



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 02:43 PM UTC

PDB ID : 1CFG / pdb_00001cfg
Title : MEMBRANE-BINDING PEPTIDE FROM THE C2 DOMAIN OF FACTOR
VIII FORMS AN AMPHIPATHIC STRUCTURE AS DETERMINED BY
NMR SPECTROSCOPY
Authors : Baleja, J.D.; Gilbert, G.E.
Deposited on : 1994-11-10

This is a Full wwPDB NMR Structure Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

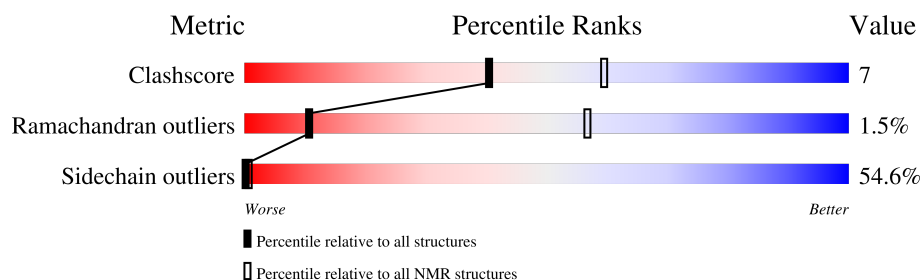
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	22	23% 32% 5% 41%

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models).

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:7-A:19 (13)	0.26	17

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 4 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 194 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called COAGULATION FACTOR VIII.

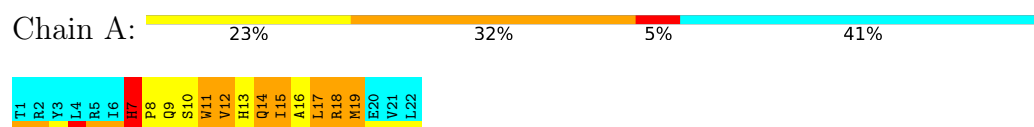
Mol	Chain	Residues	Atoms					Trace
1	A	22	Total	C	N	O	S	0
			194	125	38	30	1	

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: COAGULATION FACTOR VIII

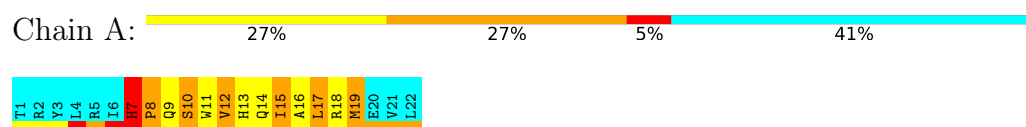


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

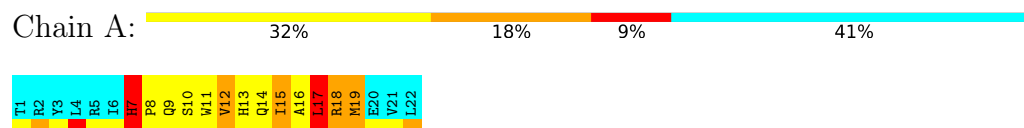
4.2.1 Score per residue for model 1

- Molecule 1: COAGULATION FACTOR VIII



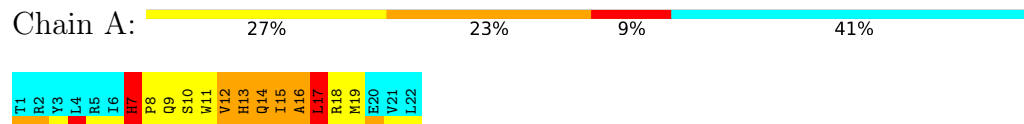
4.2.2 Score per residue for model 2

- Molecule 1: COAGULATION FACTOR VIII



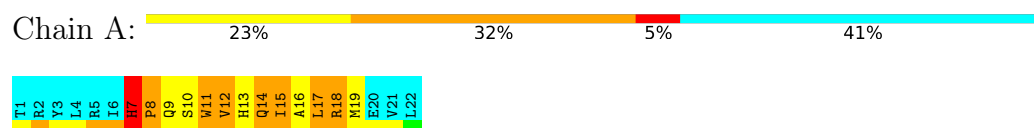
4.2.4 Score per residue for model 4

- Molecule 1: COAGULATION FACTOR VIII



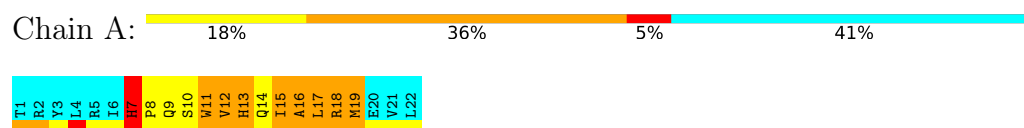
4.2.5 Score per residue for model 5

- Molecule 1: COAGULATION FACTOR VIII



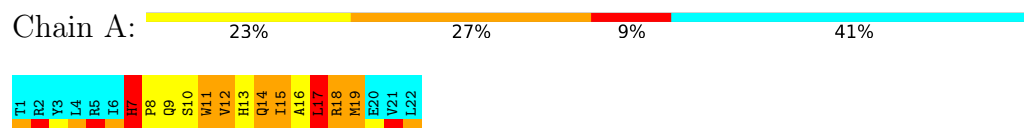
4.2.6 Score per residue for model 6

- Molecule 1: COAGULATION FACTOR VIII



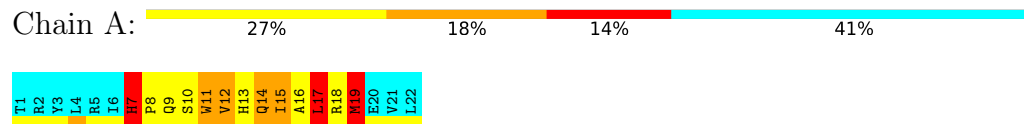
4.2.7 Score per residue for model 7

- Molecule 1: COAGULATION FACTOR VIII



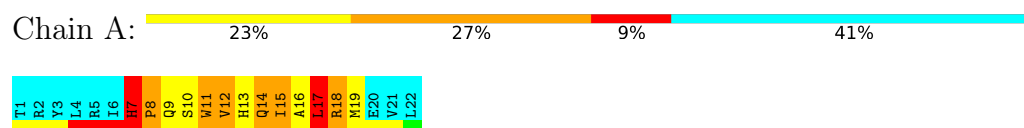
4.2.9 Score per residue for model 9

- Molecule 1: COAGULATION FACTOR VIII



4.2.10 Score per residue for model 10

- Molecule 1: COAGULATION FACTOR VIII



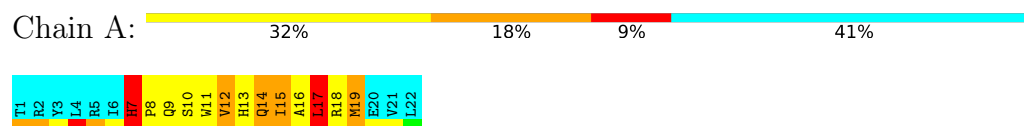
4.2.11 Score per residue for model 11

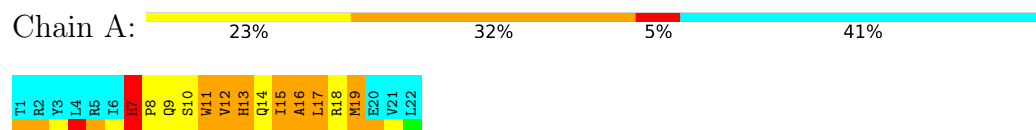
- Molecule 1: COAGULATION FACTOR VIII



4.2.12 Score per residue for model 12

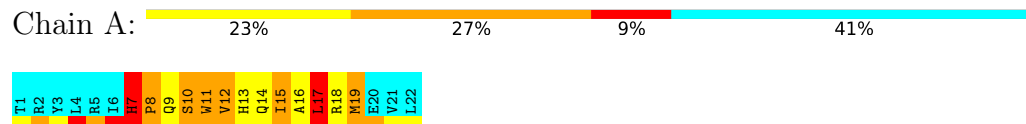
- Molecule 1: COAGULATION FACTOR VIII





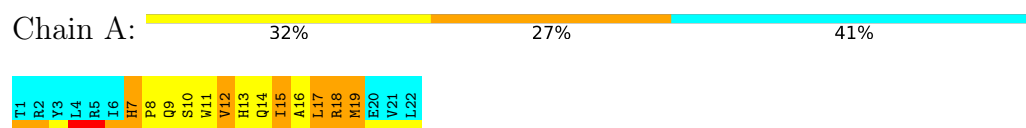
4.2.14 Score per residue for model 14

- Molecule 1: COAGULATION FACTOR VIII



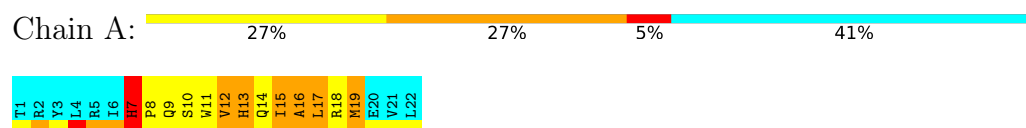
4.2.15 Score per residue for model 15

- Molecule 1: COAGULATION FACTOR VIII



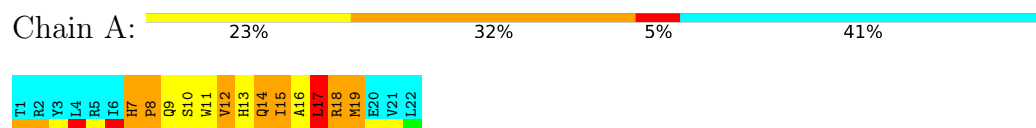
4.2.16 Score per residue for model 16

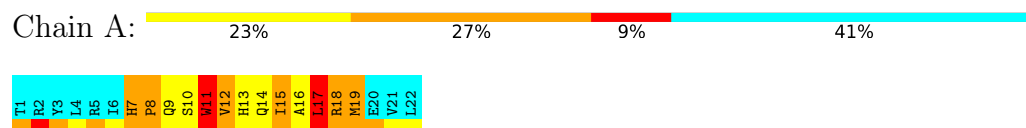
- Molecule 1: COAGULATION FACTOR VIII



4.2.17 Score per residue for model 17 (medoid)

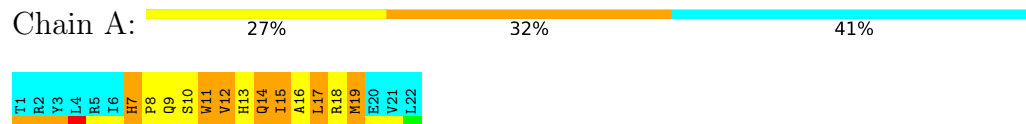
- Molecule 1: COAGULATION FACTOR VIII





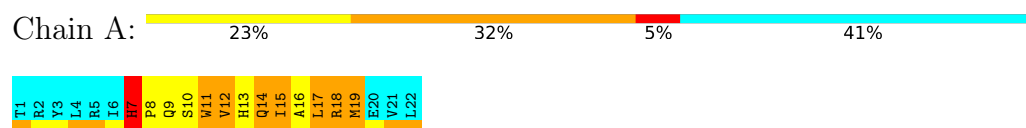
4.2.19 Score per residue for model 19

- Molecule 1: COAGULATION FACTOR VIII



4.2.20 Score per residue for model 20

- Molecule 1: COAGULATION FACTOR VIII



5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 20 were deposited, based on the following criterion: ?.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided.

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	3.34±0.03	19±1/117 (16.0± 0.6%)	5.53±0.10	47±1/160 (29.4± 0.8%)
All	All	3.34	375/2340 (16.0%)	5.53	942/3200 (29.4%)

All 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	7	HIS	CA-CB	9.38	1.63	1.53	16	20
1	A	13	HIS	CG-ND1	8.62	1.47	1.38	12	20
1	A	7	HIS	CG-ND1	8.58	1.47	1.38	20	20
1	A	8	PRO	N-CA	7.14	1.56	1.47	2	20
1	A	12	VAL	CA-C	6.47	1.60	1.52	9	20
1	A	13	HIS	CA-C	6.40	1.60	1.52	13	20
1	A	18	ARG	CA-C	6.34	1.60	1.52	2	20
1	A	13	HIS	CA-CB	6.33	1.63	1.53	1	

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	11	TRP	CA-CB-CG	15.90	143.80	113.60	7	20
1	A	15	ILE	CA-C-N	12.73	136.99	120.44	11	20
1	A	15	ILE	C-N-CA	12.73	136.99	120.44	11	20
1	A	8	PRO	CA-C-N	12.38	136.87	120.28	13	20
1	A	8	PRO	C-N-CA	12.38	136.87	120.28	13	20
1	A	12	VAL	CA-C-N	12.29	136.42	120.44	3	20
1	A	12	VAL	C-N-CA	12.29	136.42	120.44	3	20
1	A	16	ALA	CA-C-N	12.03	136.79	120.44	19	20
1	A	16	ALA	C-N-CA	12.03	136.79	120.44	19	20
1	A	17	LEU	CA-C-N	11.85	136.16	120.28	17	20
1	A	17	LEU	C-N-CA	11.85	136.16	120.28	17	20
1	A	10	SER	CA-C-N	11.50	135.69	120.28	11	20
1	A	10	SER	C-N-CA	11.50	135.69	120.28	11	20
1	A	11	TRP	CA-C-N	11.49	135.03	120.56	20	20
1	A	11	TRP	C-N-CA	11.49	135.03	120.56	20	20
1									

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	13	HIS	CE1-NE2-CD2	-6.11	102.89	109.00	4	20
1	A	8	PRO	CA-CB-CG	5.69	115.32	104.50	7	11
1	A	18	ARG	CA-CB-CG	5.60	125.30	114.10	3	1
1	A	7	HIS	N-CA-C	5.54	118.69	108.94	2	1
1	A	10	SER	N-CA-CB	5.53	118.09	110.07	1	19
1	A	9	GLN	CB-CG-CD	5.47	121.89	112.60	17	1
1	A	11	TRP	CB-CA-C	-5.31	101.97	110.79	3	7
1	A	9	GLN	OE1-CD-NE2	-5.30	117.30	122.60	2	13
1	A	9	GLN	CB-CA-C	-5.27	102.04	110.79	5	2
1	A	11	TRP	N-CA-C	-5.27	105.62	111.36	14	2
1	A	13	HIS	CG-ND1-CE1	-5.15	100.55	109.30	12	20
1	A	7	HIS	CG-ND1-CE1	-5.12	100.60	109.30	16	15
1	A	14	GLN	OE1-CD-NE2	-5.11	117.49	122.60	4	3
1	A	13	HIS	CA-CB-CG	-5.08	108.72	113.80	14	1

There are no chirality outliers.

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:HIS:N	1:A:7:HIS:ND1	0.43	2.65	12	2
1:A:17:LEU:C	1:A:17:LEU:HD12	0.42	2.39	14	1
1:A:14:GLN:HA	1:A:17:LEU:HD12	0.41	1.92	11	1
1:A:19:MET:HE2	1:A:19:MET:HA	0.41	1.92	9	1
1:A:7:HIS:N	1:A:8:PRO:CD	0.41	2.84	14	2

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	13/22 (59%)	12±1 (90±8%)	1±1 (8±9%)	0±0 (2±3%)	11	57
All	All	260/440 (59%)	235 (90%)	21 (8%)	4 (2%)	11	57

All 2 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	7	HIS	3
1	A	8	PRO	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	
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Mol	Chain	Res	Type	Models (Total)
1	A	12	VAL	20
1	A	15	ILE	20
1	A	17	LEU	20
1	A	7	HIS	18
1	A	19	MET	16
1	A	11	TRP	12
1	A	14	GLN	11
1	A	18	ARG	11
1	A	10	SER	2
1	A	9	GLN	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 oligosaccharides 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