



Full wwPDB NMR Structure Validation Report ⓘ

Aug 9, 2020 – 01:39 AM BST

PDB ID : 6RZC
Title : Winter flounder 4 in SDS micelles
Authors : Mason, A.J.; Clarke, M.
Deposited on : 2019-06-13

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 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 : 2.13.1
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

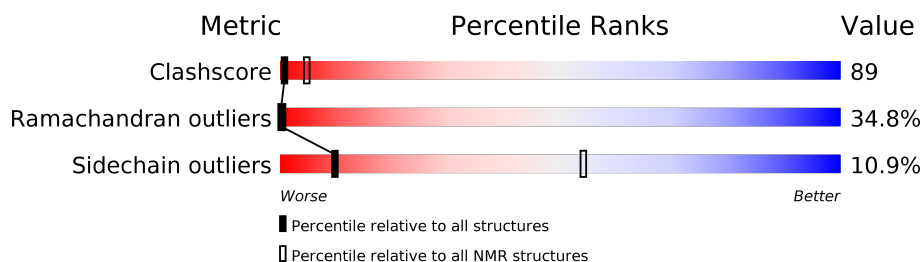
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 30%.

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 ≥ 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 | 25 | <div> <div></div> <div>12%</div> <div>20%</div> <div>32%</div> <div>36%</div> </div> |

2 Ensemble composition and analysis

This entry contains 100 models. Model 77 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:10-A:25 (16) | 0.59 | 77 |

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 6 clusters and 2 single-model clusters were found.

| Cluster number | Models |
|-----------------------|---|
| 1 | 4, 6, 7, 8, 10, 11, 12, 13, 21, 26, 30, 32, 39, 43, 44, 49, 53, 54, 56, 63, 65, 67, 68, 71, 77, 78, 79, 81, 85, 91, 93, 100 |
| 2 | 1, 2, 3, 16, 19, 24, 28, 29, 37, 42, 45, 48, 50, 62, 70, 72, 73, 83, 84, 86, 88, 94, 97 |
| 3 | 14, 15, 25, 27, 34, 35, 38, 46, 52, 55, 57, 60, 61, 69, 74, 76, 82, 89, 92, 96, 98, 99 |
| 4 | 17, 20, 22, 33, 40, 41, 51, 75, 87, 90 |
| 5 | 5, 9, 18, 23, 36, 47, 66, 80, 95 |
| 6 | 31, 59 |
| Single-model clusters | 58; 64 |

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 386 atoms, of which 189 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Pleurocidin-like peptide WF4.

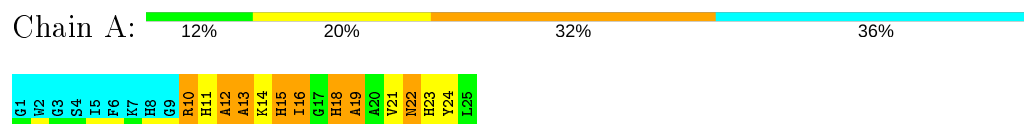
| Mol | Chain | Residues | Atoms | | | | | Trace |
|-----|-------|----------|-------|-----|-----|----|----|-------|
| 1 | A | 25 | Total | C | H | N | O | 0 |
| | | | 386 | 127 | 189 | 42 | 28 | |

4 Residue-property plots

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: Pleurocidin-like peptide WF4

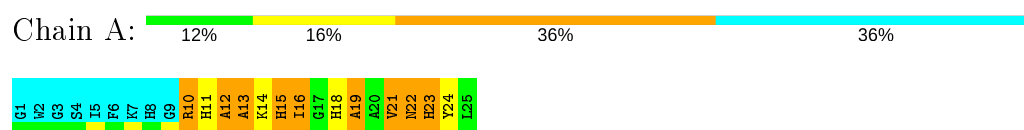


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

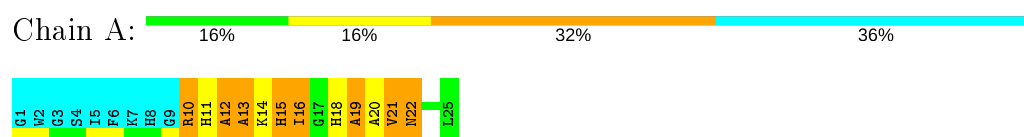
4.2.1 Score per residue for model 1

- Molecule 1: Pleurocidin-like peptide WF4



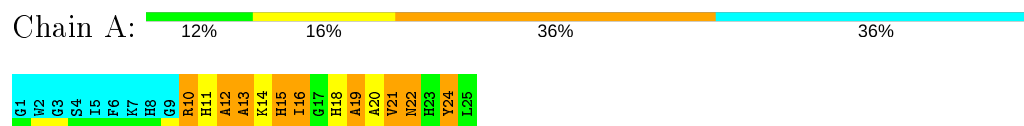
4.2.2 Score per residue for model 2

- Molecule 1: Pleurocidin-like peptide WF4



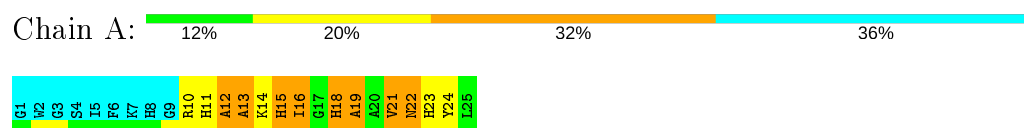
4.2.3 Score per residue for model 3

- Molecule 1: Pleurocidin-like peptide WF4



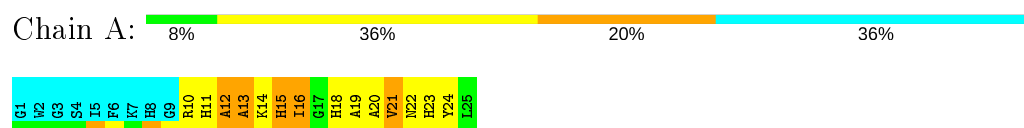
4.2.4 Score per residue for model 4

- Molecule 1: Pleurocidin-like peptide WF4



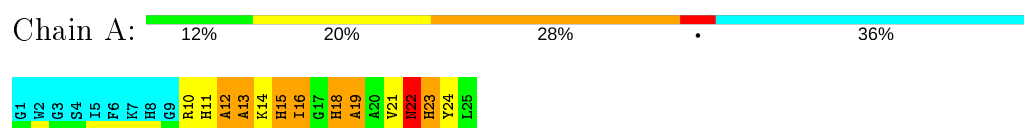
4.2.5 Score per residue for model 5

- Molecule 1: Pleurocidin-like peptide WF4



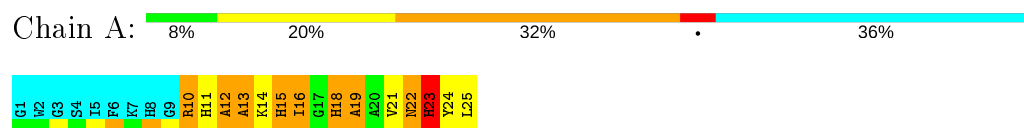
4.2.6 Score per residue for model 6

- Molecule 1: Pleurocidin-like peptide WF4



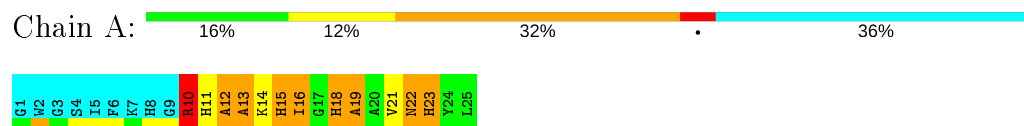
4.2.7 Score per residue for model 7

- Molecule 1: Pleurocidin-like peptide WF4



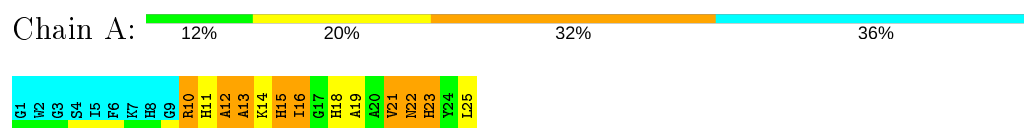
4.2.8 Score per residue for model 8

- Molecule 1: Pleurocidin-like peptide WF4



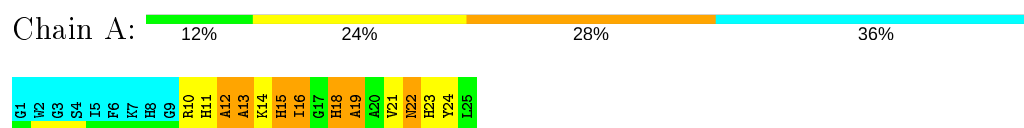
4.2.9 Score per residue for model 9

- Molecule 1: Pleurocidin-like peptide WF4



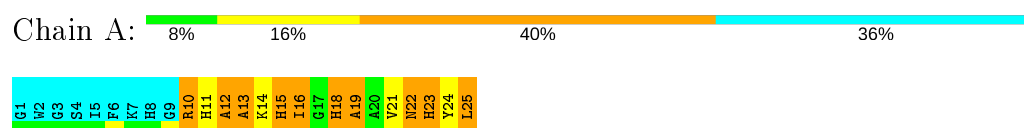
4.2.10 Score per residue for model 10

- Molecule 1: Pleurocidin-like peptide WF4



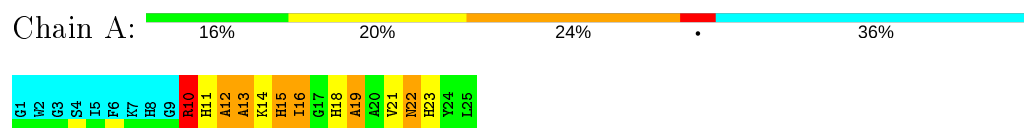
4.2.11 Score per residue for model 11

- Molecule 1: Pleurocidin-like peptide WF4



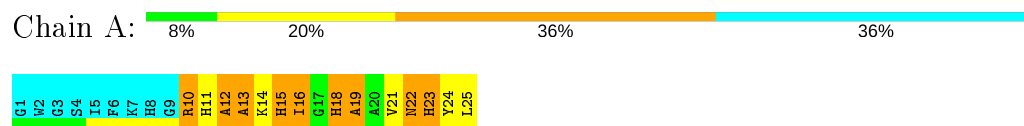
4.2.12 Score per residue for model 12

- Molecule 1: Pleurocidin-like peptide WF4



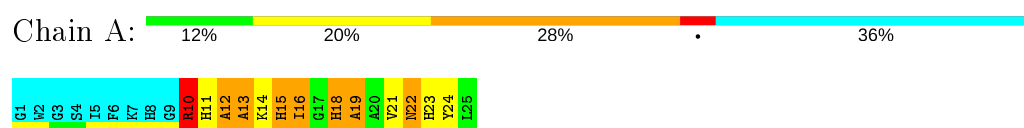
4.2.13 Score per residue for model 13

- Molecule 1: Pleurocidin-like peptide WF4



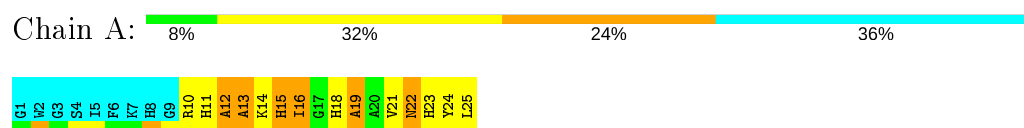
4.2.14 Score per residue for model 14

- Molecule 1: Pleurocidin-like peptide WF4



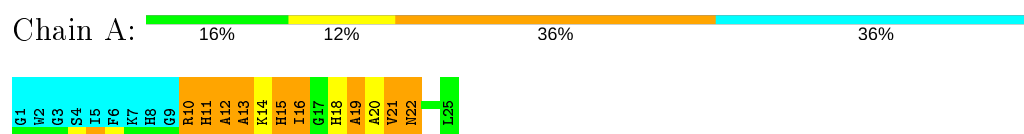
4.2.15 Score per residue for model 15

- Molecule 1: Pleurocidin-like peptide WF4



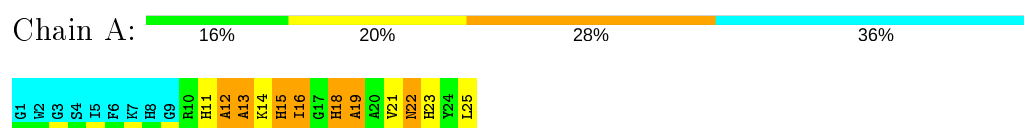
4.2.16 Score per residue for model 16

- Molecule 1: Pleurocidin-like peptide WF4



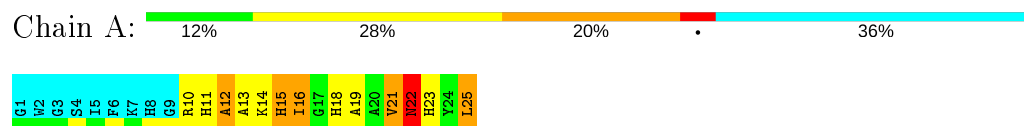
4.2.17 Score per residue for model 17

- Molecule 1: Pleurocidin-like peptide WF4



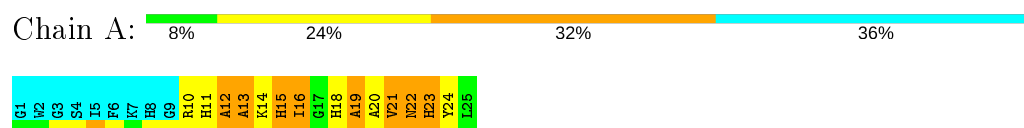
4.2.18 Score per residue for model 18

- Molecule 1: Pleurocidin-like peptide WF4



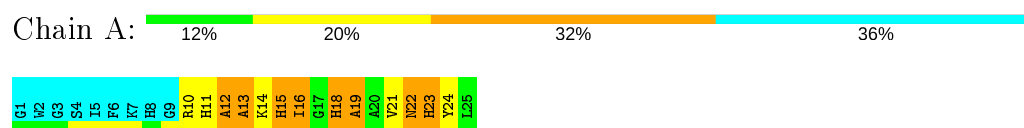
4.2.19 Score per residue for model 19

- Molecule 1: Pleurocidin-like peptide WF4



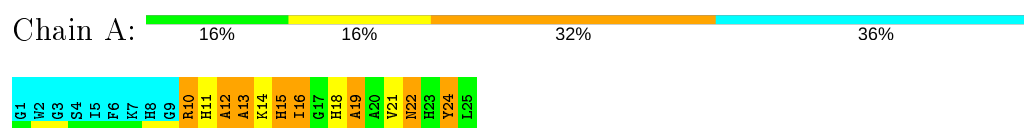
4.2.20 Score per residue for model 20

- Molecule 1: Pleurocidin-like peptide WF4



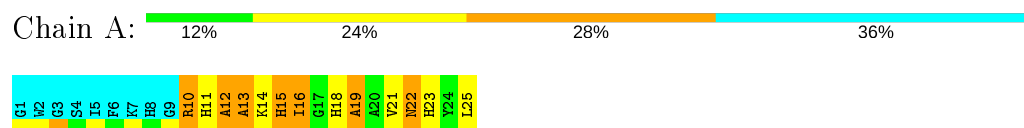
4.2.21 Score per residue for model 21

- Molecule 1: Pleurocidin-like peptide WF4



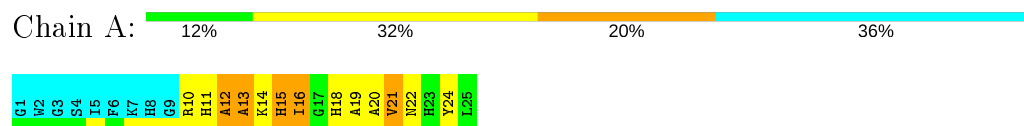
4.2.22 Score per residue for model 22

- Molecule 1: Pleurocidin-like peptide WF4



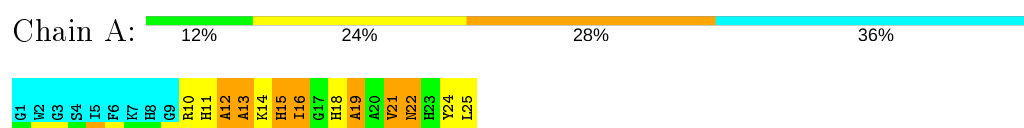
4.2.23 Score per residue for model 23

- Molecule 1: Pleurocidin-like peptide WF4



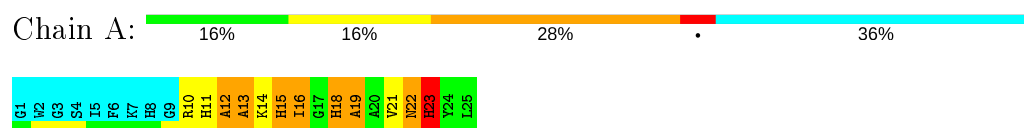
4.2.24 Score per residue for model 24

- Molecule 1: Pleurocidin-like peptide WF4



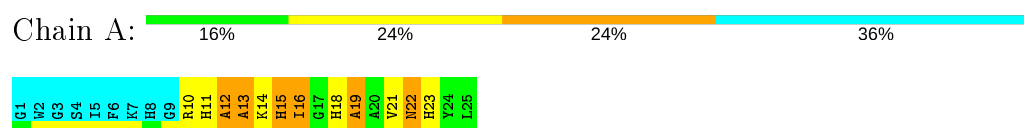
4.2.25 Score per residue for model 25

- Molecule 1: Pleurocidin-like peptide WF4



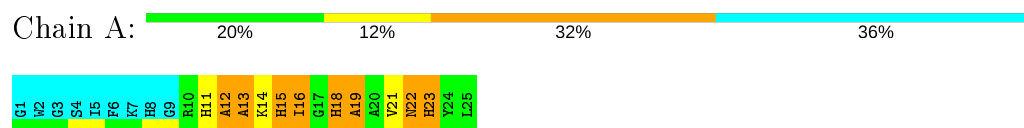
4.2.26 Score per residue for model 26

- Molecule 1: Pleurocidin-like peptide WF4



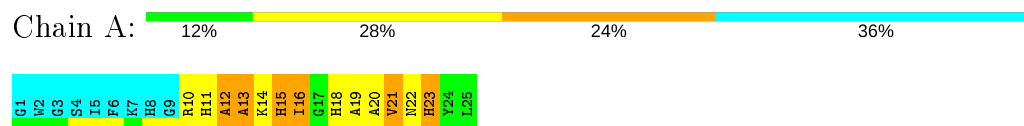
4.2.27 Score per residue for model 27

- Molecule 1: Pleurocidin-like peptide WF4



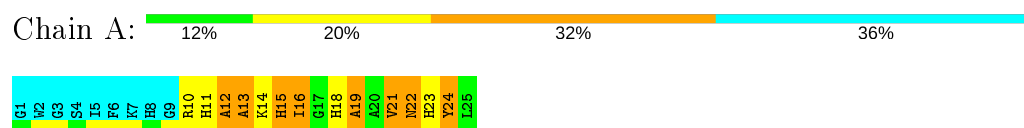
4.2.28 Score per residue for model 28

- Molecule 1: Pleurocidin-like peptide WF4



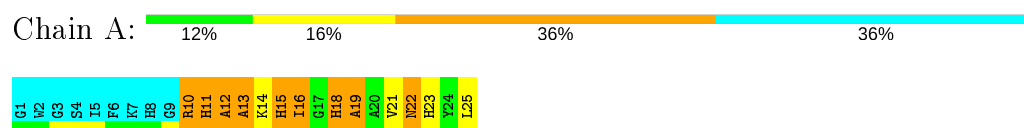
4.2.29 Score per residue for model 29

- Molecule 1: Pleurocidin-like peptide WF4



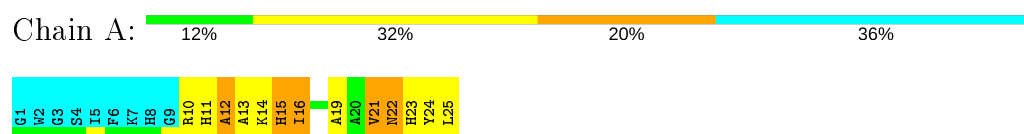
4.2.30 Score per residue for model 30

- Molecule 1: Pleurocidin-like peptide WF4



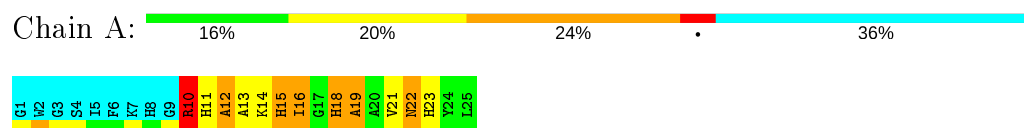
4.2.31 Score per residue for model 31

- Molecule 1: Pleurocidin-like peptide WF4



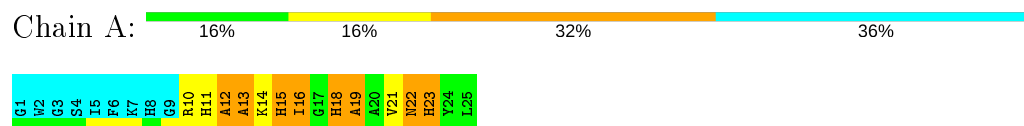
4.2.32 Score per residue for model 32

- Molecule 1: Pleurocidin-like peptide WF4



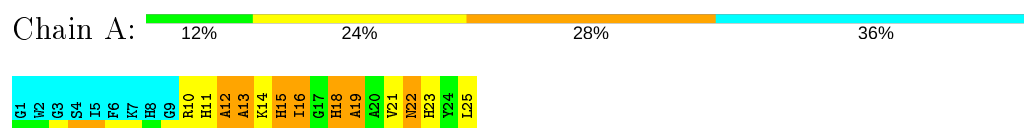
4.2.33 Score per residue for model 33

- Molecule 1: Pleurocidin-like peptide WF4



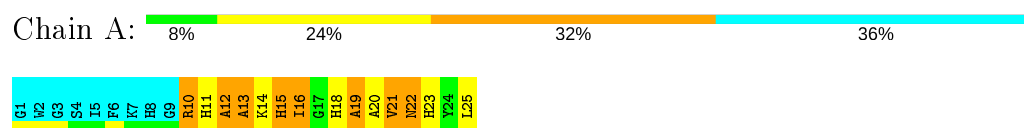
4.2.34 Score per residue for model 34

- Molecule 1: Pleurocidin-like peptide WF4



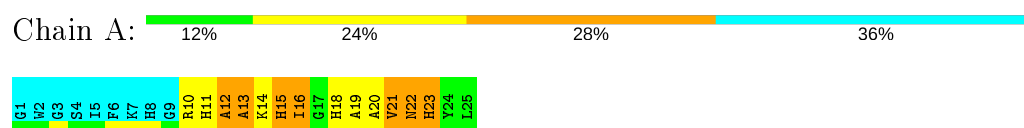
4.2.35 Score per residue for model 35

- Molecule 1: Pleurocidin-like peptide WF4



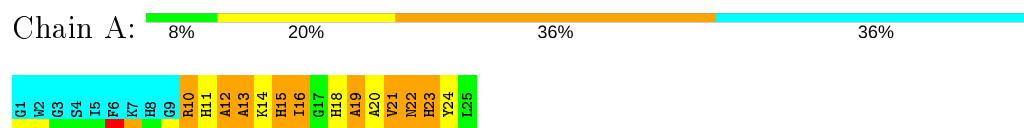
4.2.36 Score per residue for model 36

- Molecule 1: Pleurocidin-like peptide WF4



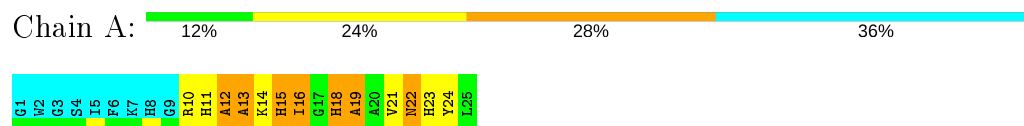
4.2.37 Score per residue for model 37

- Molecule 1: Pleurocidin-like peptide WF4



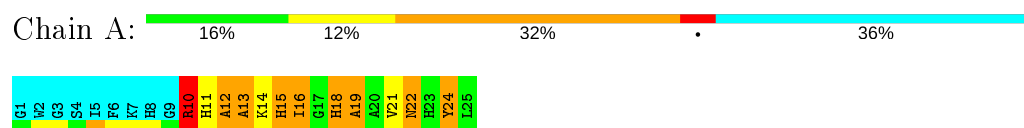
4.2.38 Score per residue for model 38

- Molecule 1: Pleurocidin-like peptide WF4



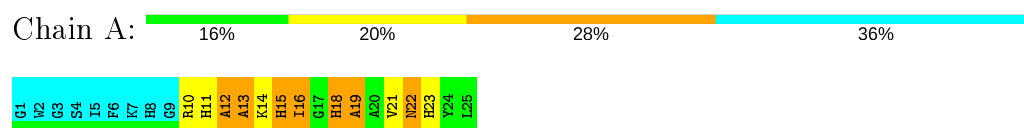
4.2.39 Score per residue for model 39

- Molecule 1: Pleurocidin-like peptide WF4



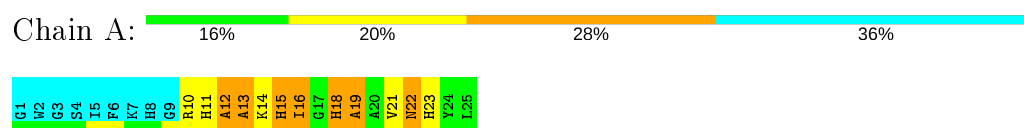
4.2.40 Score per residue for model 40

- Molecule 1: Pleurocidin-like peptide WF4



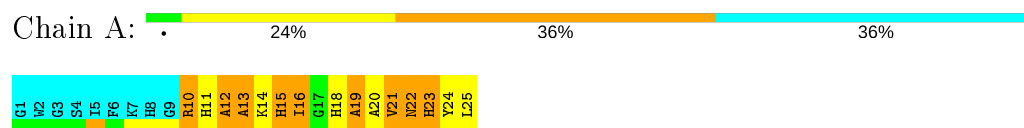
4.2.41 Score per residue for model 41

- Molecule 1: Pleurocidin-like peptide WF4



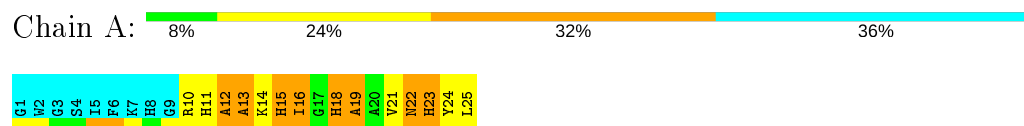
4.2.42 Score per residue for model 42

- Molecule 1: Pleurocidin-like peptide WF4



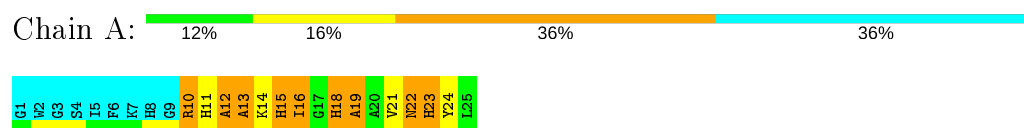
4.2.43 Score per residue for model 43

- Molecule 1: Pleurocidin-like peptide WF4



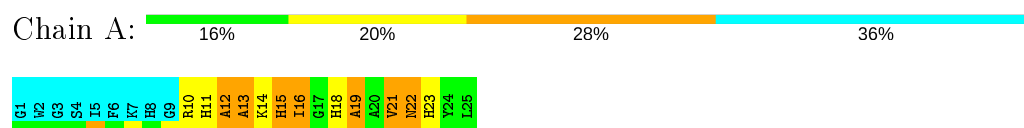
4.2.44 Score per residue for model 44

- Molecule 1: Pleurocidin-like peptide WF4



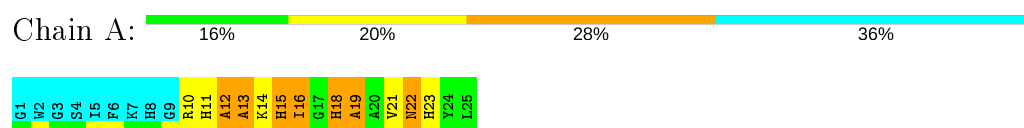
4.2.45 Score per residue for model 45

- Molecule 1: Pleurocidin-like peptide WF4



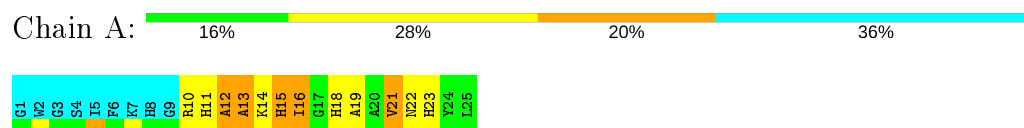
4.2.46 Score per residue for model 46

- Molecule 1: Pleurocidin-like peptide WF4



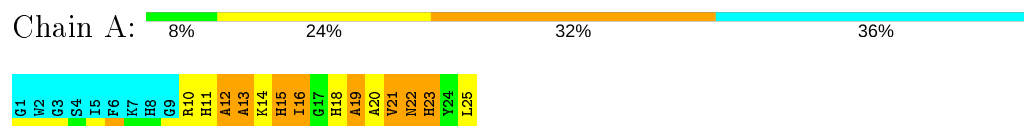
4.2.47 Score per residue for model 47

- Molecule 1: Pleurocidin-like peptide WF4



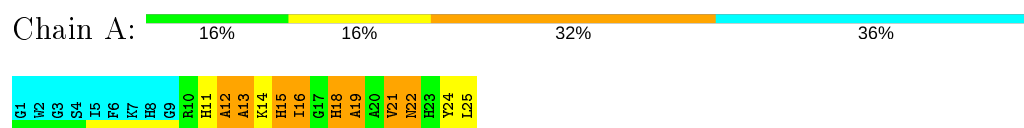
4.2.48 Score per residue for model 48

- Molecule 1: Pleurocidin-like peptide WF4



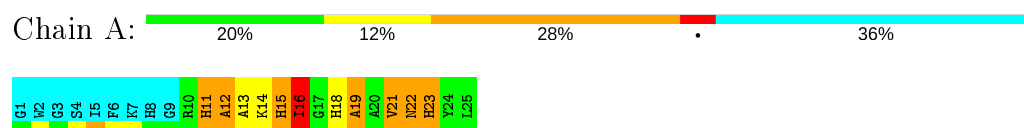
4.2.49 Score per residue for model 49

- Molecule 1: Pleurocidin-like peptide WF4



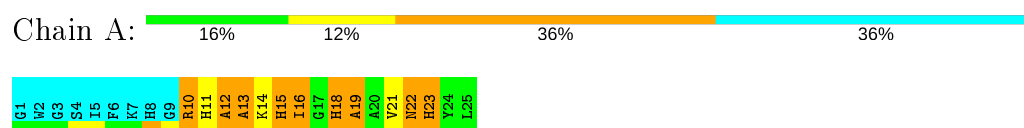
4.2.50 Score per residue for model 50

- Molecule 1: Pleurocidin-like peptide WF4



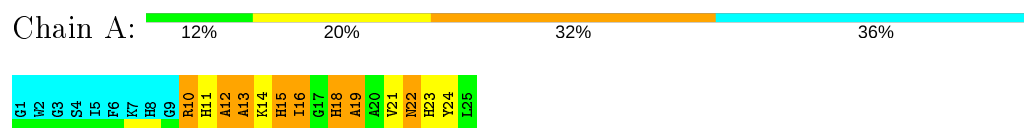
4.2.51 Score per residue for model 51

- Molecule 1: Pleurocidin-like peptide WF4



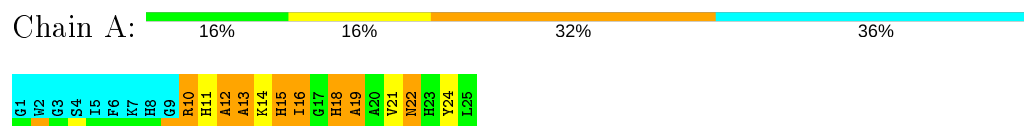
4.2.52 Score per residue for model 52

- Molecule 1: Pleurocidin-like peptide WF4



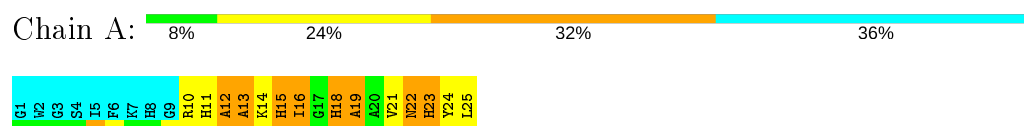
4.2.53 Score per residue for model 53

- Molecule 1: Pleurocidin-like peptide WF4



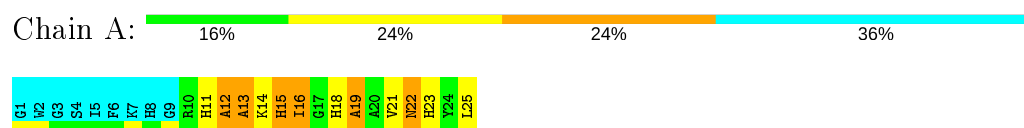
4.2.54 Score per residue for model 54

- Molecule 1: Pleurocidin-like peptide WF4



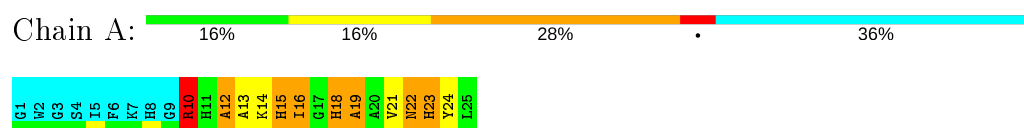
4.2.55 Score per residue for model 55

- Molecule 1: Pleurocidin-like peptide WF4



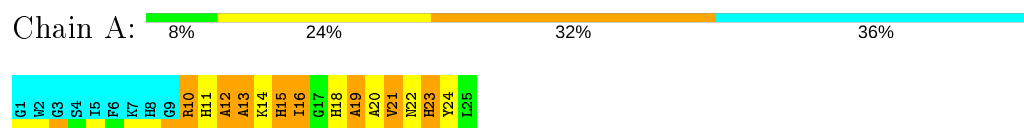
4.2.56 Score per residue for model 56

- Molecule 1: Pleurocidin-like peptide WF4



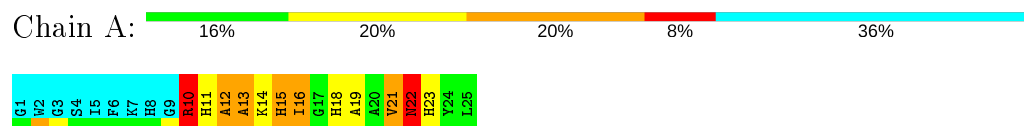
4.2.57 Score per residue for model 57

- Molecule 1: Pleurocidin-like peptide WF4



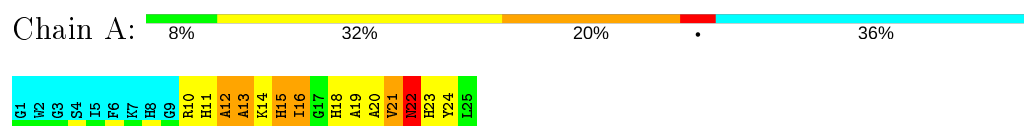
4.2.58 Score per residue for model 58

- Molecule 1: Pleurocidin-like peptide WF4



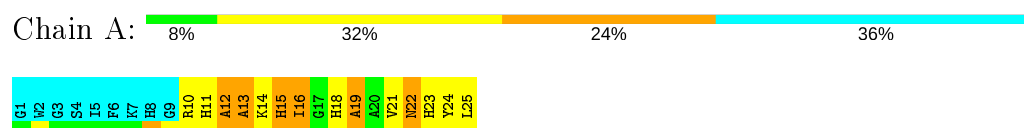
4.2.59 Score per residue for model 59

- Molecule 1: Pleurocidin-like peptide WF4



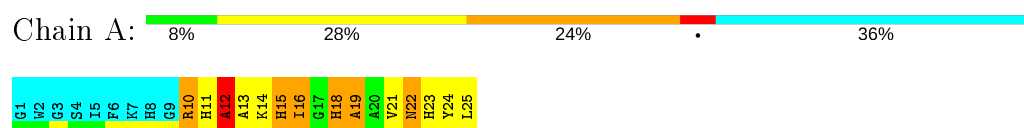
4.2.60 Score per residue for model 60

- Molecule 1: Pleurocidin-like peptide WF4



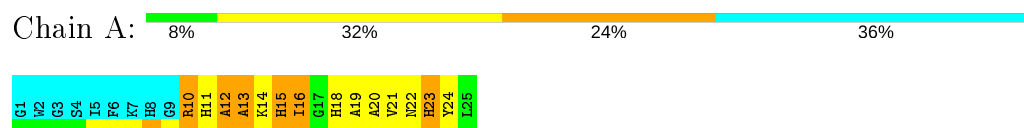
4.2.61 Score per residue for model 61

- Molecule 1: Pleurocidin-like peptide WF4



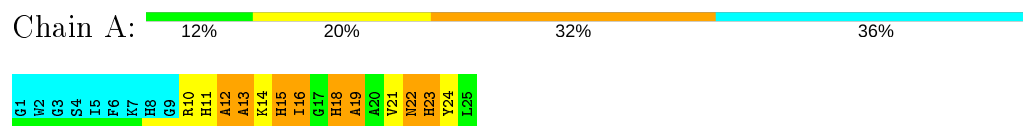
4.2.62 Score per residue for model 62

- Molecule 1: Pleurocidin-like peptide WF4



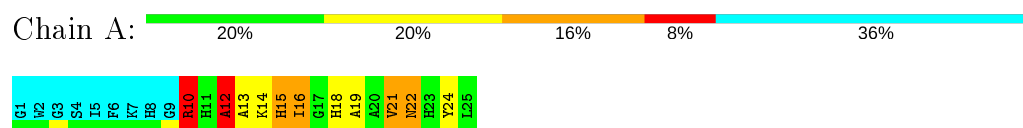
4.2.63 Score per residue for model 63

- Molecule 1: Pleurocidin-like peptide WF4



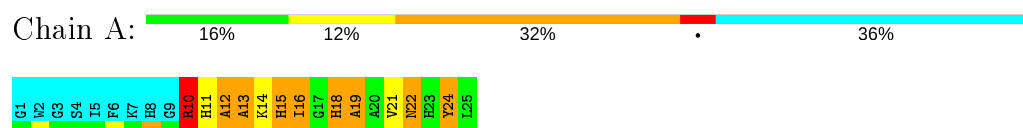
4.2.64 Score per residue for model 64

- Molecule 1: Pleurocidin-like peptide WF4



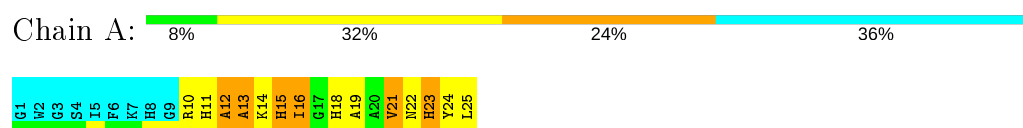
4.2.65 Score per residue for model 65

- Molecule 1: Pleurocidin-like peptide WF4



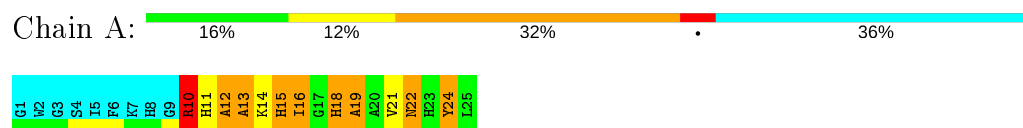
4.2.66 Score per residue for model 66

- Molecule 1: Pleurocidin-like peptide WF4



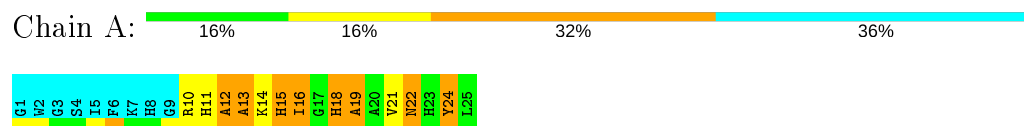
4.2.67 Score per residue for model 67

- Molecule 1: Pleurocidin-like peptide WF4



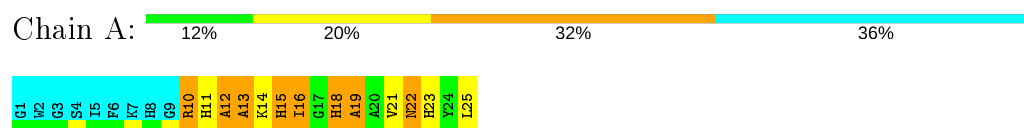
4.2.68 Score per residue for model 68

- Molecule 1: Pleurocidin-like peptide WF4



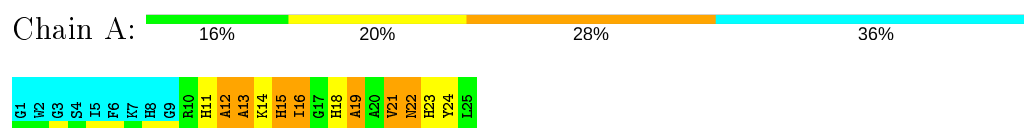
4.2.69 Score per residue for model 69

- Molecule 1: Pleurocidin-like peptide WF4



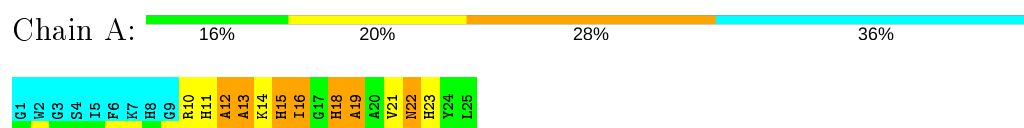
4.2.70 Score per residue for model 70

- Molecule 1: Pleurocidin-like peptide WF4



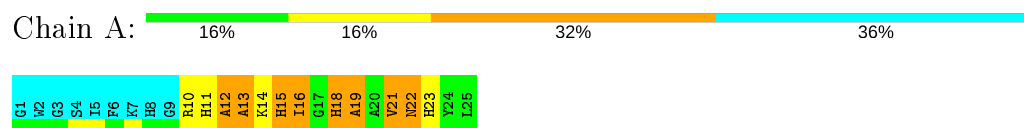
4.2.71 Score per residue for model 71

- Molecule 1: Pleurocidin-like peptide WF4



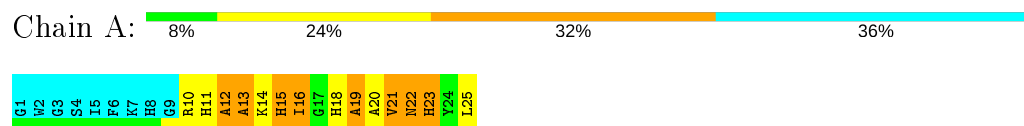
4.2.72 Score per residue for model 72

- Molecule 1: Pleurocidin-like peptide WF4



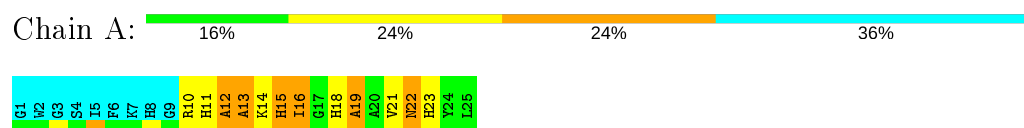
4.2.73 Score per residue for model 73

- Molecule 1: Pleurocidin-like peptide WF4



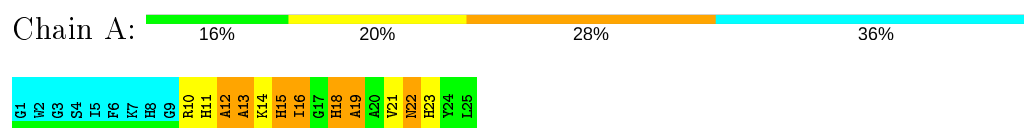
4.2.74 Score per residue for model 74

- Molecule 1: Pleurocidin-like peptide WF4



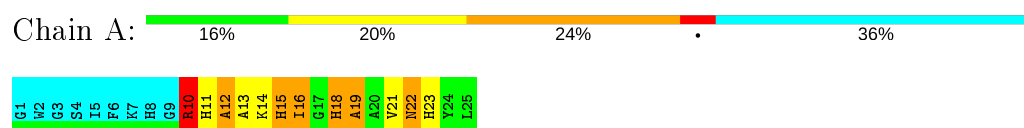
4.2.75 Score per residue for model 75

- Molecule 1: Pleurocidin-like peptide WF4



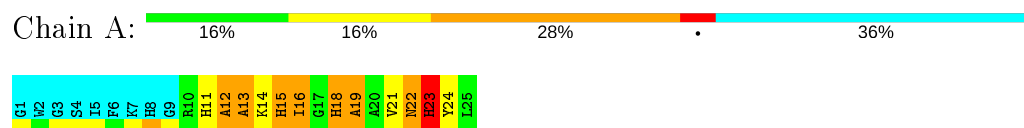
4.2.76 Score per residue for model 76

- Molecule 1: Pleurocidin-like peptide WF4



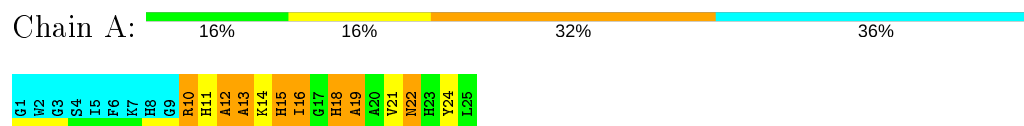
4.2.77 Score per residue for model 77 (medoid)

- Molecule 1: Pleurocidin-like peptide WF4



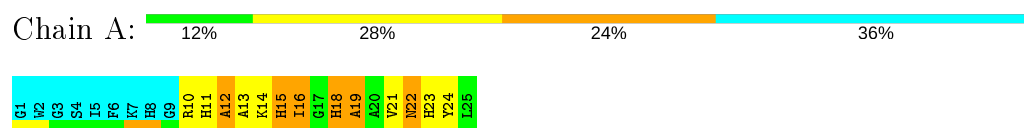
4.2.78 Score per residue for model 78

- Molecule 1: Pleurocidin-like peptide WF4



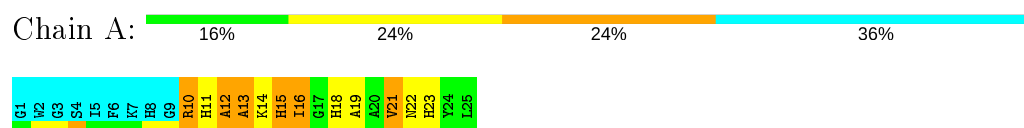
4.2.79 Score per residue for model 79

- Molecule 1: Pleurocidin-like peptide WF4



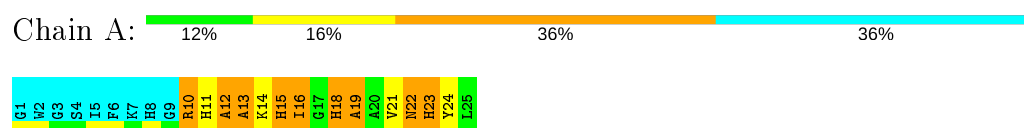
4.2.80 Score per residue for model 80

- Molecule 1: Pleurocidin-like peptide WF4



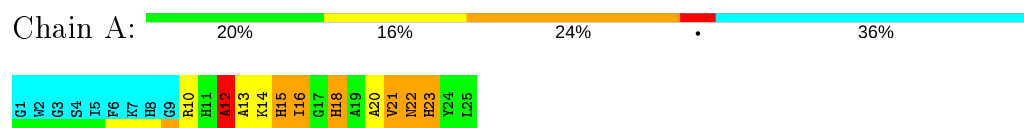
4.2.81 Score per residue for model 81

- Molecule 1: Pleurocidin-like peptide WF4



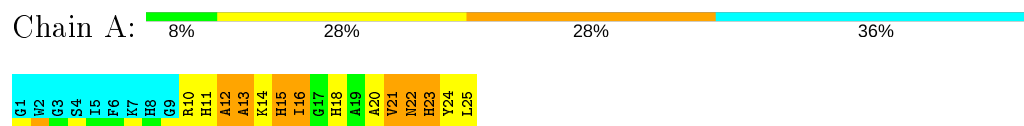
4.2.82 Score per residue for model 82

- Molecule 1: Pleurocidin-like peptide WF4



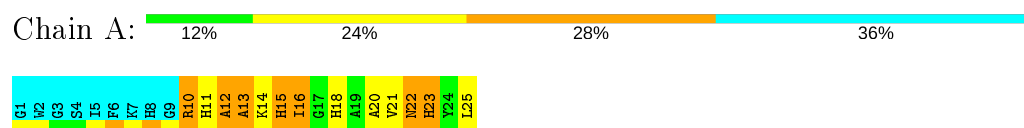
4.2.83 Score per residue for model 83

- Molecule 1: Pleurocidin-like peptide WF4



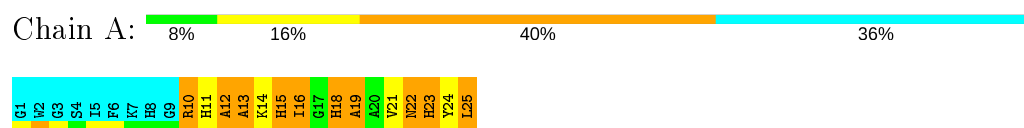
4.2.84 Score per residue for model 84

- Molecule 1: Pleurocidin-like peptide WF4



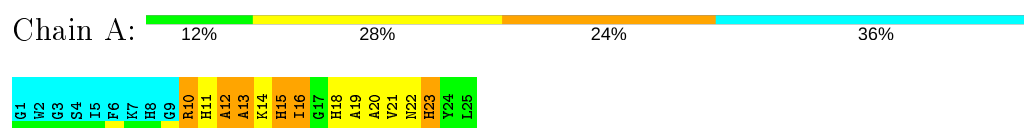
4.2.85 Score per residue for model 85

- Molecule 1: Pleurocidin-like peptide WF4



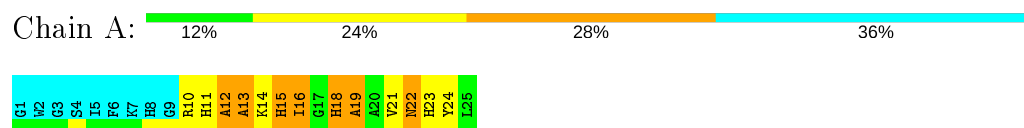
4.2.86 Score per residue for model 86

- Molecule 1: Pleurocidin-like peptide WF4



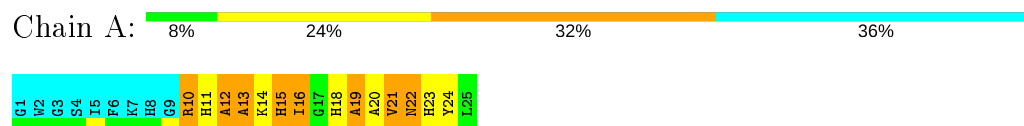
4.2.87 Score per residue for model 87

- Molecule 1: Pleurocidin-like peptide WF4



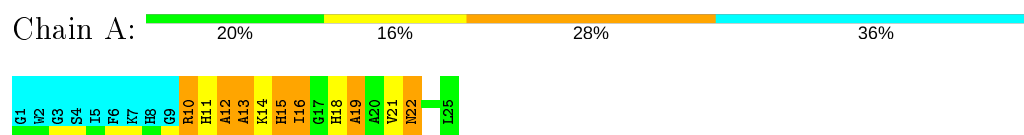
4.2.88 Score per residue for model 88

- Molecule 1: Pleurocidin-like peptide WF4



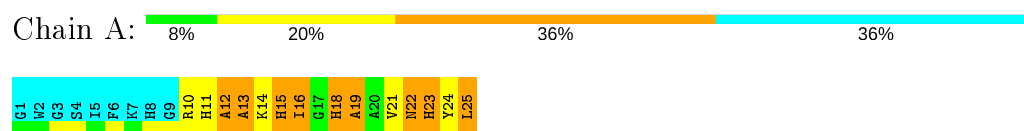
4.2.89 Score per residue for model 89

- Molecule 1: Pleurocidin-like peptide WF4



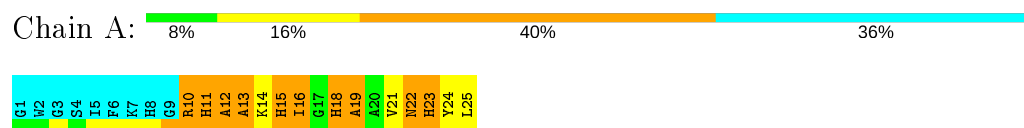
4.2.90 Score per residue for model 90

- Molecule 1: Pleurocidin-like peptide WF4



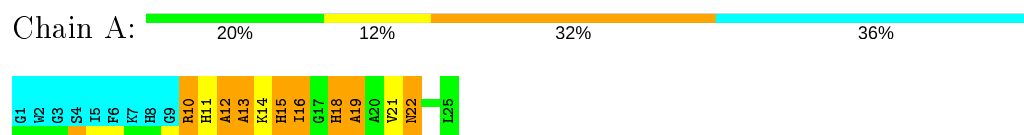
4.2.91 Score per residue for model 91

- Molecule 1: Pleurocidin-like peptide WF4



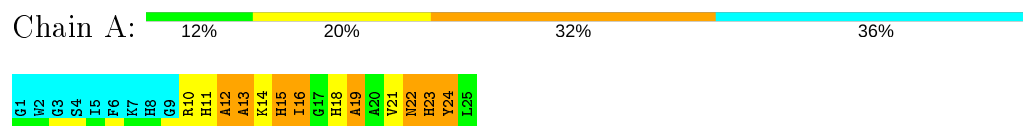
4.2.92 Score per residue for model 92

- Molecule 1: Pleurocidin-like peptide WF4



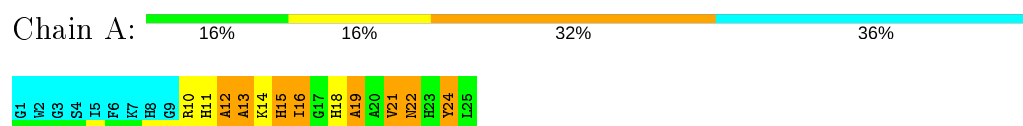
4.2.93 Score per residue for model 93

- Molecule 1: Pleurocidin-like peptide WF4



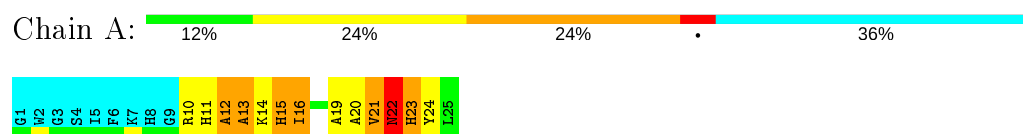
4.2.94 Score per residue for model 94

- Molecule 1: Pleurocidin-like peptide WF4



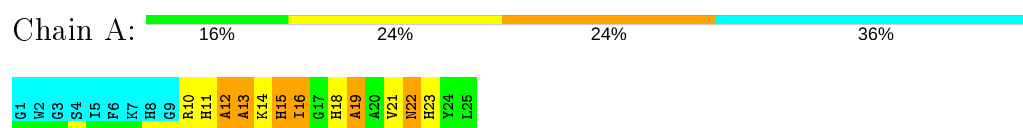
4.2.95 Score per residue for model 95

- Molecule 1: Pleurocidin-like peptide WF4



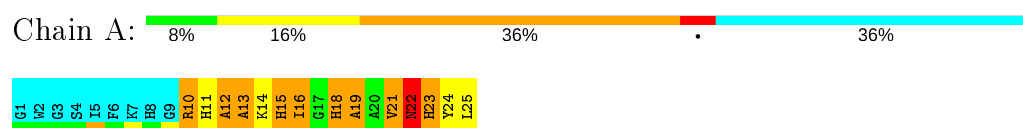
4.2.96 Score per residue for model 96

- Molecule 1: Pleurocidin-like peptide WF4



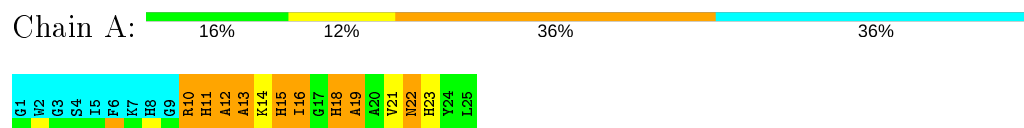
4.2.97 Score per residue for model 97

- Molecule 1: Pleurocidin-like peptide WF4



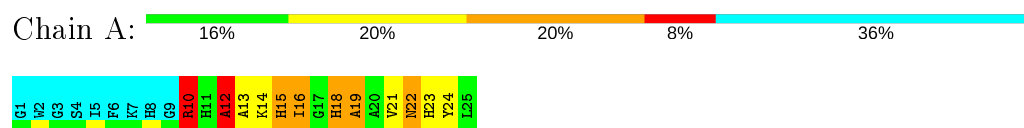
4.2.98 Score per residue for model 98

- Molecule 1: Pleurocidin-like peptide WF4



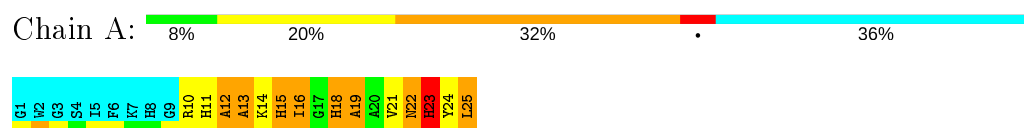
4.2.99 Score per residue for model 99

- Molecule 1: Pleurocidin-like peptide WF4



4.2.100 Score per residue for model 100

- Molecule 1: Pleurocidin-like peptide WF4



5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 100 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 |
|---------------|-----------------------|---------|
| DYNAMO | structure calculation | |
| DYNAMO | refinement | |

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) | working_cs.cif |
| Number of chemical shift lists | 1 |
| Total number of shifts | 107 |
| Number of shifts mapped to atoms | 107 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 30% |

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 | 0.97±0.01 | 1±0/131 (0.7± 0.2%) | 1.07±0.02 | 1±0/176 (0.6± 0.0%) |
| All | All | 0.97 | 93/13100 (0.7%) | 1.07 | 100/17600 (0.6%) |

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 | 0.9±0.3 |
| All | All | 0 | 89 |

All unique bond outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 12 | ALA | CA-CB | -5.66 | 1.40 | 1.52 | 91 | 93 |

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 13 | ALA | N-CA-C | -6.03 | 94.73 | 111.00 | 57 | 100 |

There are no chirality outliers.

All unique planar outliers are listed below.

| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1 | A | 10 | ARG | Sidechain | 89 |

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 | 127 | 123 | 123 | 22±2 |
| All | All | 12700 | 12300 | 12300 | 2219 |

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 89.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|----------------|----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:12:ALA:C | 1:A:14:LYS:N | 1.07 | 2.06 | 49 | 100 |
| 1:A:12:ALA:C | 1:A:14:LYS:H | 0.99 | 1.51 | 33 | 100 |
| 1:A:12:ALA:CA | 1:A:14:LYS:H | 0.73 | 1.96 | 69 | 100 |
| 1:A:14:LYS:O | 1:A:16:ILE:N | 0.72 | 2.22 | 62 | 100 |
| 1:A:12:ALA:N | 1:A:14:LYS:H | 0.70 | 1.84 | 79 | 100 |
| 1:A:12:ALA:O | 1:A:14:LYS:N | 0.67 | 2.28 | 36 | 100 |
| 1:A:12:ALA:H | 1:A:14:LYS:H | 0.65 | 1.34 | 79 | 11 |
| 1:A:14:LYS:NZ | 1:A:18:HIS:NE2 | 0.59 | 2.50 | 97 | 1 |
| 1:A:22:ASN:ND2 | 1:A:22:ASN:N | 0.59 | 2.50 | 59 | 2 |
| 1:A:12:ALA:O | 1:A:14:LYS:O | 0.58 | 2.21 | 62 | 100 |
| 1:A:23:HIS:ND1 | 1:A:24:TYR:N | 0.58 | 2.51 | 54 | 2 |
| 1:A:11:HIS:NE2 | 1:A:15:HIS:NE2 | 0.58 | 2.51 | 79 | 1 |
| 1:A:23:HIS:ND1 | 1:A:23:HIS:N | 0.58 | 2.50 | 25 | 6 |
| 1:A:14:LYS:NZ | 1:A:15:HIS:CE1 | 0.58 | 2.72 | 4 | 8 |
| 1:A:14:LYS:NZ | 1:A:18:HIS:CD2 | 0.57 | 2.72 | 97 | 3 |
| 1:A:14:LYS:CG | 1:A:15:HIS:H | 0.56 | 2.13 | 31 | 100 |
| 1:A:18:HIS:O | 1:A:19:ALA:HB2 | 0.56 | 2.00 | 4 | 61 |
| 1:A:11:HIS:ND1 | 1:A:11:HIS:N | 0.56 | 2.51 | 30 | 2 |
| 1:A:22:ASN:N | 1:A:22:ASN:ND2 | 0.56 | 2.49 | 95 | 1 |
| 1:A:23:HIS:CG | 1:A:24:TYR:N | 0.56 | 2.74 | 63 | 20 |
| 1:A:22:ASN:ND2 | 1:A:23:HIS:CD2 | 0.56 | 2.74 | 36 | 2 |
| 1:A:18:HIS:O | 1:A:19:ALA:HB3 | 0.56 | 2.01 | 64 | 2 |
| 1:A:14:LYS:NZ | 1:A:15:HIS:NE2 | 0.55 | 2.54 | 50 | 4 |
| 1:A:11:HIS:NE2 | 1:A:15:HIS:CD2 | 0.55 | 2.74 | 79 | 1 |
| 1:A:14:LYS:C | 1:A:16:ILE:N | 0.54 | 2.61 | 44 | 100 |
| 1:A:23:HIS:N | 1:A:23:HIS:ND1 | 0.54 | 2.54 | 27 | 3 |
| 1:A:12:ALA:H | 1:A:14:LYS:N | 0.53 | 2.01 | 18 | 5 |

Continued on next page...

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:25:LEU:HD12 | 1:A:25:LEU:N | 0.53 | 2.19 | 30 | 4 |
| 1:A:10:ARG:NH2 | 1:A:11:HIS:NE2 | 0.53 | 2.57 | 65 | 2 |
| 1:A:21:VAL:O | 1:A:22:ASN:CB | 0.53 | 2.57 | 79 | 84 |
| 1:A:23:HIS:CG | 1:A:24:TYR:H | 0.52 | 2.22 | 4 | 18 |
| 1:A:22:ASN:ND2 | 1:A:23:HIS:H | 0.52 | 2.03 | 95 | 3 |
| 1:A:25:LEU:N | 1:A:25:LEU:HD12 | 0.52 | 2.19 | 60 | 2 |
| 1:A:10:ARG:O | 1:A:11:HIS:CG | 0.51 | 2.63 | 39 | 13 |
| 1:A:22:ASN:HD22 | 1:A:22:ASN:N | 0.51 | 2.03 | 18 | 3 |
| 1:A:10:ARG:CD | 1:A:10:ARG:N | 0.51 | 2.73 | 32 | 3 |
| 1:A:25:LEU:N | 1:A:25:LEU:CD2 | 0.51 | 2.74 | 11 | 2 |
| 1:A:18:HIS:ND1 | 1:A:18:HIS:O | 0.51 | 2.44 | 36 | 3 |
| 1:A:11:HIS:O | 1:A:12:ALA:HB2 | 0.51 | 2.06 | 18 | 4 |
| 1:A:15:HIS:CG | 1:A:15:HIS:O | 0.51 | 2.64 | 11 | 32 |
| 1:A:25:LEU:CD2 | 1:A:25:LEU:N | 0.51 | 2.73 | 61 | 1 |
| 1:A:18:HIS:CD2 | 1:A:22:ASN:O | 0.51 | 2.64 | 82 | 3 |
| 1:A:23:HIS:CD2 | 1:A:24:TYR:N | 0.51 | 2.79 | 85 | 1 |
| 1:A:25:LEU:N | 1:A:25:LEU:CD1 | 0.50 | 2.74 | 22 | 4 |
| 1:A:19:ALA:C | 1:A:21:VAL:H | 0.50 | 2.10 | 29 | 30 |
| 1:A:18:HIS:ND1 | 1:A:22:ASN:O | 0.50 | 2.44 | 45 | 2 |
| 1:A:25:LEU:HD23 | 1:A:25:LEU:N | 0.50 | 2.21 | 11 | 1 |
| 1:A:22:ASN:O | 1:A:23:HIS:CG | 0.50 | 2.65 | 52 | 9 |
| 1:A:11:HIS:ND1 | 1:A:12:ALA:N | 0.50 | 2.59 | 98 | 3 |
| 1:A:18:HIS:O | 1:A:22:ASN:N | 0.50 | 2.45 | 58 | 2 |
| 1:A:15:HIS:CD2 | 1:A:21:VAL:O | 0.50 | 2.65 | 28 | 2 |
| 1:A:15:HIS:ND1 | 1:A:21:VAL:O | 0.50 | 2.45 | 82 | 9 |
| 1:A:14:LYS:C | 1:A:16:ILE:H | 0.50 | 2.10 | 34 | 94 |
| 1:A:22:ASN:O | 1:A:23:HIS:CD2 | 0.50 | 2.65 | 31 | 3 |
| 1:A:23:HIS:CG | 1:A:23:HIS:O | 0.50 | 2.65 | 5 | 9 |
| 1:A:25:LEU:CD1 | 1:A:25:LEU:N | 0.50 | 2.75 | 60 | 2 |
| 1:A:18:HIS:CG | 1:A:22:ASN:O | 0.50 | 2.65 | 29 | 3 |
| 1:A:24:TYR:O | 1:A:24:TYR:CG | 0.50 | 2.65 | 38 | 6 |
| 1:A:15:HIS:CD2 | 1:A:15:HIS:O | 0.50 | 2.65 | 73 | 4 |
| 1:A:14:LYS:CG | 1:A:15:HIS:N | 0.49 | 2.75 | 56 | 94 |
| 1:A:12:ALA:H | 1:A:14:LYS:HB3 | 0.49 | 1.66 | 16 | 89 |
| 1:A:10:ARG:O | 1:A:11:HIS:ND1 | 0.49 | 2.45 | 69 | 12 |
| 1:A:15:HIS:O | 1:A:15:HIS:ND1 | 0.49 | 2.44 | 28 | 3 |
| 1:A:24:TYR:CG | 1:A:24:TYR:O | 0.49 | 2.65 | 87 | 4 |
| 1:A:24:TYR:CD2 | 1:A:24:TYR:O | 0.49 | 2.66 | 78 | 5 |
| 1:A:15:HIS:O | 1:A:15:HIS:CG | 0.49 | 2.65 | 46 | 21 |
| 1:A:22:ASN:O | 1:A:23:HIS:ND1 | 0.49 | 2.45 | 1 | 1 |
| 1:A:24:TYR:O | 1:A:24:TYR:CD1 | 0.49 | 2.65 | 42 | 16 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:24:TYR:O | 1:A:24:TYR:CD2 | 0.49 | 2.66 | 93 | 8 |
| 1:A:14:LYS:HZ2 | 1:A:15:HIS:CE1 | 0.49 | 2.26 | 84 | 3 |
| 1:A:24:TYR:CD1 | 1:A:24:TYR:O | 0.49 | 2.66 | 39 | 8 |
| 1:A:23:HIS:CD2 | 1:A:23:HIS:O | 0.49 | 2.66 | 38 | 3 |
| 1:A:11:HIS:N | 1:A:11:HIS:ND1 | 0.49 | 2.58 | 91 | 1 |
| 1:A:22:ASN:OD1 | 1:A:23:HIS:CE1 | 0.49 | 2.66 | 52 | 2 |
| 1:A:23:HIS:O | 1:A:23:HIS:CG | 0.48 | 2.65 | 14 | 6 |
| 1:A:14:LYS:O | 1:A:16:ILE:HG22 | 0.48 | 2.09 | 36 | 87 |
| 1:A:19:ALA:CB | 1:A:24:TYR:N | 0.48 | 2.77 | 23 | 2 |
| 1:A:11:HIS:O | 1:A:11:HIS:ND1 | 0.48 | 2.46 | 50 | 1 |
| 1:A:11:HIS:O | 1:A:12:ALA:CB | 0.48 | 2.62 | 61 | 4 |
| 1:A:18:HIS:O | 1:A:22:ASN:CA | 0.48 | 2.62 | 64 | 2 |
| 1:A:18:HIS:CD2 | 1:A:18:HIS:O | 0.47 | 2.67 | 23 | 1 |
| 1:A:12:ALA:H | 1:A:14:LYS:CB | 0.47 | 2.22 | 61 | 4 |
| 1:A:11:HIS:C | 1:A:13:ALA:H | 0.47 | 2.13 | 69 | 88 |
| 1:A:14:LYS:HZ1 | 1:A:22:ASN:ND2 | 0.47 | 2.07 | 71 | 1 |
| 1:A:10:ARG:O | 1:A:11:HIS:CD2 | 0.47 | 2.66 | 92 | 2 |
| 1:A:11:HIS:O | 1:A:12:ALA:HB3 | 0.47 | 2.10 | 34 | 88 |
| 1:A:23:HIS:O | 1:A:24:TYR:CG | 0.47 | 2.67 | 4 | 1 |
| 1:A:22:ASN:ND2 | 1:A:23:HIS:N | 0.47 | 2.62 | 18 | 3 |
| 1:A:10:ARG:N | 1:A:10:ARG:CD | 0.47 | 2.78 | 56 | 2 |
| 1:A:19:ALA:C | 1:A:21:VAL:N | 0.46 | 2.69 | 58 | 64 |
| 1:A:22:ASN:O | 1:A:23:HIS:CB | 0.46 | 2.64 | 33 | 10 |
| 1:A:15:HIS:CD2 | 1:A:23:HIS:CE1 | 0.46 | 3.03 | 31 | 2 |
| 1:A:18:HIS:O | 1:A:19:ALA:CB | 0.46 | 2.63 | 32 | 30 |
| 1:A:25:LEU:HD22 | 1:A:25:LEU:N | 0.46 | 2.26 | 61 | 1 |
| 1:A:21:VAL:O | 1:A:21:VAL:HG12 | 0.46 | 2.11 | 11 | 20 |
| 1:A:23:HIS:C | 1:A:24:TYR:CG | 0.45 | 2.90 | 4 | 1 |
| 1:A:11:HIS:CD2 | 1:A:11:HIS:O | 0.45 | 2.69 | 73 | 2 |
| 1:A:23:HIS:ND1 | 1:A:23:HIS:O | 0.45 | 2.49 | 5 | 3 |
| 1:A:15:HIS:ND1 | 1:A:15:HIS:O | 0.45 | 2.50 | 65 | 4 |
| 1:A:10:ARG:O | 1:A:11:HIS:O | 0.45 | 2.35 | 98 | 2 |
| 1:A:15:HIS:O | 1:A:15:HIS:CD2 | 0.45 | 2.69 | 83 | 5 |
| 1:A:23:HIS:O | 1:A:24:TYR:CD1 | 0.45 | 2.70 | 4 | 1 |
| 1:A:18:HIS:C | 1:A:18:HIS:ND1 | 0.45 | 2.70 | 29 | 2 |
| 1:A:10:ARG:C | 1:A:11:HIS:CG | 0.45 | 2.91 | 11 | 2 |
| 1:A:21:VAL:HG12 | 1:A:21:VAL:O | 0.45 | 2.12 | 44 | 18 |
| 1:A:24:TYR:CD1 | 1:A:25:LEU:N | 0.44 | 2.86 | 90 | 1 |
| 1:A:18:HIS:O | 1:A:18:HIS:ND1 | 0.44 | 2.50 | 9 | 2 |
| 1:A:23:HIS:C | 1:A:25:LEU:N | 0.44 | 2.71 | 84 | 10 |
| 1:A:25:LEU:N | 1:A:25:LEU:HD23 | 0.44 | 2.26 | 90 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:19:ALA:O | 1:A:20:ALA:HB3 | 0.44 | 2.12 | 88 | 10 |
| 1:A:22:ASN:C | 1:A:23:HIS:CG | 0.44 | 2.91 | 12 | 1 |
| 1:A:10:ARG:C | 1:A:11:HIS:ND1 | 0.44 | 2.71 | 88 | 2 |
| 1:A:23:HIS:CD2 | 1:A:24:TYR:H | 0.44 | 2.31 | 91 | 3 |
| 1:A:23:HIS:O | 1:A:23:HIS:CD2 | 0.44 | 2.71 | 73 | 2 |
| 1:A:19:ALA:CB | 1:A:23:HIS:O | 0.43 | 2.66 | 54 | 1 |
| 1:A:14:LYS:HZ1 | 1:A:15:HIS:CE1 | 0.43 | 2.30 | 94 | 1 |
| 1:A:19:ALA:O | 1:A:21:VAL:N | 0.43 | 2.52 | 29 | 4 |
| 1:A:18:HIS:HD1 | 1:A:18:HIS:C | 0.43 | 2.17 | 45 | 2 |
| 1:A:16:ILE:O | 1:A:20:ALA:N | 0.43 | 2.52 | 36 | 4 |
| 1:A:22:ASN:C | 1:A:23:HIS:ND1 | 0.43 | 2.72 | 30 | 1 |
| 1:A:25:LEU:HD12 | 1:A:25:LEU:C | 0.43 | 2.33 | 85 | 2 |
| 1:A:11:HIS:HD1 | 1:A:11:HIS:C | 0.43 | 2.16 | 76 | 1 |
| 1:A:22:ASN:CG | 1:A:23:HIS:CD2 | 0.43 | 2.91 | 1 | 1 |
| 1:A:23:HIS:O | 1:A:23:HIS:ND1 | 0.43 | 2.52 | 27 | 1 |
| 1:A:15:HIS:CE1 | 1:A:21:VAL:O | 0.43 | 2.72 | 82 | 1 |
| 1:A:23:HIS:CD2 | 1:A:25:LEU:C | 0.43 | 2.92 | 35 | 1 |
| 1:A:11:HIS:C | 1:A:13:ALA:N | 0.42 | 2.73 | 95 | 29 |
| 1:A:23:HIS:CE1 | 1:A:25:LEU:O | 0.42 | 2.73 | 85 | 1 |
| 1:A:25:LEU:C | 1:A:25:LEU:HD12 | 0.41 | 2.36 | 18 | 1 |
| 1:A:14:LYS:HZ3 | 1:A:18:HIS:CD2 | 0.41 | 2.33 | 77 | 1 |
| 1:A:11:HIS:CD2 | 1:A:14:LYS:NZ | 0.41 | 2.89 | 47 | 1 |
| 1:A:21:VAL:O | 1:A:22:ASN:OD1 | 0.41 | 2.39 | 9 | 1 |
| 1:A:23:HIS:O | 1:A:25:LEU:N | 0.41 | 2.54 | 97 | 1 |
| 1:A:14:LYS:HZ1 | 1:A:18:HIS:CD2 | 0.40 | 2.29 | 97 | 1 |
| 1:A:21:VAL:O | 1:A:22:ASN:CG | 0.40 | 2.60 | 56 | 1 |
| 1:A:25:LEU:C | 1:A:25:LEU:HD23 | 0.40 | 2.37 | 43 | 1 |
| 1:A:25:LEU:HD23 | 1:A:25:LEU:C | 0.40 | 2.36 | 9 | 2 |
| 1:A:14:LYS:HZ3 | 1:A:15:HIS:CE1 | 0.40 | 2.34 | 4 | 1 |
| 1:A:12:ALA:O | 1:A:13:ALA:C | 0.40 | 2.60 | 91 | 1 |

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 | 15/25 (60%) | 4±1 (26±5%) | 6±1 (40±7%) | 5±1 (35±6%) | 0 | 0 |
| All | All | 1500/2500 (60%) | 383 (26%) | 595 (40%) | 522 (35%) | 0 | 0 |

All 11 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 | 15 | HIS | 100 |
| 1 | A | 16 | ILE | 100 |
| 1 | A | 22 | ASN | 100 |
| 1 | A | 19 | ALA | 84 |
| 1 | A | 23 | HIS | 41 |
| 1 | A | 21 | VAL | 41 |
| 1 | A | 10 | ARG | 22 |
| 1 | A | 24 | TYR | 12 |
| 1 | A | 12 | ALA | 11 |
| 1 | A | 20 | ALA | 8 |
| 1 | A | 11 | HIS | 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 | 11/17 (65%) | 10±1 (89±6%) | 1±1 (11±6%) | 10 | 54 |
| All | All | 1100/1700 (65%) | 980 (89%) | 120 (11%) | 10 | 54 |

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 | 18 | HIS | 78 |
| 1 | A | 23 | HIS | 14 |
| 1 | A | 25 | LEU | 11 |
| 1 | A | 10 | ARG | 8 |
| 1 | A | 22 | ASN | 6 |
| 1 | A | 11 | HIS | 2 |
| 1 | A | 16 | ILE | 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

The completeness of assignment taking into account all chemical shift lists is 30% for the well-defined parts and 29% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *WF4-chemicalshift.php*

7.1.1 Bookkeeping

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 | 107 |
| Number of shifts mapped to atoms | 107 |
| 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

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 30%, i.e. 60 atoms were assigned a chemical shift out of a possible 201. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|--------------|----------------|-----------------|-----------------|
| Backbone | 31/80 (39%) | 31/32 (97%) | 0/32 (0%) | 0/16 (0%) |
| Sidechain | 29/85 (34%) | 29/50 (58%) | 0/30 (0%) | 0/5 (0%) |
| Aromatic | 0/36 (0%) | 0/20 (0%) | 0/12 (0%) | 0/4 (0%) |
| Overall | 60/201 (30%) | 60/102 (59%) | 0/74 (0%) | 0/25 (0%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 29%, i.e. 88 atoms were assigned a chemical shift out of a possible 308. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|--------------|----------------|-----------------|-----------------|
| Backbone | 47/125 (38%) | 47/50 (94%) | 0/50 (0%) | 0/25 (0%) |
| Sidechain | 41/119 (34%) | 41/71 (58%) | 0/42 (0%) | 0/6 (0%) |
| Aromatic | 0/64 (0%) | 0/35 (0%) | 0/23 (0%) | 0/6 (0%) |
| Overall | 88/308 (29%) | 88/156 (56%) | 0/115 (0%) | 0/37 (0%) |

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 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:

