



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 07:44 pm BST

PDB ID : 1HFF  
Title : NMR solution structures of the vMIP-II 1-10 peptide from Kaposi's sarcoma-associated herpesvirus.  
Authors : Crump, M.P.; Elisseeva, E.; Gong, J.H.; Clark-Lewis, I.; Sykes, B.D.  
Deposited on : 2000-12-01

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.

---

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  
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 : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

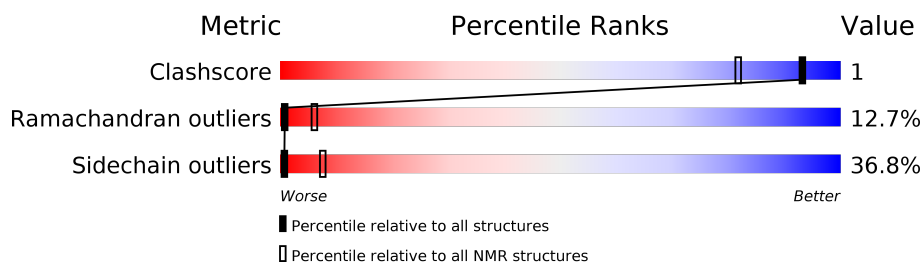
# 1 Overall quality at a glance

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	10	

## 2 Ensemble composition and analysis ⓘ

This entry contains 55 models.

Cyrange was unable to find well-defined residues.

Error message: The number of core atoms ( 6) was below the domain threshold value ( 8).

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 163 atoms, of which 80 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II.

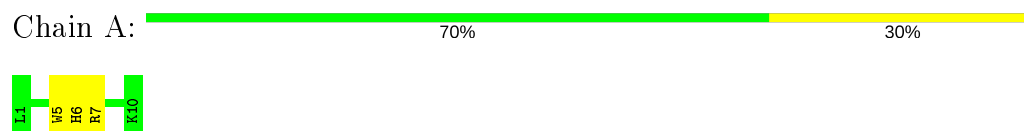
Mol	Chain	Residues	Atoms					Trace
1	A	10	Total	C	H	N	O	0
			163	52	80	17	14	

## 4 Residue-property plots

### 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: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



### 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: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



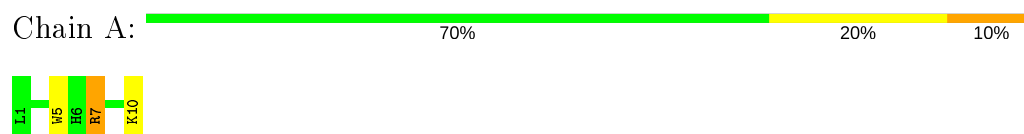
#### 4.2.2 Score per residue for model 2

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



### 4.2.3 Score per residue for model 3

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



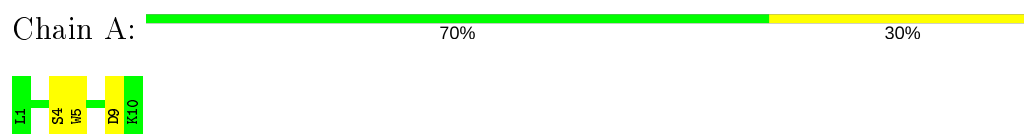
### 4.2.4 Score per residue for model 4

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



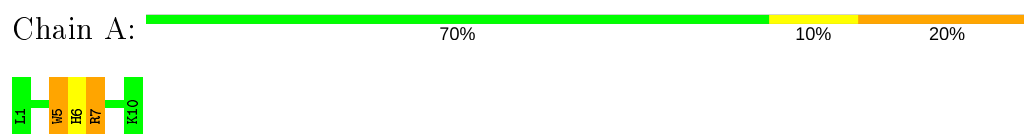
### 4.2.5 Score per residue for model 5

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



### 4.2.6 Score per residue for model 6

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



### 4.2.7 Score per residue for model 7

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.8 Score per residue for model 8

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



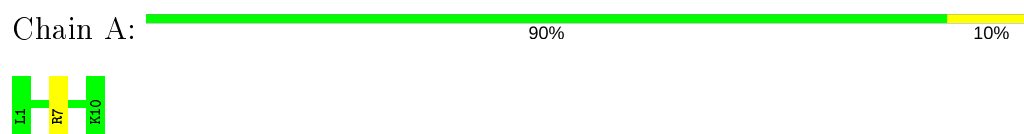
#### 4.2.9 Score per residue for model 9

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



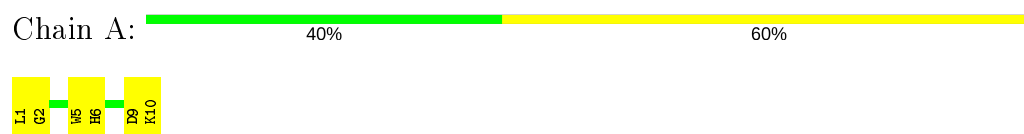
#### 4.2.10 Score per residue for model 10

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



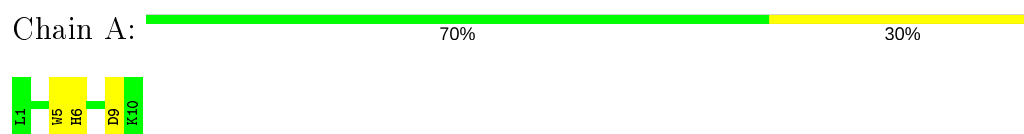
#### 4.2.11 Score per residue for model 11

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



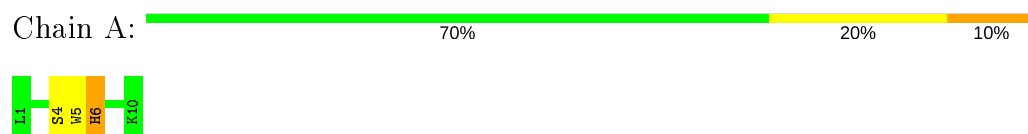
#### 4.2.12 Score per residue for model 12

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



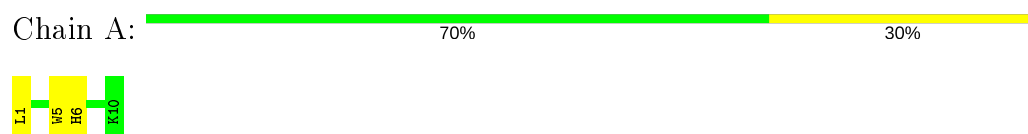
#### 4.2.13 Score per residue for model 13

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



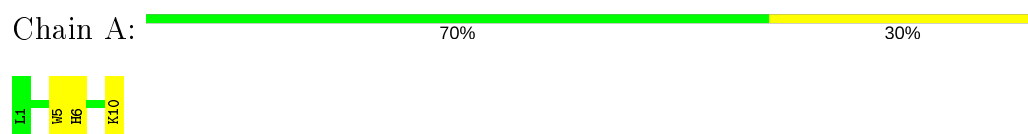
#### 4.2.14 Score per residue for model 14

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



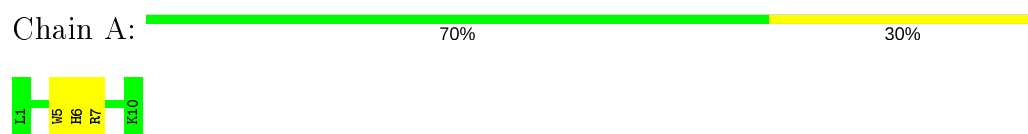
#### 4.2.15 Score per residue for model 15

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



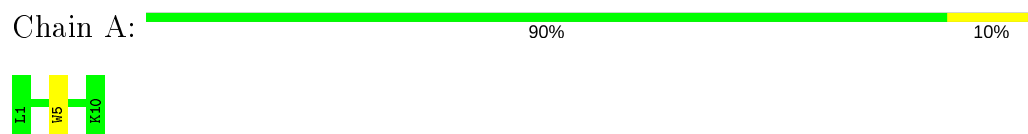
#### 4.2.16 Score per residue for model 16

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.17 Score per residue for model 17

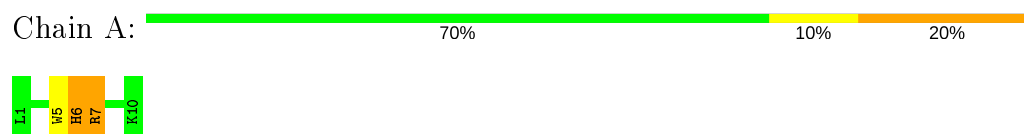
- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II





#### 4.2.18 Score per residue for model 18

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.19 Score per residue for model 19

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



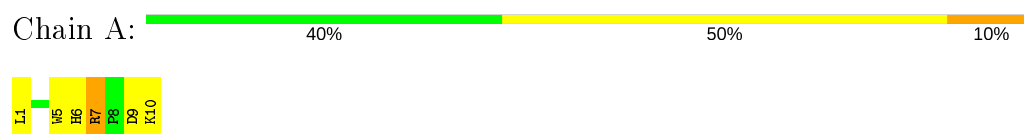
#### 4.2.20 Score per residue for model 20

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



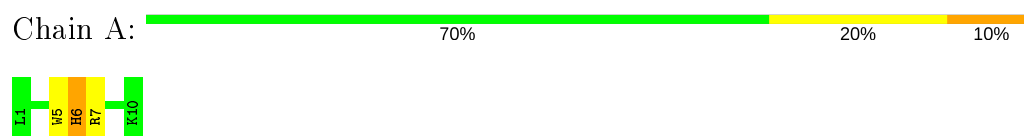
#### 4.2.21 Score per residue for model 21

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.22 Score per residue for model 22

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



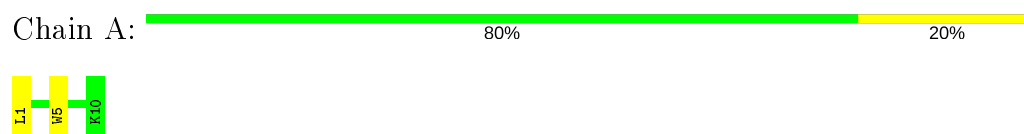
#### 4.2.23 Score per residue for model 23

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



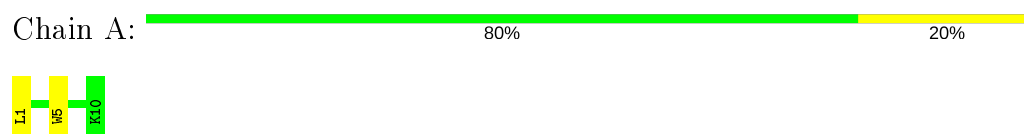
#### 4.2.24 Score per residue for model 24

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.25 Score per residue for model 25

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.26 Score per residue for model 26

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



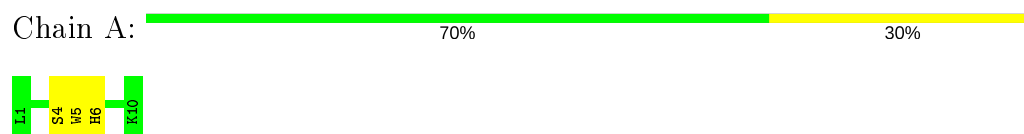
#### 4.2.27 Score per residue for model 27

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.28 Score per residue for model 28

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



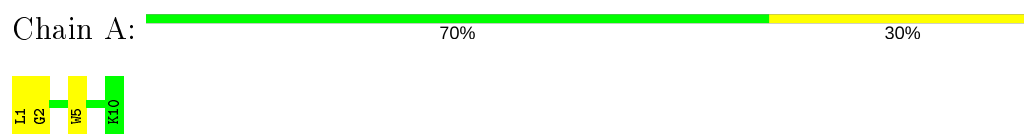
#### 4.2.29 Score per residue for model 29

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



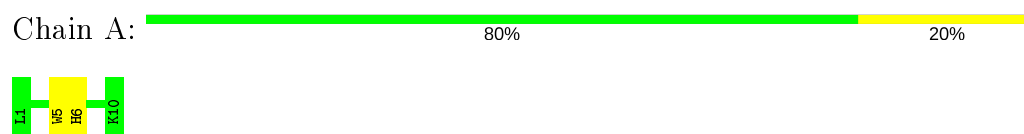
#### 4.2.30 Score per residue for model 30

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.31 Score per residue for model 31

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.32 Score per residue for model 32

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.33 Score per residue for model 33

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



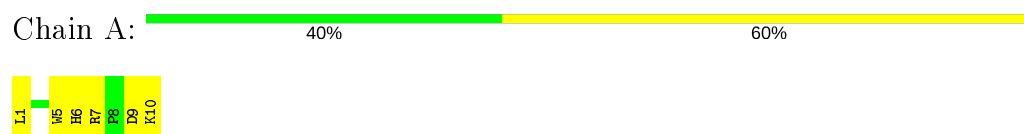
#### 4.2.34 Score per residue for model 34

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



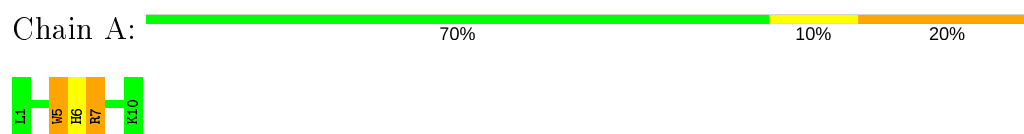
#### 4.2.35 Score per residue for model 35

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.36 Score per residue for model 36

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



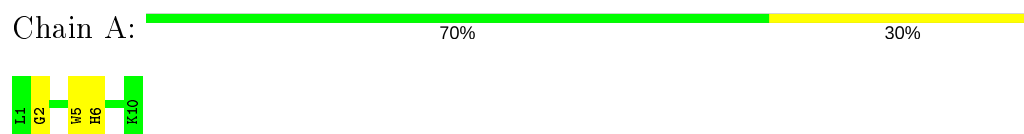
#### 4.2.37 Score per residue for model 37

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.38 Score per residue for model 38

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



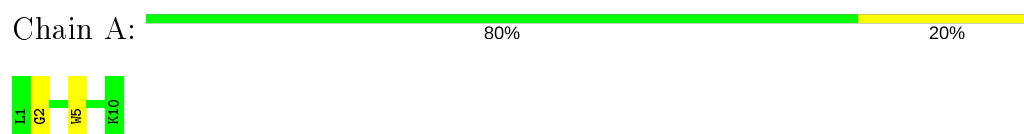
#### 4.2.39 Score per residue for model 39

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.40 Score per residue for model 40

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



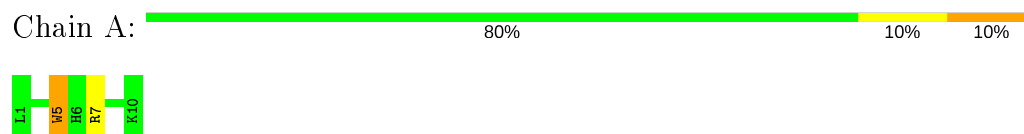
#### 4.2.41 Score per residue for model 41

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.42 Score per residue for model 42

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.43 Score per residue for model 43

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



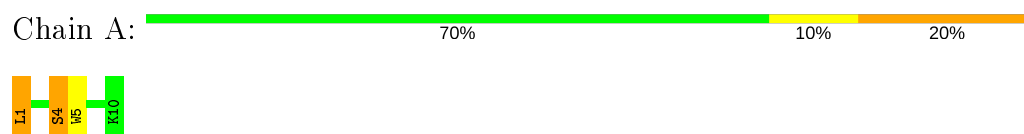
#### 4.2.44 Score per residue for model 44

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



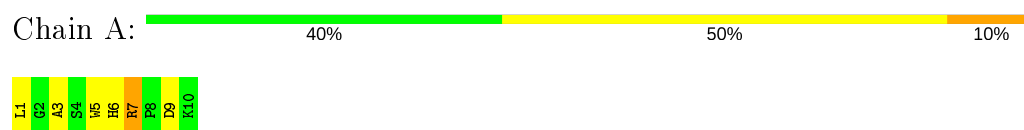
#### 4.2.45 Score per residue for model 45

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.46 Score per residue for model 46

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.47 Score per residue for model 47

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



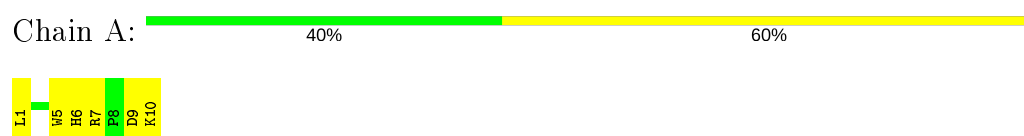
#### 4.2.48 Score per residue for model 48

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



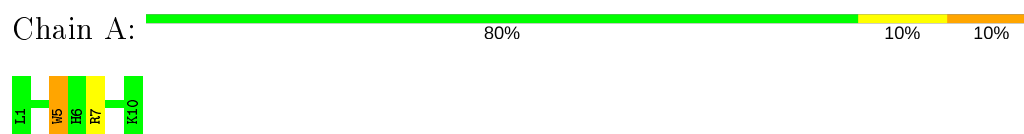
#### 4.2.49 Score per residue for model 49

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.50 Score per residue for model 50

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.51 Score per residue for model 51

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



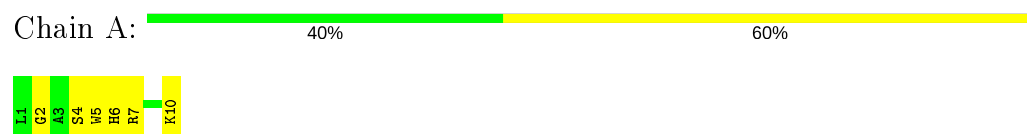
#### 4.2.52 Score per residue for model 52

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



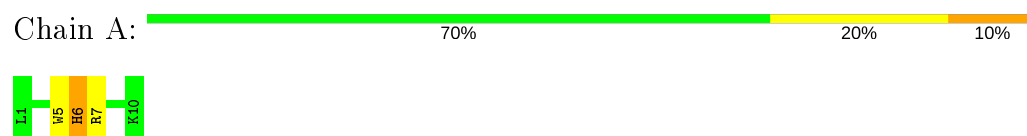
#### 4.2.53 Score per residue for model 53

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



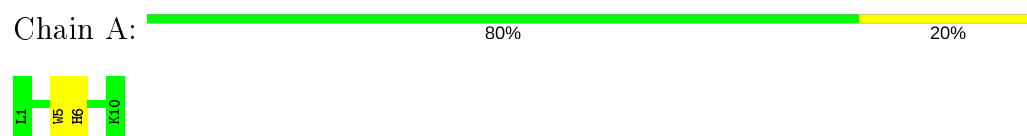
#### 4.2.54 Score per residue for model 54

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II



#### 4.2.55 Score per residue for model 55

- Molecule 1: VIRAL MACROPHAGE INFLAMMATORY PROTEIN-II





## 5 Refinement protocol and experimental data overview ⓘ

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

Of the 55 calculated structures, 55 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
X-PLOR	refinement	
X-PLOR	structure solution	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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	83	80	80	0±1
All	All	4565	4400	4400	12

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 1.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:LEU:HD13	1:A:1:LEU:N	0.60	2.11	45	1
1:A:1:LEU:O	1:A:1:LEU:HD12	0.55	2.01	21	2
1:A:1:LEU:HD13	1:A:1:LEU:H1	0.46	1.69	45	1
1:A:5:TRP:CZ3	1:A:7:ARG:HG2	0.43	2.48	36	1
1:A:1:LEU:HD12	1:A:1:LEU:C	0.43	2.34	21	1
1:A:6:HIS:O	1:A:7:ARG:CB	0.42	2.67	36	6

### 6.3 Torsion angles

#### 6.3.1 Protein backbone

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	8/10 (80%)	4±1 (54±13%)	3±1 (33±15%)	1±1 (13±11%)	1	6
All	All	440/550 (80%)	239 (54%)	145 (33%)	56 (13%)	1	6

All 7 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	ARG	19
1	A	9	ASP	9
1	A	6	HIS	8
1	A	2	GLY	7
1	A	4	SER	6
1	A	3	ALA	4
1	A	5	TRP	3

### 6.3.2 Protein sidechains ⓘ

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	8/8 (100%)	5±1 (63±15%)	3±1 (37±15%)	1	7
All	All	440/440 (100%)	278 (63%)	162 (37%)	1	7

All 7 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	5	TRP	54
1	A	6	HIS	38
1	A	7	ARG	19
1	A	1	LEU	19
1	A	4	SER	15
1	A	10	LYS	14
1	A	9	ASP	3

### 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

No chemical shift data were provided