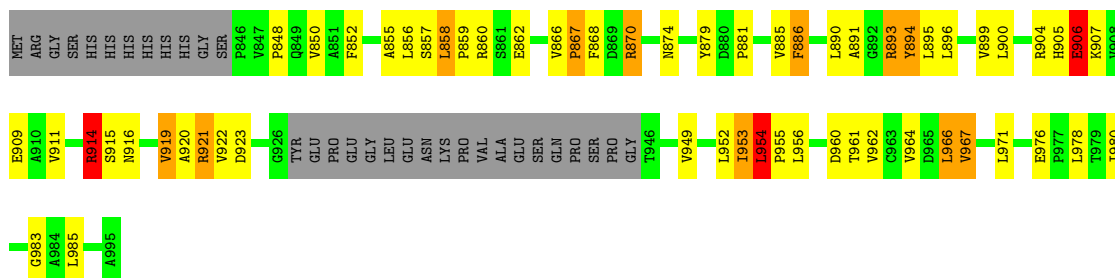
Chain C:  43% 31% 5% 19%



#### 4.2.5 Score per residue for model 5

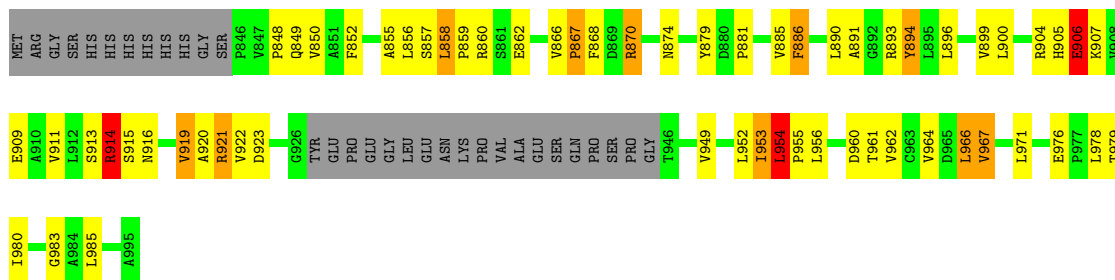
- Molecule 1: EMILIN-1

Chain A:  44% 28% 7% 19%



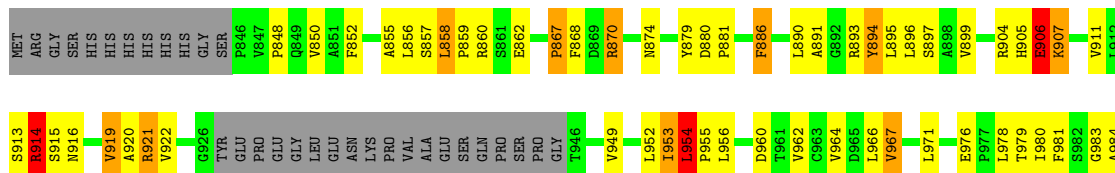
- Molecule 1: EMILIN-1

Chain B:  43% 30% 6% 19%



- Molecule 1: EMILIN-1

Chain C:  44% 28% 6% 19%

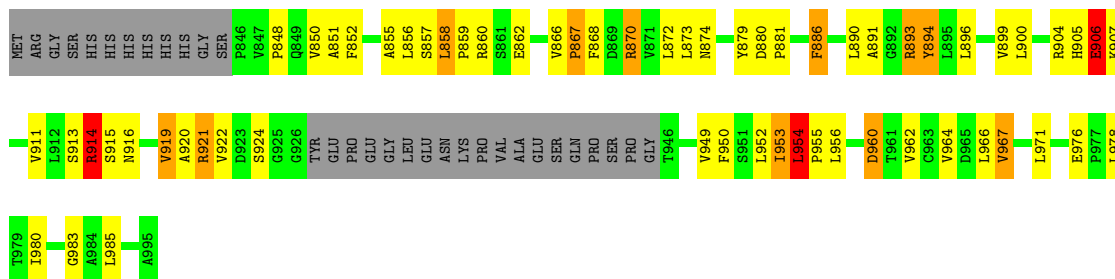




#### 4.2.6 Score per residue for model 6

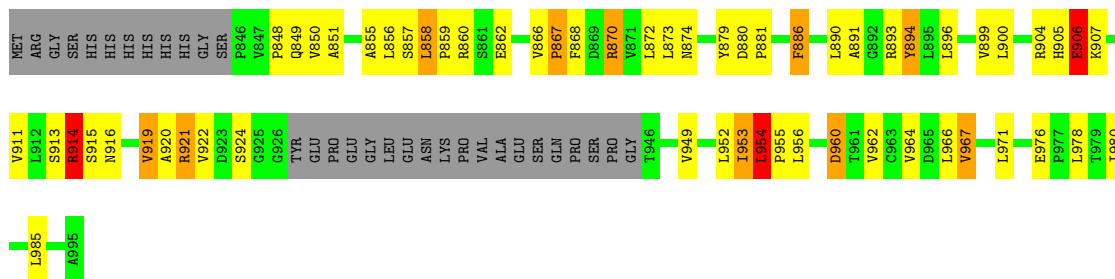
- Molecule 1: EMILIN-1

Chain A: 43% 29% 7% 19%



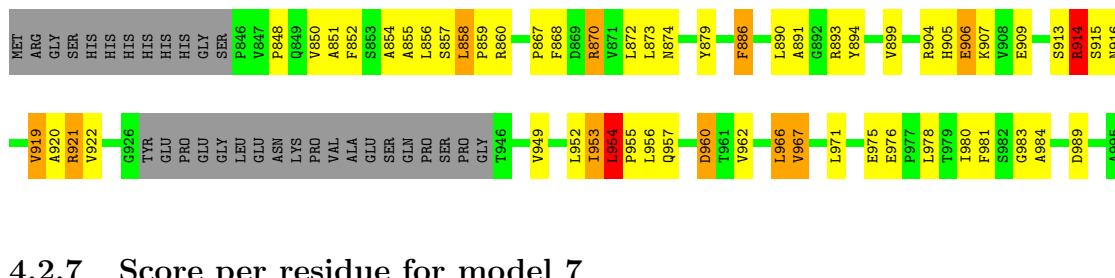
- Molecule 1: EMILIN-1

Chain B: 44% 28% 6% 19%



- Molecule 1: EMILIN-1

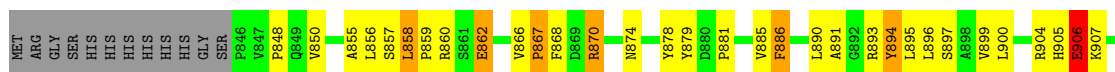
Chain C: 46% 28% 6% 19%



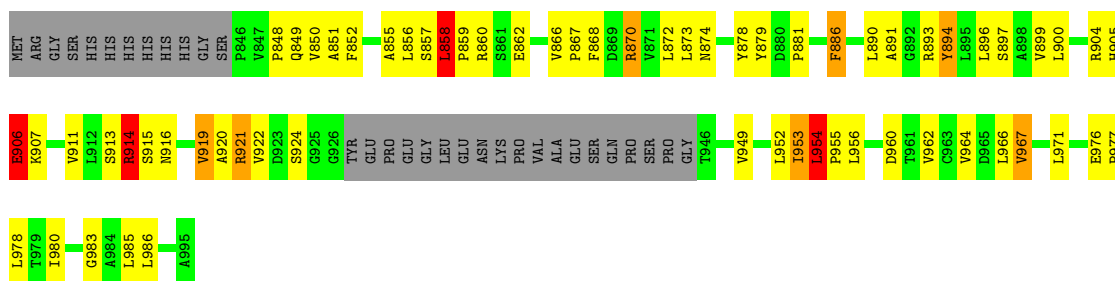
#### 4.2.7 Score per residue for model 7

- Molecule 1: EMILIN-1

Chain A: 44% 28% 6% 19%

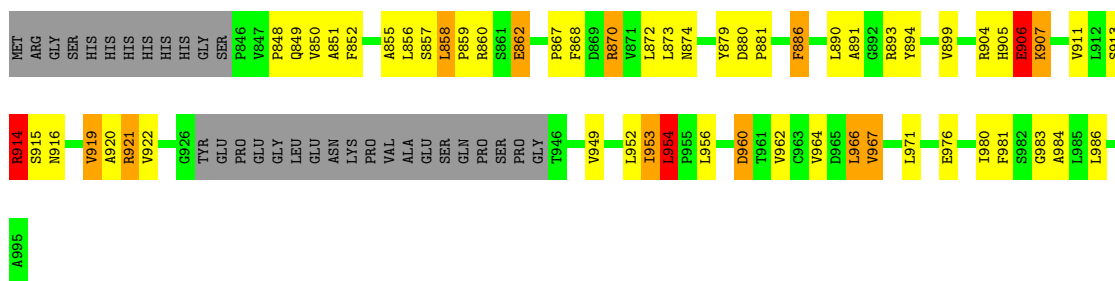






- Molecule 1: EMILIN-1

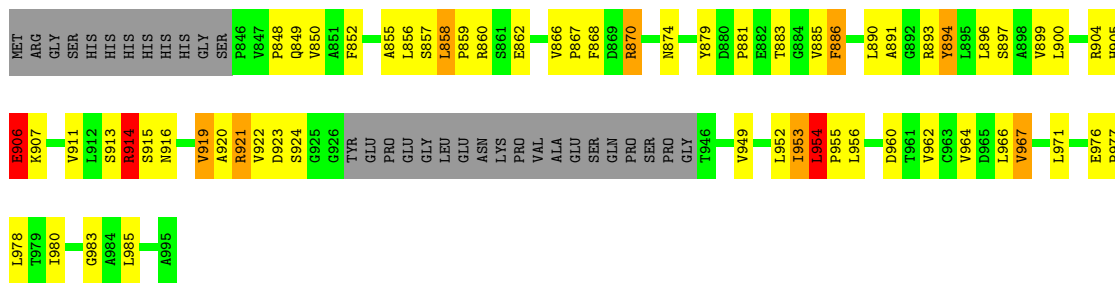
Chain C: 46% 27% 7% 19%



#### 4.2.9 Score per residue for model 9

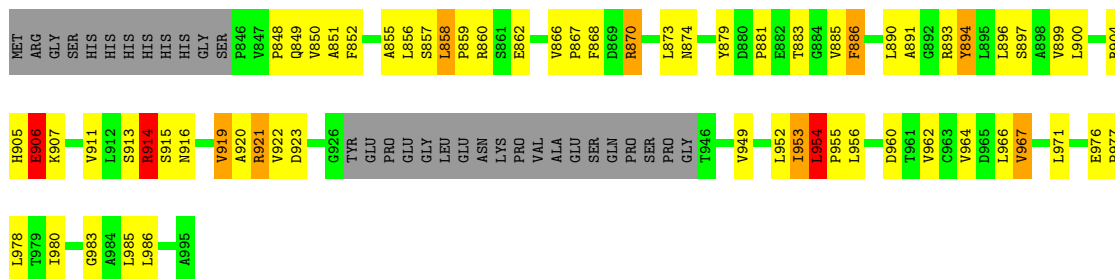
- Molecule 1: EMILIN-1

Chain A: 43% 31% 5% 19%



- Molecule 1: EMILIN-1

Chain B: 41% 33% 5% 19%





T980  
F981  
G982  
G983  
A984  
L985  
A986

## 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

No chemical shift data was provided.



## 6 Model quality

### 6.1 Standard geometry

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

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	860	ARG	Sidechain	10
1	A	870	ARG	Sidechain	10
1	A	893	ARG	Sidechain	10
1	A	904	ARG	Sidechain	10
1	A	914	ARG	Sidechain	10
1	A	921	ARG	Sidechain	10
1	B	860	ARG	Sidechain	10
1	B	870	ARG	Sidechain	10
1	B	893	ARG	Sidechain	10
1	B	904	ARG	Sidechain	10
1	B	914	ARG	Sidechain	10
1	B	921	ARG	Sidechain	10
1	C	860	ARG	Sidechain	10

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Mol	Chain	Res	Type	Group	Models (Total)
1	C	870	ARG	Sidechain	10
1	C	893	ARG	Sidechain	10
1	C	904	ARG	Sidechain	10
1	C	914	ARG	Sidechain	10
1	C	921	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.

All 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
1:B:890:LEU:HD22	1:B:985:LEU:HD13	0.86	1.46	4	8
1:A:920:ALA:HB3	1:A:949:VAL:HG12	0.84	1.47	1	10
1:C:848:PRO:O	1:C:850:VAL:HG23	0.79	1.76	2	10
1:B:886:PHE:HB3	1:B:962:VAL:HG22	0.78	1.55	1	10
1:C:911:VAL:HG23	1:C:964:VAL:HG22	0.78	1.55	5	4
1:C:914:ARG:NH1	1:C:956:LEU:HD23	0.78	1.92	7	6
1:C:894:TYR:CE1	1:C:954:LEU:HD23	0.78	2.14	4	1
1:C:886:PHE:HB3	1:C:962:VAL:HG22	0.78	1.55	9	10
1:C:894:TYR:CE2	1:C:954:LEU:HD23	0.77	2.15	3	4
1:B:856:LEU:HD11	1:B:858:LEU:HD23	0.77	1.56	2	4
1:A:856:LEU:HD11	1:A:858:LEU:HD23	0.77	1.56	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:886:PHE:HB3	1:A:962:VAL:HG22	0.76	1.57	10	10
1:A:914:ARG:NH1	1:A:956:LEU:HD23	0.76	1.95	10	8
1:A:953:ILE:HD11	1:C:872:LEU:HD13	0.76	1.55	4	4
1:C:886:PHE:CB	1:C:962:VAL:HG22	0.76	2.09	1	10
1:B:914:ARG:NH1	1:B:956:LEU:HD23	0.76	1.95	10	8
1:A:855:ALA:HB3	1:A:870:ARG:CB	0.75	2.12	6	10
1:C:914:ARG:CZ	1:C:956:LEU:HD23	0.74	2.12	6	3
1:B:855:ALA:HB3	1:B:870:ARG:CB	0.74	2.12	8	10
1:C:896:LEU:HD23	1:C:897:SER:N	0.74	1.98	1	5
1:A:848:PRO:O	1:A:850:VAL:HG23	0.73	1.84	1	10
1:B:886:PHE:CB	1:B:962:VAL:HG22	0.73	2.14	9	10
1:A:856:LEU:HD23	1:A:867:PRO:O	0.73	1.84	2	5
1:C:914:ARG:NH1	1:C:956:LEU:HD13	0.73	1.99	8	2
1:B:894:TYR:OH	1:B:896:LEU:HD12	0.72	1.85	8	8
1:A:894:TYR:OH	1:A:896:LEU:HD12	0.72	1.85	8	8
1:A:886:PHE:CB	1:A:962:VAL:HG22	0.71	2.14	9	10
1:C:954:LEU:HD22	1:C:954:LEU:O	0.71	1.85	2	10
1:B:856:LEU:HD23	1:B:867:PRO:O	0.71	1.84	2	5
1:C:920:ALA:HB3	1:C:949:VAL:CG1	0.71	2.15	9	9
1:B:848:PRO:O	1:B:850:VAL:HG23	0.71	1.84	1	10
1:C:856:LEU:HD23	1:C:867:PRO:O	0.71	1.86	10	5
1:A:954:LEU:HD22	1:A:954:LEU:O	0.71	1.86	10	10
1:C:894:TYR:OH	1:C:956:LEU:HD22	0.71	1.86	3	3
1:B:954:LEU:HD22	1:B:954:LEU:O	0.70	1.86	10	10
1:A:914:ARG:CZ	1:A:956:LEU:HD23	0.70	2.16	10	1
1:B:914:ARG:CZ	1:B:956:LEU:HD23	0.69	2.16	10	1
1:B:862:GLU:OE1	1:B:866:VAL:HG22	0.68	1.88	8	4
1:C:955:PRO:C	1:C:956:LEU:HD12	0.68	2.07	4	7
1:C:856:LEU:HD11	1:C:858:LEU:CD2	0.68	2.18	2	8
1:C:911:VAL:HG22	1:C:964:VAL:HG13	0.68	1.66	9	4
1:B:856:LEU:HD11	1:B:858:LEU:CD2	0.68	2.19	5	5
1:A:862:GLU:OE1	1:A:866:VAL:HG22	0.68	1.88	8	4
1:B:916:ASN:HB2	1:B:919:VAL:HG21	0.68	1.66	3	10
1:B:858:LEU:HD22	1:B:862:GLU:OE2	0.67	1.90	4	3
1:A:856:LEU:HD11	1:A:858:LEU:CD2	0.67	2.19	5	4
1:A:858:LEU:HD22	1:A:862:GLU:OE2	0.67	1.90	4	3
1:C:855:ALA:HB3	1:C:870:ARG:CB	0.66	2.20	6	10
1:A:858:LEU:HD22	1:A:862:GLU:OE1	0.66	1.91	10	2
1:B:955:PRO:C	1:B:956:LEU:HD12	0.66	2.11	9	10
1:C:890:LEU:HD12	1:C:891:ALA:N	0.65	2.06	1	1
1:B:911:VAL:HG22	1:B:964:VAL:HG13	0.65	1.67	9	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:856:LEU:HD12	1:A:978:LEU:HD23	0.65	1.68	9	7
1:B:858:LEU:HD22	1:B:862:GLU:OE1	0.65	1.91	10	2
1:A:921:ARG:HG3	1:A:922:VAL:HG23	0.65	1.67	6	10
1:B:921:ARG:HG3	1:B:922:VAL:HG23	0.65	1.69	10	10
1:A:916:ASN:HB2	1:A:919:VAL:HG21	0.65	1.67	3	10
1:A:955:PRO:C	1:A:956:LEU:HD12	0.65	2.11	9	10
1:B:856:LEU:HD12	1:B:978:LEU:HD23	0.64	1.68	9	6
1:A:911:VAL:HG22	1:A:964:VAL:HG13	0.64	1.67	9	9
1:C:894:TYR:CZ	1:C:954:LEU:HD23	0.64	2.27	7	3
1:B:920:ALA:HB3	1:B:949:VAL:CG1	0.64	2.21	1	5
1:B:855:ALA:HB2	1:B:872:LEU:HD11	0.64	1.67	8	3
1:C:916:ASN:HB2	1:C:919:VAL:HG21	0.64	1.70	8	10
1:A:895:LEU:HD23	1:B:952:LEU:HD11	0.64	1.68	5	2
1:A:855:ALA:HB2	1:A:872:LEU:HD11	0.64	1.67	8	3
1:A:920:ALA:HB3	1:A:949:VAL:CG1	0.63	2.22	1	3
1:A:858:LEU:HD22	1:A:862:GLU:CD	0.62	2.15	10	3
1:C:921:ARG:HG3	1:C:922:VAL:HG23	0.61	1.72	4	10
1:B:858:LEU:HD22	1:B:862:GLU:CD	0.61	2.15	10	3
1:B:855:ALA:HB3	1:B:870:ARG:HB2	0.60	1.73	6	10
1:C:850:VAL:HG11	1:C:890:LEU:HD21	0.60	1.73	3	5
1:A:855:ALA:HB3	1:A:870:ARG:HB2	0.60	1.73	10	10
1:A:909:GLU:OE2	1:A:966:LEU:HD12	0.60	1.97	5	4
1:B:909:GLU:OE2	1:B:966:LEU:HD12	0.60	1.97	5	4
1:C:856:LEU:HD12	1:C:978:LEU:HG	0.59	1.73	4	1
1:A:953:ILE:HD11	1:C:872:LEU:CD1	0.59	2.27	4	1
1:C:911:VAL:HG13	1:C:964:VAL:HG22	0.59	1.74	1	2
1:C:954:LEU:N	1:C:954:LEU:CD1	0.58	2.67	4	10
1:B:920:ALA:HB1	1:B:923:ASP:HB2	0.58	1.75	5	4
1:A:920:ALA:HB1	1:A:923:ASP:HB2	0.58	1.75	5	4
1:A:856:LEU:HD13	1:A:857:SER:N	0.58	2.14	5	10
1:C:855:ALA:HB3	1:C:870:ARG:HB2	0.57	1.74	3	10
1:B:856:LEU:HD13	1:B:857:SER:N	0.57	2.15	5	10
1:A:856:LEU:CD1	1:A:978:LEU:HD23	0.57	2.29	4	4
1:C:953:ILE:HD12	1:C:954:LEU:N	0.57	2.14	9	5
1:B:986:LEU:CD1	1:C:986:LEU:HD11	0.57	2.30	9	3
1:C:966:LEU:HD23	1:C:966:LEU:O	0.57	1.99	2	1
1:B:977:PRO:C	1:B:978:LEU:HD12	0.57	2.20	10	3
1:C:909:GLU:OE2	1:C:966:LEU:HD12	0.57	2.00	10	4
1:B:856:LEU:CD1	1:B:978:LEU:HD23	0.56	2.29	4	4
1:A:954:LEU:CD1	1:A:954:LEU:N	0.56	2.69	1	10
1:A:899:VAL:HG21	1:A:980:ILE:HB	0.56	1.78	5	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:914:ARG:NE	1:C:956:LEU:HD22	0.56	2.16	8	1
1:B:954:LEU:CD1	1:B:954:LEU:N	0.55	2.68	1	10
1:C:883:THR:OG1	1:C:885:VAL:HG23	0.55	2.00	10	1
1:A:977:PRO:C	1:A:978:LEU:HD12	0.55	2.21	10	4
1:B:899:VAL:HG21	1:B:980:ILE:HB	0.55	1.77	9	10
1:C:911:VAL:CG2	1:C:964:VAL:HG22	0.55	2.29	5	3
1:A:916:ASN:CB	1:A:919:VAL:HG21	0.55	2.32	3	7
1:B:885:VAL:HG13	1:B:961:THR:HG21	0.55	1.79	5	3
1:A:885:VAL:HG13	1:A:961:THR:HG21	0.55	1.79	5	3
1:B:890:LEU:HD11	1:B:985:LEU:CD1	0.54	2.32	2	2
1:C:911:VAL:HG23	1:C:964:VAL:CG2	0.54	2.31	5	3
1:A:890:LEU:HD11	1:A:985:LEU:CD1	0.54	2.32	2	2
1:B:916:ASN:CB	1:B:919:VAL:HG21	0.54	2.31	3	9
1:C:914:ARG:HD3	1:C:962:VAL:HG12	0.54	1.79	8	3
1:B:856:LEU:C	1:B:856:LEU:HD13	0.53	2.23	4	3
1:A:856:LEU:C	1:A:856:LEU:HD13	0.53	2.23	4	4
1:C:856:LEU:HD13	1:C:857:SER:N	0.53	2.19	7	10
1:C:899:VAL:HG21	1:C:980:ILE:HB	0.53	1.79	5	10
1:C:858:LEU:HD22	1:C:862:GLU:HG3	0.53	1.80	9	2
1:C:890:LEU:HD22	1:C:985:LEU:CD1	0.53	2.27	5	1
1:A:896:LEU:HD23	1:A:897:SER:N	0.53	2.19	2	7
1:A:921:ARG:NH1	1:A:962:VAL:HG11	0.52	2.19	3	3
1:C:856:LEU:HD13	1:C:856:LEU:C	0.52	2.24	9	7
1:C:855:ALA:HB2	1:C:872:LEU:HD11	0.52	1.80	2	4
1:C:971:LEU:HD23	1:C:971:LEU:O	0.52	2.04	2	1
1:A:911:VAL:HG13	1:A:964:VAL:HG22	0.52	1.81	9	3
1:B:896:LEU:HD23	1:B:897:SER:N	0.52	2.19	2	7
1:C:978:LEU:HD12	1:C:978:LEU:N	0.52	2.19	2	6
1:B:921:ARG:NH1	1:B:962:VAL:HG11	0.52	2.19	8	3
1:C:894:TYR:OH	1:C:896:LEU:HD12	0.52	2.05	10	1
1:B:879:TYR:CG	1:B:879:TYR:O	0.52	2.63	1	7
1:B:955:PRO:O	1:B:956:LEU:HD12	0.51	2.05	4	6
1:C:856:LEU:C	1:C:856:LEU:HD13	0.51	2.25	5	3
1:C:852:PHE:CD1	1:C:879:TYR:CE1	0.51	2.99	9	1
1:A:978:LEU:N	1:A:978:LEU:HD12	0.51	2.21	1	5
1:B:856:LEU:HD13	1:B:856:LEU:C	0.51	2.26	1	7
1:B:920:ALA:HB1	1:B:923:ASP:CB	0.51	2.36	4	3
1:A:858:LEU:CD2	1:A:866:VAL:HG12	0.51	2.36	1	1
1:C:879:TYR:O	1:C:879:TYR:CG	0.51	2.63	9	10
1:B:911:VAL:HG13	1:B:964:VAL:HG22	0.51	1.81	9	3
1:B:858:LEU:CD2	1:B:866:VAL:HG12	0.51	2.36	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:896:LEU:C	1:B:896:LEU:HD23	0.51	2.26	9	7
1:C:879:TYR:CE2	1:C:981:PHE:CD1	0.51	2.99	6	9
1:A:879:TYR:CG	1:A:879:TYR:O	0.50	2.63	1	10
1:C:916:ASN:CB	1:C:919:VAL:HG21	0.50	2.34	6	8
1:A:856:LEU:HD13	1:A:856:LEU:C	0.50	2.27	7	6
1:A:879:TYR:CE2	1:A:981:PHE:CD1	0.50	2.99	1	1
1:A:920:ALA:HB1	1:A:923:ASP:CB	0.50	2.36	4	3
1:C:886:PHE:HB2	1:C:962:VAL:HG22	0.50	1.84	2	2
1:C:906:GLU:O	1:C:907:LYS:CB	0.50	2.60	3	10
1:A:896:LEU:C	1:A:896:LEU:HD23	0.50	2.27	9	7
1:C:905:HIS:O	1:C:906:GLU:CB	0.50	2.60	8	10
1:B:879:TYR:CE2	1:B:981:PHE:CD1	0.50	3.00	1	1
1:B:978:LEU:HD12	1:B:978:LEU:N	0.49	2.21	1	4
1:A:900:LEU:HD12	1:A:924:SER:HB2	0.49	1.83	8	5
1:A:955:PRO:O	1:A:956:LEU:HD12	0.49	2.06	4	5
1:B:905:HIS:O	1:B:906:GLU:CB	0.49	2.60	1	10
1:C:954:LEU:N	1:C:954:LEU:HD12	0.49	2.23	1	10
1:A:905:HIS:O	1:A:906:GLU:CB	0.49	2.60	1	10
1:A:966:LEU:O	1:A:966:LEU:HD23	0.49	2.08	2	1
1:A:858:LEU:HD12	1:A:858:LEU:C	0.49	2.28	6	5
1:B:894:TYR:CD2	1:B:954:LEU:HD23	0.49	2.43	5	5
1:C:850:VAL:HG13	1:C:878:TYR:CE2	0.49	2.43	1	1
1:B:879:TYR:CB	1:B:886:PHE:CD2	0.48	2.95	9	10
1:A:879:TYR:CB	1:A:886:PHE:CD2	0.48	2.96	9	10
1:B:900:LEU:HD12	1:B:924:SER:HB2	0.48	1.83	8	4
1:A:894:TYR:CD2	1:A:954:LEU:HD23	0.48	2.42	5	5
1:A:906:GLU:O	1:A:907:LYS:CB	0.48	2.61	7	10
1:B:966:LEU:HD23	1:B:966:LEU:O	0.48	2.08	2	1
1:B:858:LEU:C	1:B:858:LEU:HD12	0.48	2.28	6	5
1:B:851:ALA:HB3	1:B:873:LEU:HG	0.48	1.86	6	4
1:A:883:THR:OG1	1:A:885:VAL:HG23	0.48	2.08	9	1
1:B:953:ILE:HD12	1:B:955:PRO:HD3	0.48	1.86	2	1
1:B:906:GLU:O	1:B:907:LYS:CB	0.48	2.62	10	10
1:C:879:TYR:CB	1:C:886:PHE:CD2	0.47	2.98	3	10
1:B:900:LEU:HD22	1:B:900:LEU:N	0.47	2.24	6	8
1:C:879:TYR:CB	1:C:886:PHE:CG	0.47	2.97	2	8
1:A:856:LEU:HG	1:A:866:VAL:HG11	0.47	1.87	4	2
1:C:868:PHE:CD1	1:C:868:PHE:N	0.47	2.82	3	9
1:B:856:LEU:HG	1:B:866:VAL:HG11	0.47	1.87	4	2
1:B:953:ILE:O	1:B:954:LEU:HB3	0.47	2.09	2	10
1:A:900:LEU:HD22	1:A:900:LEU:N	0.47	2.24	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:883:THR:OG1	1:B:885:VAL:HG23	0.47	2.09	9	1
1:C:952:LEU:O	1:C:953:ILE:O	0.47	2.33	10	10
1:C:953:ILE:O	1:C:954:LEU:HB3	0.47	2.10	10	9
1:A:851:ALA:HB3	1:A:873:LEU:HG	0.47	1.85	6	3
1:B:858:LEU:HD12	1:B:858:LEU:O	0.47	2.09	8	1
1:A:954:LEU:N	1:A:954:LEU:HD12	0.47	2.24	7	10
1:A:896:LEU:HD23	1:A:896:LEU:C	0.47	2.29	2	2
1:B:921:ARG:HH12	1:B:962:VAL:HG11	0.47	1.70	3	1
1:A:868:PHE:CD1	1:A:868:PHE:N	0.47	2.83	8	10
1:B:879:TYR:O	1:B:879:TYR:CG	0.47	2.67	4	3
1:A:858:LEU:HD12	1:A:858:LEU:O	0.47	2.09	8	1
1:A:953:ILE:O	1:A:954:LEU:HB3	0.47	2.10	2	10
1:B:954:LEU:N	1:B:954:LEU:HD12	0.47	2.25	1	10
1:B:896:LEU:HD23	1:B:896:LEU:C	0.47	2.29	2	2
1:C:858:LEU:C	1:C:858:LEU:HD12	0.47	2.29	5	2
1:A:879:TYR:CB	1:A:886:PHE:CG	0.46	2.98	7	9
1:B:879:TYR:CB	1:B:886:PHE:CG	0.46	2.98	8	9
1:B:990:PRO:HD2	1:B:992:LEU:HD12	0.46	1.86	1	1
1:B:868:PHE:N	1:B:868:PHE:CD1	0.46	2.83	8	8
1:C:896:LEU:HD11	1:C:981:PHE:CE1	0.46	2.46	3	1
1:C:920:ALA:O	1:C:949:VAL:HG12	0.46	2.10	10	4
1:C:850:VAL:CG1	1:C:890:LEU:HD21	0.46	2.40	3	3
1:A:868:PHE:CD1	1:A:881:PRO:CG	0.46	2.99	5	3
1:B:868:PHE:CD1	1:B:881:PRO:CG	0.46	2.99	5	3
1:A:905:HIS:O	1:A:906:GLU:CG	0.46	2.64	5	10
1:C:905:HIS:O	1:C:906:GLU:CG	0.46	2.64	1	8
1:B:894:TYR:CD1	1:B:895:LEU:N	0.46	2.84	2	5
1:B:905:HIS:O	1:B:906:GLU:CG	0.46	2.64	5	10
1:A:953:ILE:HD12	1:A:955:PRO:HD3	0.46	1.87	2	1
1:C:852:PHE:CD1	1:C:852:PHE:N	0.46	2.84	3	6
1:B:868:PHE:CD1	1:B:868:PHE:N	0.46	2.83	5	2
1:C:868:PHE:CD1	1:C:881:PRO:CG	0.45	2.99	3	5
1:C:896:LEU:C	1:C:896:LEU:HD23	0.45	2.31	2	2
1:A:852:PHE:HA	1:A:874:ASN:HB3	0.45	1.88	1	1
1:C:894:TYR:CD1	1:C:895:LEU:N	0.45	2.85	5	4
1:A:894:TYR:CD1	1:A:895:LEU:N	0.45	2.84	2	5
1:A:990:PRO:HD2	1:A:992:LEU:HD12	0.45	1.86	1	1
1:C:977:PRO:C	1:C:978:LEU:HD12	0.45	2.32	7	2
1:A:879:TYR:HB2	1:A:886:PHE:CD2	0.45	2.47	1	1
1:B:852:PHE:HA	1:B:874:ASN:HB3	0.45	1.89	1	1
1:B:900:LEU:N	1:B:900:LEU:CD2	0.44	2.81	6	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:913:SER:OG	1:A:919:VAL:HG11	0.44	2.12	10	2
1:A:900:LEU:N	1:A:900:LEU:CD2	0.44	2.81	6	9
1:A:914:ARG:O	1:A:915:SER:CB	0.44	2.66	10	10
1:B:913:SER:OG	1:B:919:VAL:HG11	0.44	2.13	10	2
1:A:858:LEU:HD23	1:A:866:VAL:HG13	0.44	1.90	10	2
1:C:886:PHE:O	1:C:961:THR:HG23	0.44	2.11	3	1
1:C:954:LEU:HB2	1:C:956:LEU:HD13	0.44	1.88	10	1
1:C:868:PHE:CD1	1:C:881:PRO:HG2	0.44	2.47	2	7
1:C:854:ALA:HB1	1:C:868:PHE:CD2	0.44	2.48	6	1
1:C:858:LEU:CD2	1:C:866:VAL:HG12	0.44	2.42	9	1
1:A:952:LEU:O	1:A:953:ILE:O	0.44	2.36	2	10
1:C:879:TYR:HB2	1:C:886:PHE:CD2	0.44	2.48	9	5
1:A:921:ARG:HH12	1:A:962:VAL:HG11	0.44	1.70	3	1
1:B:855:ALA:HB3	1:B:870:ARG:HB3	0.44	1.88	6	2
1:C:856:LEU:HD21	1:C:858:LEU:HD23	0.44	1.89	10	1
1:B:879:TYR:HB2	1:B:886:PHE:CD2	0.44	2.47	1	1
1:B:914:ARG:HD3	1:B:962:VAL:HG12	0.44	1.89	6	3
1:C:850:VAL:CG1	1:C:878:TYR:CE2	0.44	3.01	1	1
1:B:858:LEU:CD2	1:B:866:VAL:HG13	0.44	2.43	7	3
1:C:913:SER:OG	1:C:919:VAL:HG11	0.43	2.12	9	5
1:C:879:TYR:O	1:C:879:TYR:CD2	0.43	2.70	6	8
1:B:857:SER:O	1:B:858:LEU:O	0.43	2.36	2	10
1:B:952:LEU:O	1:B:953:ILE:O	0.43	2.36	2	10
1:C:851:ALA:HB3	1:C:873:LEU:HG	0.43	1.89	3	5
1:C:896:LEU:HD23	1:C:896:LEU:C	0.43	2.34	5	2
1:A:858:LEU:CD2	1:A:866:VAL:HG13	0.43	2.44	3	3
1:A:920:ALA:O	1:A:949:VAL:HG12	0.43	2.13	3	1
1:A:906:GLU:CG	1:A:907:LYS:N	0.43	2.82	4	10
1:A:966:LEU:C	1:A:967:VAL:HG23	0.43	2.34	4	10
1:B:914:ARG:O	1:B:915:SER:CB	0.43	2.66	9	10
1:B:966:LEU:C	1:B:967:VAL:HG23	0.43	2.34	10	10
1:C:857:SER:O	1:C:858:LEU:O	0.43	2.37	6	10
1:C:966:LEU:C	1:C:967:VAL:HG23	0.43	2.34	3	10
1:C:914:ARG:HH11	1:C:962:VAL:HG13	0.43	1.73	7	3
1:C:914:ARG:NE	1:C:962:VAL:HG12	0.43	2.29	10	1
1:C:906:GLU:CG	1:C:907:LYS:N	0.43	2.82	5	7
1:A:914:ARG:HD3	1:A:962:VAL:HG12	0.43	1.90	6	4
1:A:857:SER:O	1:A:858:LEU:O	0.43	2.36	2	10
1:B:858:LEU:HD22	1:B:862:GLU:HG3	0.43	1.89	7	2
1:C:894:TYR:CE1	1:C:895:LEU:O	0.43	2.72	1	3
1:C:914:ARG:O	1:C:915:SER:CB	0.43	2.66	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:856:LEU:HD11	1:A:858:LEU:HG	0.43	1.91	8	1
1:B:879:TYR:O	1:B:879:TYR:CD2	0.43	2.72	10	9
1:B:856:LEU:HD21	1:B:858:LEU:HD23	0.43	1.91	4	1
1:B:858:LEU:HD23	1:B:866:VAL:HG13	0.42	1.90	10	2
1:A:906:GLU:O	1:A:907:LYS:HB2	0.42	2.14	5	1
1:A:855:ALA:HB3	1:A:870:ARG:HB3	0.42	1.89	6	1
1:A:856:LEU:HD21	1:A:858:LEU:HD23	0.42	1.91	4	1
1:B:856:LEU:HD11	1:B:858:LEU:HG	0.42	1.90	8	1
1:A:858:LEU:HD22	1:A:862:GLU:HG3	0.42	1.89	7	2
1:A:868:PHE:CD1	1:A:881:PRO:HG2	0.42	2.49	5	7
1:B:868:PHE:CD1	1:B:881:PRO:HG2	0.42	2.50	9	6
1:B:890:LEU:HD11	1:B:985:LEU:HD12	0.42	1.91	2	1
1:C:886:PHE:CE1	1:C:888:ALA:HB2	0.42	2.50	1	1
1:A:852:PHE:O	1:A:852:PHE:CD1	0.42	2.73	5	4
1:B:906:GLU:CG	1:B:907:LYS:N	0.42	2.82	5	10
1:C:956:LEU:HD12	1:C:956:LEU:N	0.42	2.29	4	2
1:C:880:ASP:O	1:C:884:GLY:N	0.42	2.52	1	1
1:C:852:PHE:CZ	1:C:983:GLY:O	0.42	2.73	8	5
1:B:906:GLU:O	1:B:907:LYS:HB2	0.42	2.14	5	1
1:A:880:ASP:O	1:A:884:GLY:N	0.42	2.53	1	1
1:A:913:SER:CB	1:A:919:VAL:CG1	0.42	2.98	1	6
1:B:966:LEU:O	1:B:967:VAL:CG2	0.42	2.68	3	10
1:C:913:SER:CB	1:C:919:VAL:CG1	0.42	2.97	6	8
1:A:862:GLU:OE1	1:A:866:VAL:HG13	0.42	2.15	6	1
1:A:850:VAL:CG1	1:A:878:TYR:CE2	0.42	3.03	7	1
1:B:850:VAL:CG1	1:B:878:TYR:CE2	0.42	3.03	7	1
1:B:852:PHE:O	1:B:852:PHE:CD1	0.42	2.73	1	4
1:B:852:PHE:CD1	1:B:879:TYR:CE1	0.42	3.07	1	1
1:B:879:TYR:HB3	1:B:886:PHE:CG	0.42	2.50	6	3
1:C:954:LEU:O	1:C:954:LEU:CD2	0.42	2.64	2	1
1:B:920:ALA:O	1:B:949:VAL:HG12	0.42	2.14	3	1
1:B:966:LEU:O	1:B:967:VAL:HG23	0.42	2.15	3	2
1:B:890:LEU:CD2	1:B:985:LEU:HD13	0.42	2.34	4	1
1:A:978:LEU:HD12	1:A:978:LEU:N	0.42	2.29	10	1
1:A:886:PHE:CB	1:A:962:VAL:CG2	0.42	2.98	8	3
1:A:852:PHE:CD1	1:A:879:TYR:CE1	0.41	3.07	1	1
1:B:913:SER:CB	1:B:919:VAL:CG1	0.41	2.98	1	9
1:A:852:PHE:CZ	1:A:983:GLY:O	0.41	2.73	8	1
1:B:868:PHE:O	1:B:868:PHE:CG	0.41	2.73	1	1
1:B:914:ARG:NH1	1:B:956:LEU:CD2	0.41	2.83	1	5
1:C:966:LEU:O	1:C:967:VAL:CG2	0.41	2.68	6	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:879:TYR:O	1:A:879:TYR:CD2	0.41	2.73	10	8
1:C:879:TYR:HB3	1:C:886:PHE:CG	0.41	2.49	4	4
1:A:966:LEU:O	1:A:967:VAL:CG2	0.41	2.68	3	10
1:B:862:GLU:OE1	1:B:866:VAL:HG13	0.41	2.14	6	1
1:C:886:PHE:O	1:C:961:THR:HA	0.41	2.16	7	1
1:B:954:LEU:O	1:B:954:LEU:CD2	0.41	2.64	10	1
1:A:954:LEU:O	1:A:954:LEU:CD2	0.41	2.64	10	1
1:A:914:ARG:NH1	1:A:956:LEU:CD2	0.41	2.83	1	3
1:C:848:PRO:O	1:C:849:GLN:C	0.41	2.59	1	3
1:C:852:PHE:CE2	1:C:983:GLY:O	0.41	2.73	5	4
1:C:921:ARG:CB	1:C:950:PHE:CE1	0.41	3.03	2	1
1:A:893:ARG:CZ	1:C:984:ALA:HB1	0.41	2.45	5	2
1:A:852:PHE:CE1	1:A:983:GLY:O	0.41	2.74	1	2
1:A:868:PHE:O	1:A:868:PHE:CG	0.41	2.73	1	1
1:B:852:PHE:CE1	1:B:983:GLY:O	0.41	2.74	1	1
1:B:848:PRO:O	1:B:849:GLN:C	0.41	2.59	2	8
1:C:953:ILE:HD12	1:C:955:PRO:HD3	0.41	1.91	4	1
1:A:894:TYR:CE1	1:A:895:LEU:O	0.41	2.74	2	4
1:C:852:PHE:CD1	1:C:852:PHE:O	0.41	2.74	1	1
1:A:890:LEU:HD11	1:A:985:LEU:HD12	0.41	1.91	2	1
1:B:894:TYR:CE1	1:B:895:LEU:O	0.41	2.74	10	3
1:A:856:LEU:HD21	1:A:866:VAL:CG1	0.41	2.45	4	1
1:A:858:LEU:HD23	1:A:866:VAL:CG1	0.41	2.46	4	1
1:C:852:PHE:CD1	1:C:852:PHE:C	0.41	2.93	9	1
1:C:914:ARG:NE	1:C:962:VAL:CG1	0.41	2.84	10	1
1:C:920:ALA:CB	1:C:949:VAL:HG12	0.41	2.31	9	1
1:A:893:ARG:NE	1:C:984:ALA:HB1	0.41	2.31	10	1
1:B:858:LEU:CD2	1:B:866:VAL:CG1	0.41	2.99	3	2
1:C:978:LEU:C	1:C:979:THR:HG23	0.41	2.36	5	4
1:A:856:LEU:CD2	1:A:866:VAL:CG1	0.41	2.99	4	1
1:B:856:LEU:HD21	1:B:866:VAL:CG1	0.41	2.45	4	1
1:B:986:LEU:HD11	1:C:986:LEU:HD11	0.41	1.92	4	1
1:C:868:PHE:O	1:C:868:PHE:CG	0.41	2.73	9	2
1:A:879:TYR:HB3	1:A:886:PHE:CG	0.41	2.50	6	1
1:B:879:TYR:HB2	1:B:886:PHE:CG	0.41	2.51	7	1
1:B:852:PHE:CZ	1:B:983:GLY:O	0.41	2.74	8	2
1:C:852:PHE:CD2	1:C:983:GLY:O	0.41	2.74	2	1
1:C:911:VAL:HG21	1:C:921:ARG:NH2	0.41	2.31	2	1
1:A:893:ARG:CZ	1:C:984:ALA:CB	0.41	2.99	3	4
1:A:966:LEU:O	1:A:967:VAL:HG23	0.41	2.16	6	2
1:B:852:PHE:CE2	1:B:983:GLY:O	0.41	2.74	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:978:LEU:N	1:C:978:LEU:HD12	0.41	2.31	10	1
1:A:858:LEU:CD2	1:A:866:VAL:CG1	0.40	2.99	3	2
1:C:886:PHE:CB	1:C:962:VAL:CG2	0.40	2.98	7	3
1:A:900:LEU:N	1:A:900:LEU:HD22	0.40	2.31	5	2
1:C:955:PRO:O	1:C:956:LEU:HD12	0.40	2.16	5	1
1:A:879:TYR:HB2	1:A:886:PHE:CG	0.40	2.51	7	1
1:A:978:LEU:C	1:A:979:THR:HG23	0.40	2.36	10	1
1:B:872:LEU:HD13	1:C:953:ILE:HD11	0.40	1.93	1	1
1:A:848:PRO:O	1:A:849:GLN:C	0.40	2.59	2	3
1:C:879:TYR:HB2	1:C:886:PHE:CG	0.40	2.51	7	1
1:A:900:LEU:CD2	1:A:900:LEU:N	0.40	2.84	4	1
1:C:852:PHE:CE1	1:C:983:GLY:O	0.40	2.74	7	1
1:C:858:LEU:CD2	1:C:866:VAL:CG1	0.40	2.99	2	1
1:A:916:ASN:CB	1:A:919:VAL:CG2	0.40	3.00	3	1
1:B:978:LEU:C	1:B:979:THR:HG23	0.40	2.36	3	2
1:A:893:ARG:NH1	1:A:986:LEU:CD2	0.40	2.85	4	1
1:B:858:LEU:HD23	1:B:866:VAL:CG1	0.40	2.46	4	1
1:B:900:LEU:CD2	1:B:900:LEU:N	0.40	2.85	4	1
1:A:852:PHE:CE2	1:A:983:GLY:O	0.40	2.74	9	2
1:B:852:PHE:CD1	1:B:852:PHE:O	0.40	2.74	7	1
1:A:868:PHE:CG	1:A:868:PHE:O	0.40	2.74	2	1
1:A:868:PHE:O	1:A:868:PHE:CD2	0.40	2.75	2	1
1:A:921:ARG:HB2	1:A:950:PHE:CE1	0.40	2.52	6	1
1:C:856:LEU:CD1	1:C:858:LEU:HD23	0.40	2.22	6	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	127/162 (78%)	86±1 (68±1%)	29±1 (23±1%)	12±1 (9±1%)	1	11
1	B	127/162 (78%)	86±1 (68±1%)	30±1 (23±1%)	12±1 (9±1%)	1	11
1	C	127/162 (78%)	85±1 (67±1%)	29±1 (23±1%)	12±1 (10±1%)	1	10
All	All	3810/4860 (78%)	2575 (68%)	878 (23%)	357 (9%)	1	11

All 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	858	LEU	10
1	A	859	PRO	10
1	A	867	PRO	10
1	A	874	ASN	10
1	A	891	ALA	10
1	A	906	GLU	10
1	A	919	VAL	10
1	A	953	ILE	10
1	A	954	LEU	10
1	A	967	VAL	10
1	A	971	LEU	10
1	B	858	LEU	10
1	B	859	PRO	10
1	B	867	PRO	10
1	B	874	ASN	10
1	B	891	ALA	10
1	B	906	GLU	10
1	B	919	VAL	10
1	B	953	ILE	10
1	B	954	LEU	10
1	B	967	VAL	10
1	B	971	LEU	10
1	C	858	LEU	10
1	C	859	PRO	10
1	C	867	PRO	10
1	C	874	ASN	10
1	C	891	ALA	10
1	C	906	GLU	10
1	C	919	VAL	10
1	C	953	ILE	10
1	C	954	LEU	10
1	C	967	VAL	10
1	C	971	LEU	10
1	C	960	ASP	5
1	C	905	HIS	4
1	C	907	LYS	4
1	A	960	ASP	3
1	B	960	ASP	3
1	A	878	TYR	2
1	B	878	TYR	2
1	C	952	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	C	878	TYR	1
1	A	952	LEU	1
1	B	952	LEU	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	105/131 (80%)	96±1 (92±1%)	8±1 (8±1%)	15	63
1	B	105/131 (80%)	96±1 (92±1%)	8±1 (8±1%)	15	63
1	C	105/131 (80%)	96±1 (92±1%)	9±1 (8±1%)	14	61
All	All	3150/3930 (80%)	2891 (92%)	259 (8%)	15	62

All 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	A	894	TYR	10
1	A	906	GLU	10
1	A	914	ARG	10
1	A	954	LEU	10
1	A	976	GLU	10
1	B	894	TYR	10
1	B	906	GLU	10
1	B	914	ARG	10
1	B	954	LEU	10
1	B	976	GLU	10
1	C	914	ARG	10
1	C	954	LEU	10
1	C	862	GLU	9
1	C	976	GLU	9
1	A	886	PHE	9
1	B	886	PHE	9
1	C	960	ASP	9
1	A	960	ASP	8
1	B	960	ASP	8
1	C	906	GLU	8

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Mol	Chain	Res	Type	Models (Total)
1	A	862	GLU	7
1	B	862	GLU	7
1	C	886	PHE	7
1	C	894	TYR	5
1	C	966	LEU	5
1	A	966	LEU	4
1	B	966	LEU	4
1	C	989	ASP	3
1	C	880	ASP	3
1	A	880	ASP	2
1	B	880	ASP	2
1	C	915	SER	2
1	A	913	SER	2
1	B	913	SER	2
1	C	957	GLN	2
1	C	903	HIS	2
1	C	973	HIS	2
1	A	975	GLU	1
1	B	975	GLU	1
1	C	857	SER	1
1	A	866	VAL	1
1	B	866	VAL	1
1	C	975	GLU	1
1	A	858	LEU	1
1	B	858	LEU	1
1	C	852	PHE	1

### 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

No chemical shift data were provided