



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 07:14 AM UTC

PDB ID : 6RY9 / pdb_00006ry9
BMRB ID : 34410
Title : Winter flounder 1a-1 in SDS micelles
Authors : Clarke, M.; Mason, A.J.
Deposited on : 2019-06-10

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

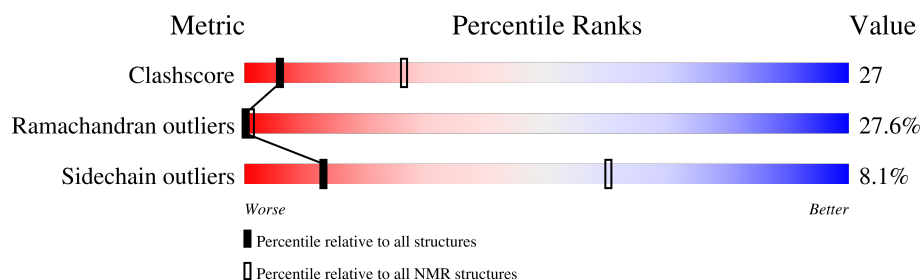
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 39%.

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	26	35% 50% 15%

2 Ensemble composition and analysis ⓘ

This entry contains 100 models.

Cyrange was unable to find well-defined residues.

Error message: Only domains with < 8 residues could be identified.

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 448 atoms, of which 240 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Pleurocidin-like prepropolypeptide.

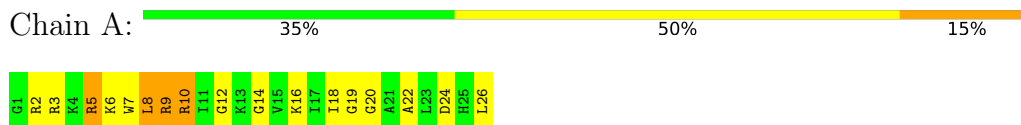
Mol	Chain	Residues	Atoms					Trace
1	A	26	Total	C	H	N	O	0
			448	132	240	48	28	

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: Pleurocidin-like prepropolypeptide

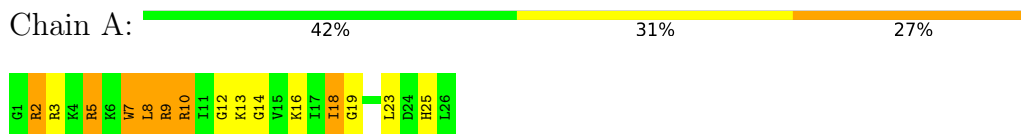


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

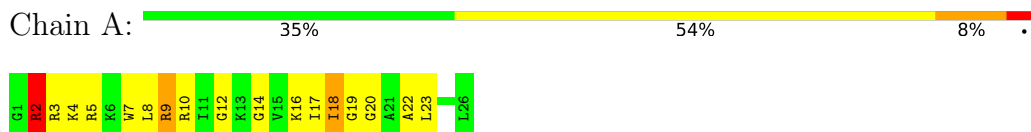
4.2.1 Score per residue for model 1

- Molecule 1: Pleurocidin-like prepropolypeptide



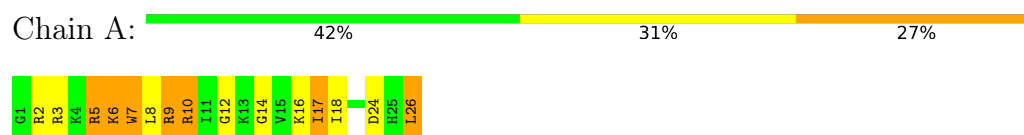
4.2.2 Score per residue for model 2

- Molecule 1: Pleurocidin-like prepropolypeptide



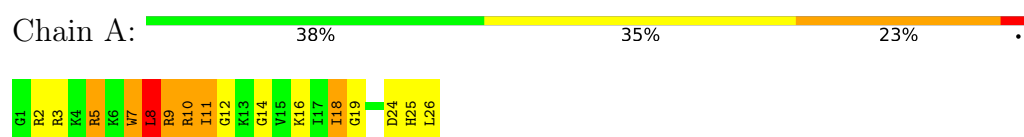
4.2.3 Score per residue for model 3

- Molecule 1: Pleurocidin-like prepropolypeptide



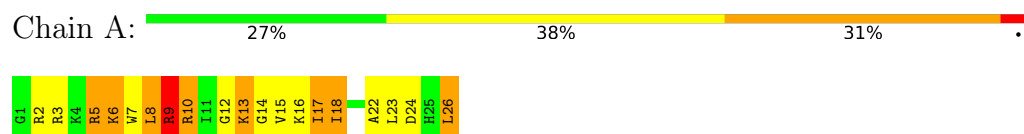
4.2.4 Score per residue for model 4

- Molecule 1: Pleurocidin-like prepropolypeptide



4.2.5 Score per residue for model 5

- Molecule 1: Pleurocidin-like prepropolypeptide



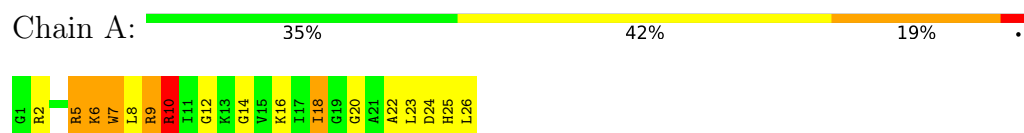
4.2.6 Score per residue for model 6

- Molecule 1: Pleurocidin-like prepropolypeptide



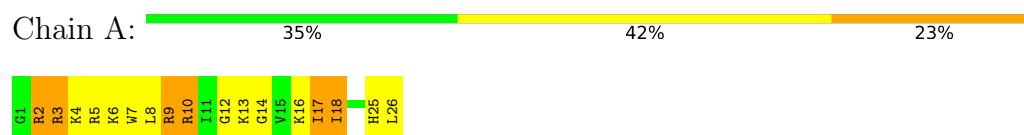
4.2.7 Score per residue for model 7

- Molecule 1: Pleurocidin-like prepropolypeptide



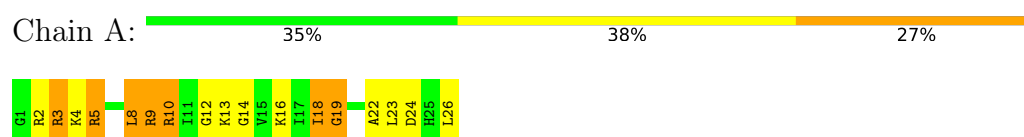
4.2.8 Score per residue for model 8

- Molecule 1: Pleurocidin-like prepropolypeptide



4.2.9 Score per residue for model 9

- Molecule 1: Pleurocidin-like prepropolypeptide



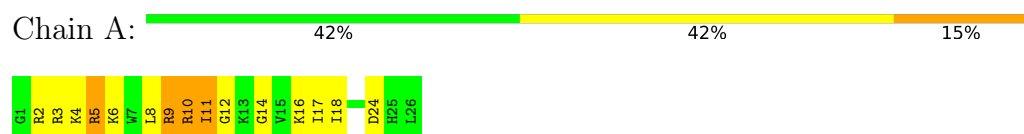
4.2.10 Score per residue for model 10

- Molecule 1: Pleurocidin-like prepropolypeptide



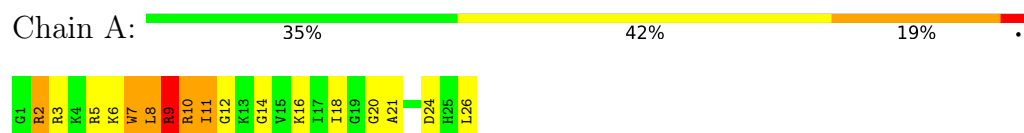
4.2.11 Score per residue for model 11

- Molecule 1: Pleurocidin-like prepropolypeptide



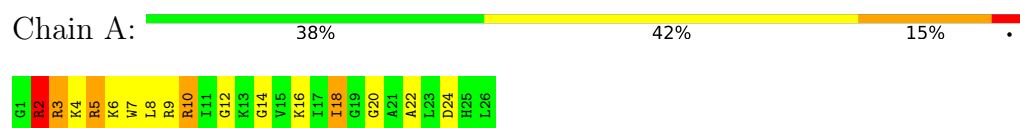
4.2.12 Score per residue for model 12

- Molecule 1: Pleurocidin-like prepropolypeptide



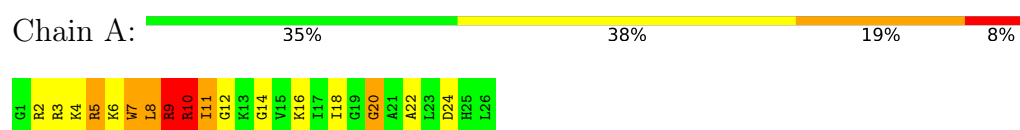
4.2.13 Score per residue for model 13

- Molecule 1: Pleurocidin-like prepropolypeptide



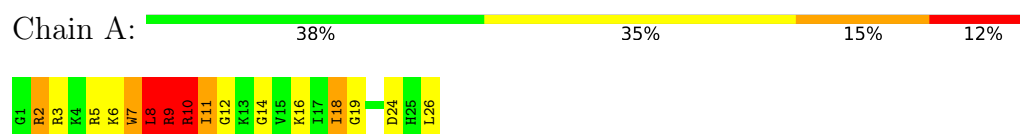
4.2.14 Score per residue for model 14

- Molecule 1: Pleurocidin-like prepropolypeptide



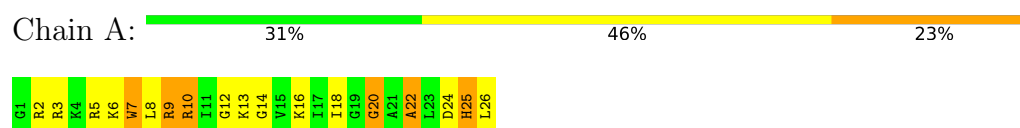
4.2.15 Score per residue for model 15

- Molecule 1: Pleurocidin-like prepropolypeptide



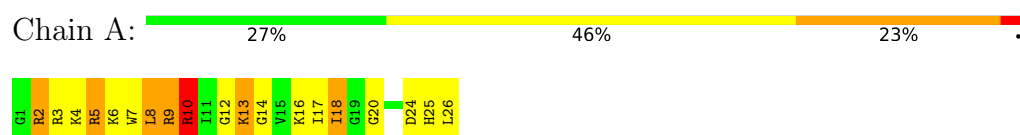
4.2.16 Score per residue for model 16

- Molecule 1: Pleurocidin-like prepropolypeptide



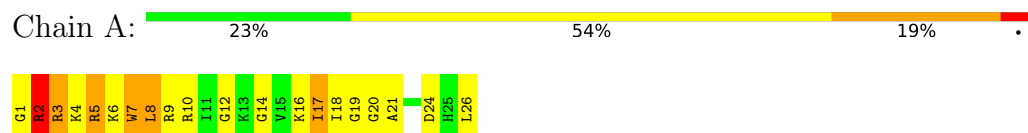
4.2.17 Score per residue for model 17

- Molecule 1: Pleurocidin-like prepropolypeptide



4.2.18 Score per residue for model 18

- Molecule 1: Pleurocidin-like prepropolypeptide



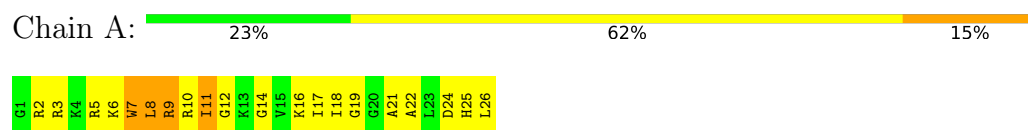
4.2.19 Score per residue for model 19

- Molecule 1: Pleurocidin-like prepropolypeptide



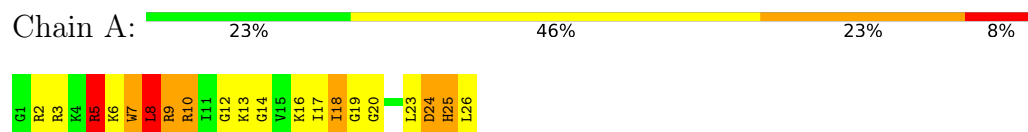
4.2.20 Score per residue for model 20

- Molecule 1: Pleurocidin-like prepropolypeptide



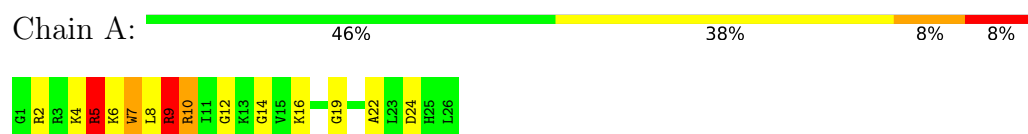
4.2.21 Score per residue for model 21

- Molecule 1: Pleurocidin-like prepropolypeptide



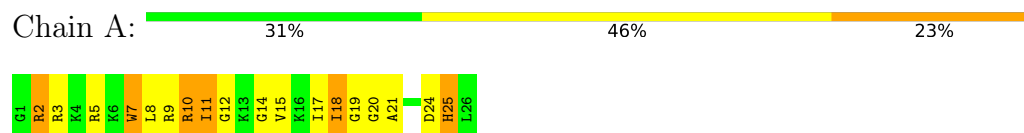
4.2.22 Score per residue for model 22

- Molecule 1: Pleurocidin-like prepropolypeptide



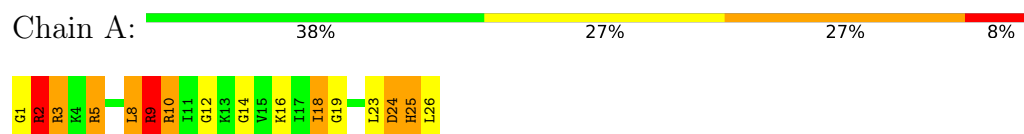
4.2.23 Score per residue for model 23

- Molecule 1: Pleurocidin-like prepropolypeptide



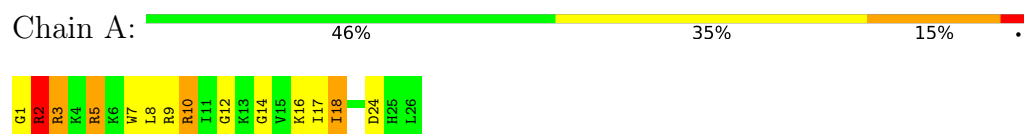
4.2.24 Score per residue for model 24

- Molecule 1: Pleurocidin-like prepropolypeptide



4.2.25 Score per residue for model 25

- Molecule 1: Pleurocidin-like prepropolypeptide



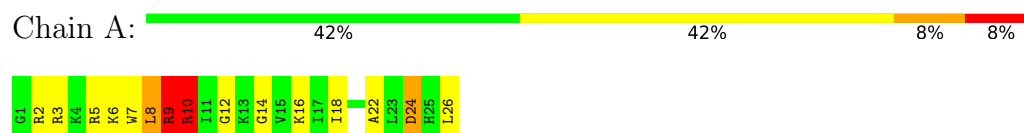
4.2.26 Score per residue for model 26

- Molecule 1: Pleurocidin-like prepropolypeptide



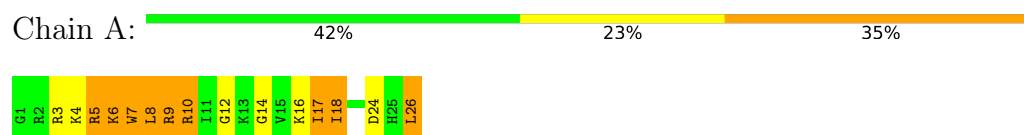
4.2.27 Score per residue for model 27

- Molecule 1: Pleurocidin-like prepropolypeptide



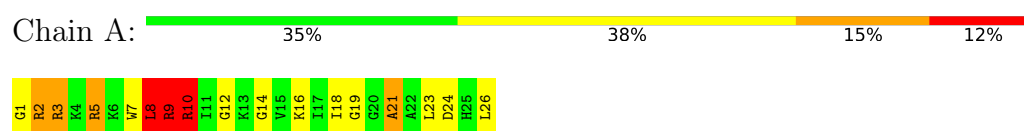
4.2.28 Score per residue for model 28

- Molecule 1: Pleurocidin-like prepropolypeptide



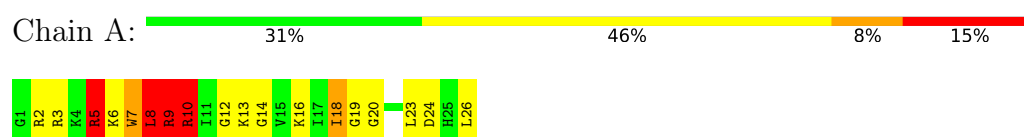
4.2.29 Score per residue for model 29

- Molecule 1: Pleurocidin-like prepropolypeptide



4.2.30 Score per residue for model 30

- Molecule 1: Pleurocidin-like prepropolypeptide



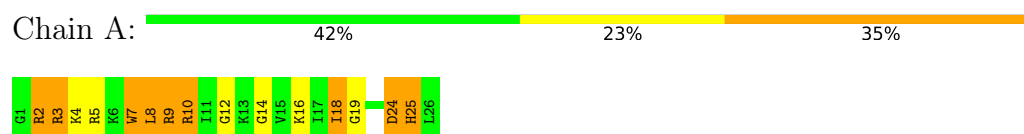
4.2.31 Score per residue for model 31

- Molecule 1: Pleurocidin-like prepropolypeptide



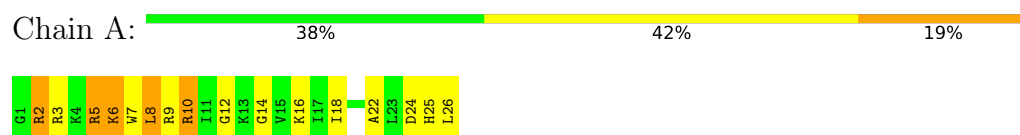
4.2.32 Score per residue for model 32

- Molecule 1: Pleurocidin-like prepropolypeptide



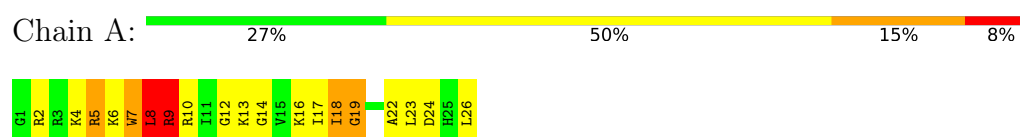
4.2.33 Score per residue for model 33

- Molecule 1: Pleurocidin-like prepropolypeptide



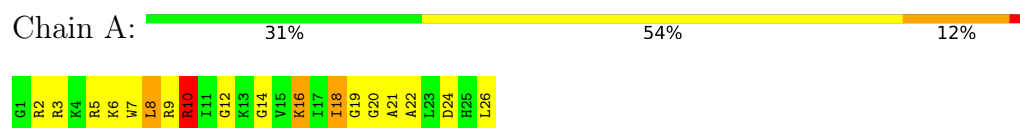
4.2.34 Score per residue for model 34

- Molecule 1: Pleurocidin-like prepropolypeptide



4.2.35 Score per residue for model 35

- Molecule 1: Pleurocidin-like prepropolypeptide



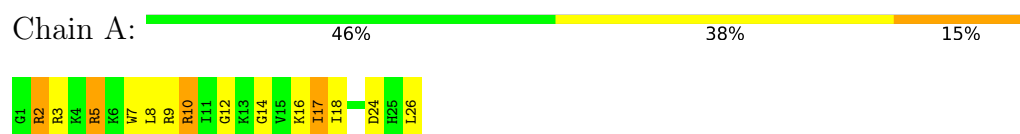
4.2.36 Score per residue for model 36

- Molecule 1: Pleurocidin-like prepropolypeptide



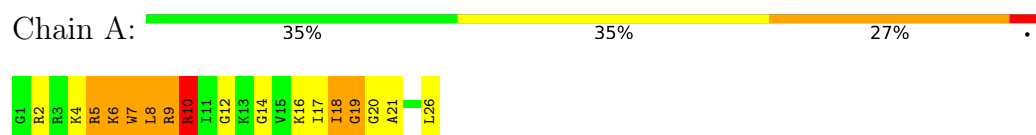
4.2.37 Score per residue for model 37

- Molecule 1: Pleurocidin-like prepropolypeptide



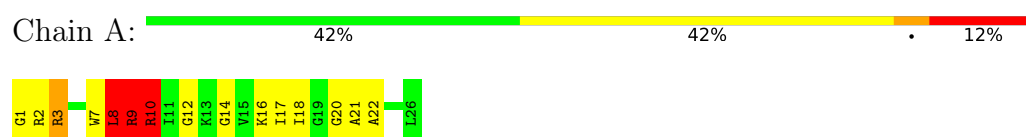
4.2.38 Score per residue for model 38

- Molecule 1: Pleurocidin-like prepropolypeptide



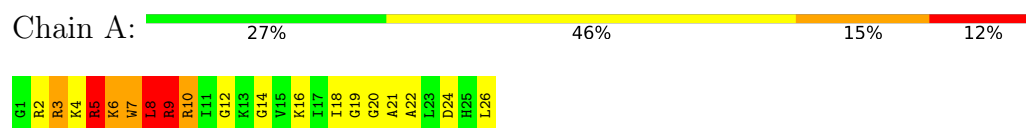
4.2.39 Score per residue for model 39

- Molecule 1: Pleurocidin-like prepropolypeptide



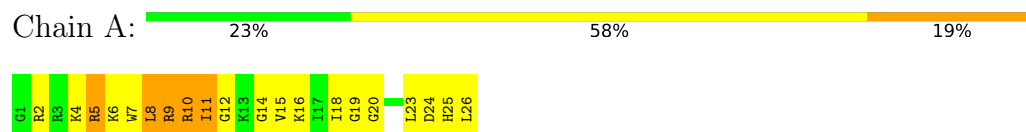
4.2.40 Score per residue for model 40

- Molecule 1: Pleurocidin-like prepropolypeptide



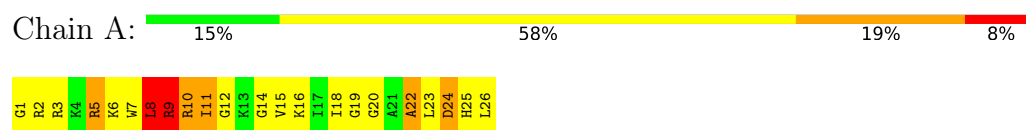
4.2.41 Score per residue for model 41

- Molecule 1: Pleurocidin-like prepropolypeptide



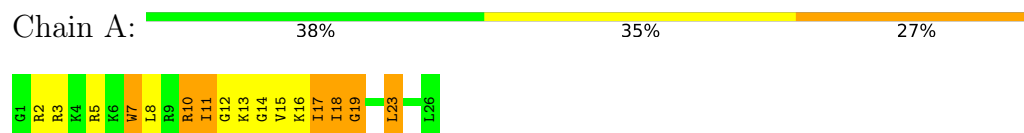
4.2.42 Score per residue for model 42

- Molecule 1: Pleurocidin-like prepropolypeptide



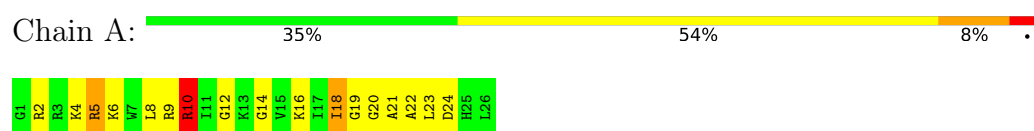
4.2.43 Score per residue for model 43

- Molecule 1: Pleurocidin-like prepropolypeptide



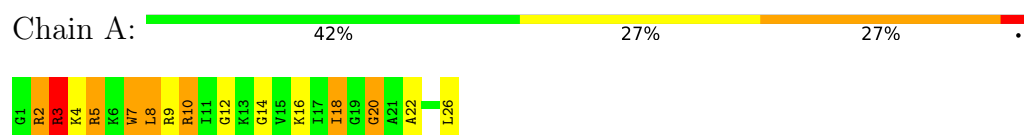
4.2.44 Score per residue for model 44

- Molecule 1: Pleurocidin-like prepropolypeptide



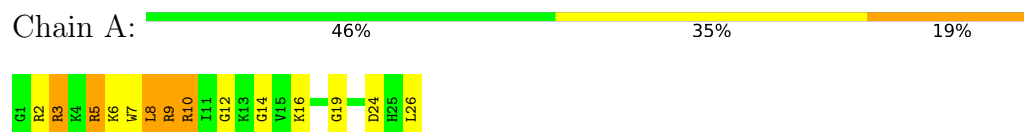
4.2.45 Score per residue for model 45

- Molecule 1: Pleurocidin-like prepropolypeptide



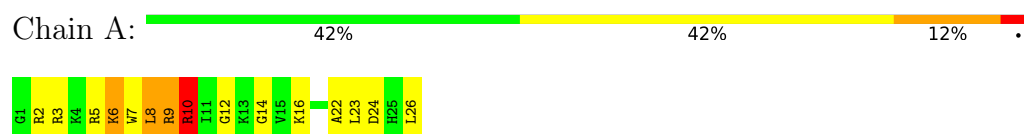
4.2.46 Score per residue for model 46

- Molecule 1: Pleurocidin-like prepropolypeptide



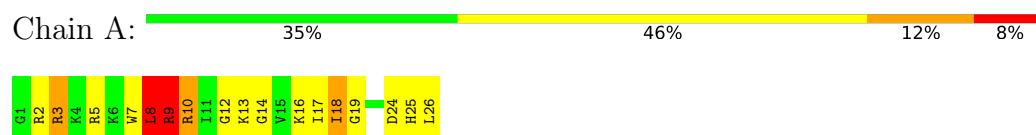
4.2.47 Score per residue for model 47

- Molecule 1: Pleurocidin-like prepropolypeptide



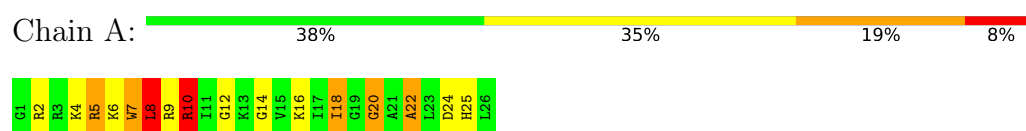
4.2.48 Score per residue for model 48

- Molecule 1: Pleurocidin-like prepropolypeptide



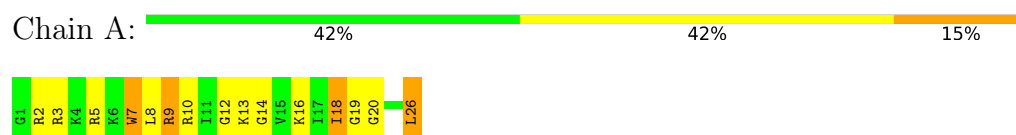
4.2.49 Score per residue for model 49

- Molecule 1: Pleurocidin-like prepropolypeptide



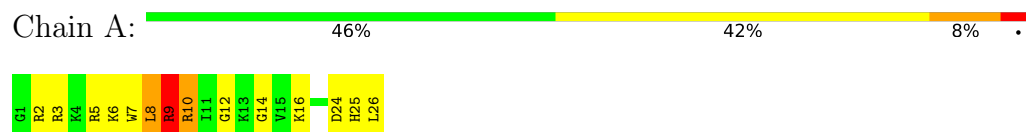
4.2.50 Score per residue for model 50

- Molecule 1: Pleurocidin-like prepropolypeptide



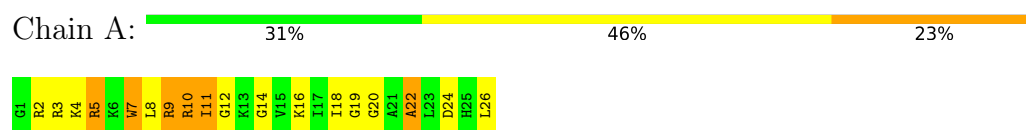
4.2.51 Score per residue for model 51

- Molecule 1: Pleurocidin-like prepropolypeptide



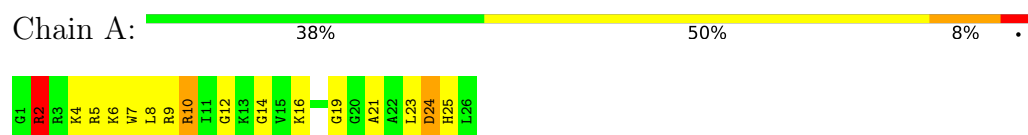
4.2.52 Score per residue for model 52

- Molecule 1: Pleurocidin-like prepropolypeptide



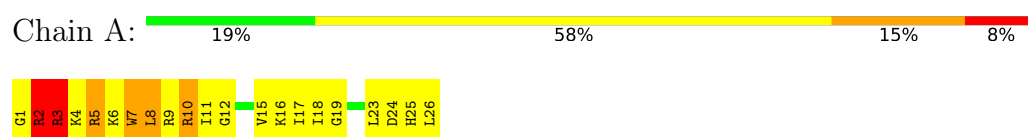
4.2.53 Score per residue for model 53

- Molecule 1: Pleurocidin-like prepropolypeptide



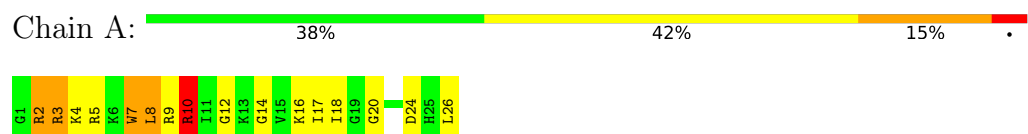
4.2.54 Score per residue for model 54

- Molecule 1: Pleurocidin-like prepropolypeptide



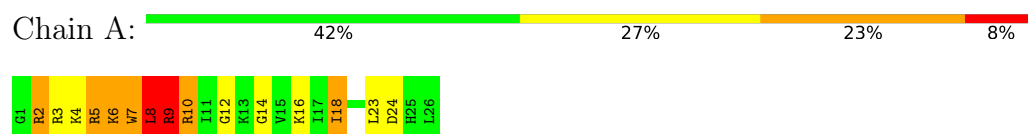
4.2.55 Score per residue for model 55

- Molecule 1: Pleurocidin-like prepropolypeptide



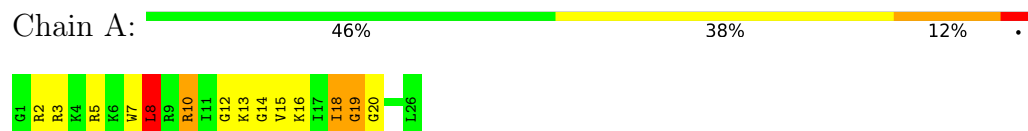
4.2.56 Score per residue for model 56

- Molecule 1: Pleurocidin-like prepropolypeptide



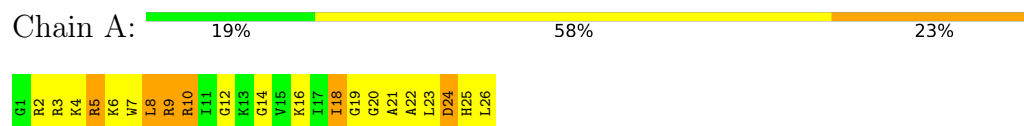
4.2.57 Score per residue for model 57

- Molecule 1: Pleurocidin-like prepropolypeptide



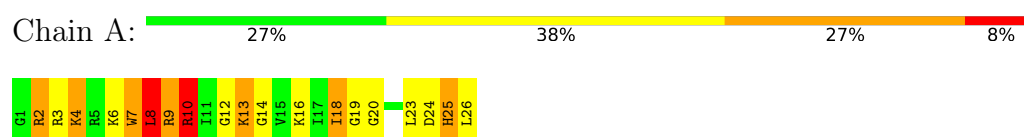
4.2.58 Score per residue for model 58

- Molecule 1: Pleurocidin-like prepropolypeptide



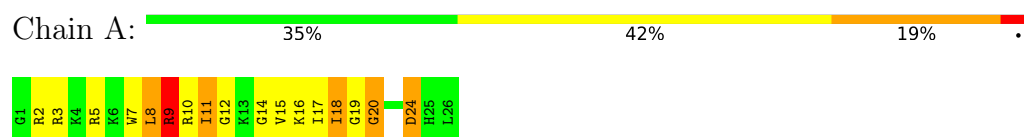
4.2.59 Score per residue for model 59

- Molecule 1: Pleurocidin-like prepropolypeptide



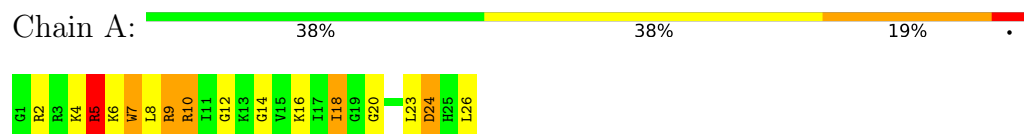
4.2.60 Score per residue for model 60

- Molecule 1: Pleurocidin-like prepropolypeptide



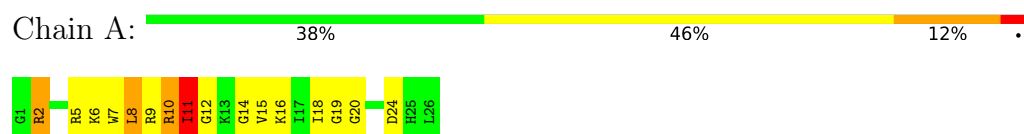
4.2.61 Score per residue for model 61

- Molecule 1: Pleurocidin-like prepropolypeptide



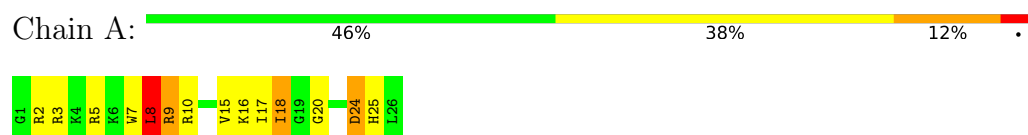
4.2.62 Score per residue for model 62

- Molecule 1: Pleurocidin-like prepropolypeptide



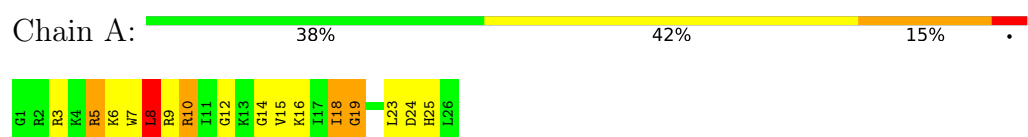
4.2.63 Score per residue for model 63

- Molecule 1: Pleurocidin-like prepropolypeptide



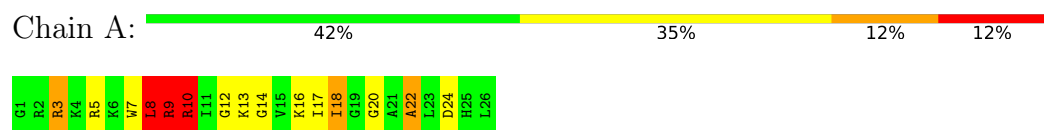
4.2.64 Score per residue for model 64

- Molecule 1: Pleurocidin-like prepropolypeptide



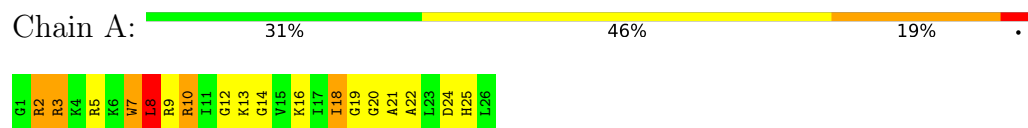
4.2.65 Score per residue for model 65

- Molecule 1: Pleurocidin-like prepropolypeptide



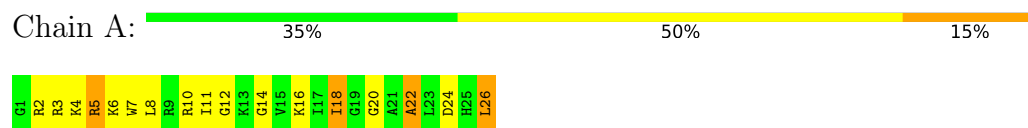
4.2.66 Score per residue for model 66

- Molecule 1: Pleurocidin-like prepropolypeptide



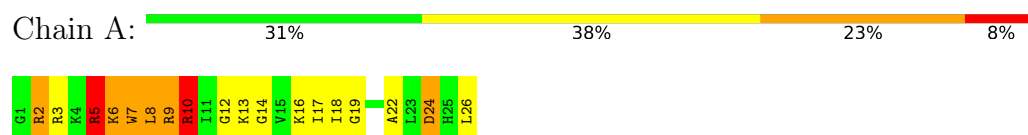
4.2.67 Score per residue for model 67

- Molecule 1: Pleurocidin-like prepropolypeptide



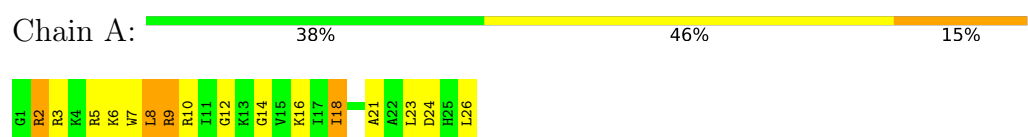
4.2.68 Score per residue for model 68

- Molecule 1: Pleurocidin-like prepropolypeptide



4.2.69 Score per residue for model 69

- Molecule 1: Pleurocidin-like prepropolypeptide



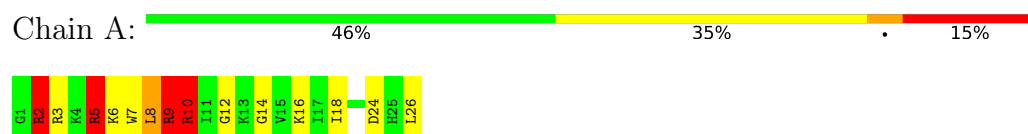
4.2.70 Score per residue for model 70

- Molecule 1: Pleurocidin-like prepropolypeptide



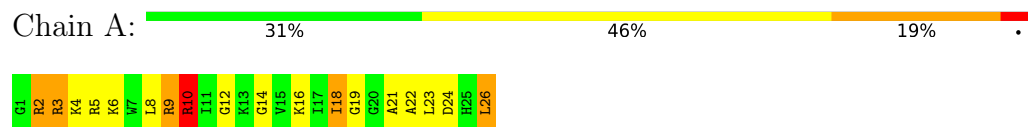
4.2.71 Score per residue for model 71

- Molecule 1: Pleurocidin-like prepropolypeptide



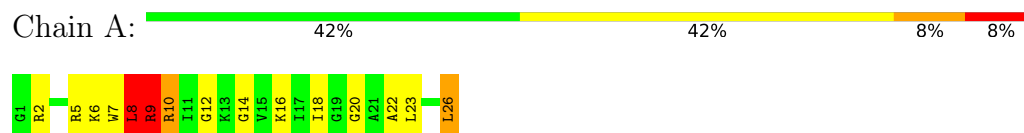
4.2.72 Score per residue for model 72

- Molecule 1: Pleurocidin-like prepropolypeptide



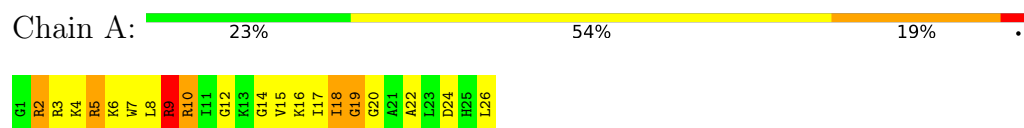
4.2.73 Score per residue for model 73

- Molecule 1: Pleurocidin-like prepropolypeptide



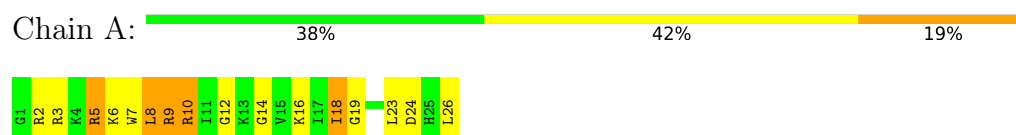
4.2.74 Score per residue for model 74

- Molecule 1: Pleurocidin-like prepropolypeptide



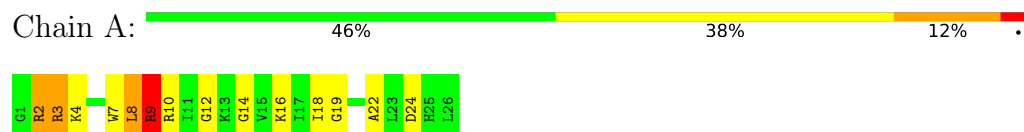
4.2.75 Score per residue for model 75

- Molecule 1: Pleurocidin-like prepropolypeptide



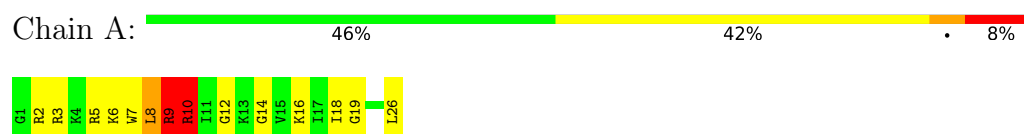
4.2.76 Score per residue for model 76

- Molecule 1: Pleurocidin-like prepropolypeptide



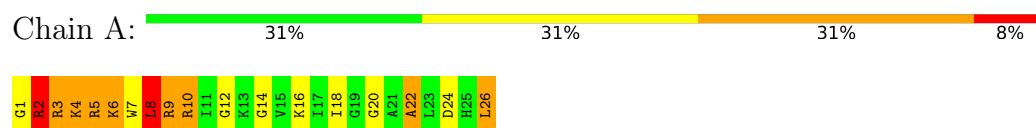
4.2.77 Score per residue for model 77

- Molecule 1: Pleurocidin-like prepropolypeptide



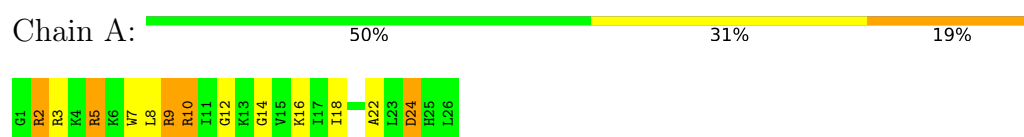
4.2.78 Score per residue for model 78

- Molecule 1: Pleurocidin-like prepropolypeptide



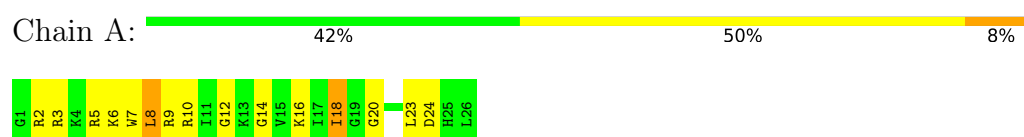
4.2.79 Score per residue for model 79

- Molecule 1: Pleurocidin-like prepropolypeptide



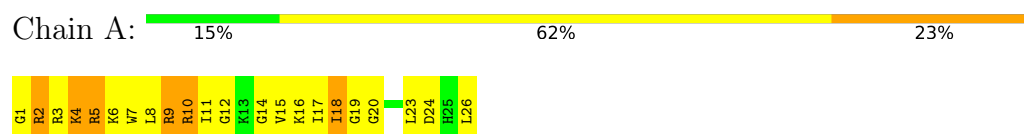
4.2.80 Score per residue for model 80

- Molecule 1: Pleurocidin-like prepropolypeptide



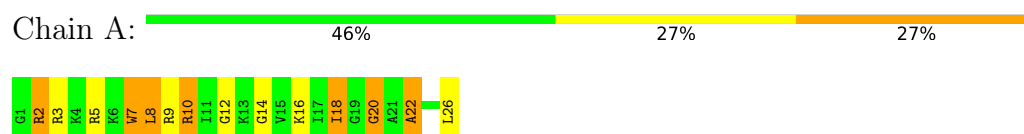
4.2.81 Score per residue for model 81

- Molecule 1: Pleurocidin-like prepropolypeptide



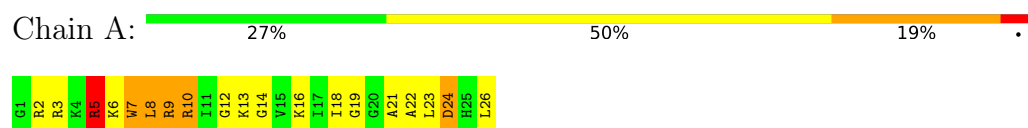
4.2.82 Score per residue for model 82

- Molecule 1: Pleurocidin-like prepropolypeptide



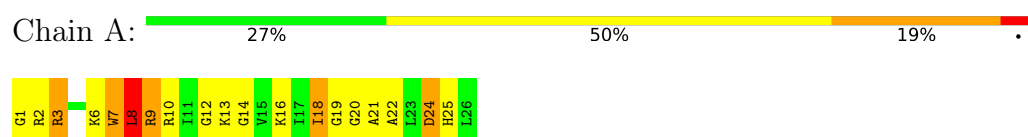
4.2.83 Score per residue for model 83

- Molecule 1: Pleurocidin-like prepropolypeptide



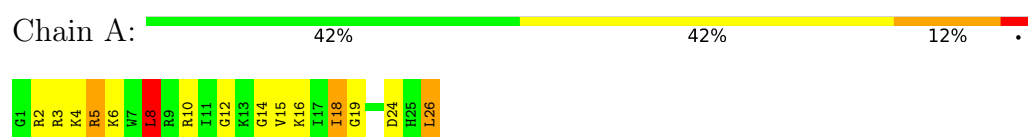
4.2.84 Score per residue for model 84

- Molecule 1: Pleurocidin-like prepropolypeptide



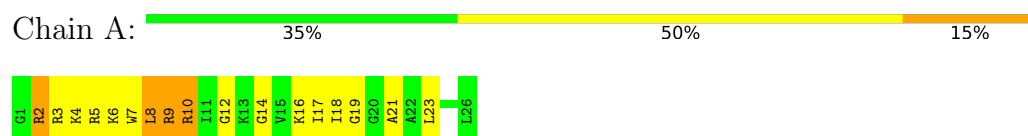
4.2.85 Score per residue for model 85

- Molecule 1: Pleurocidin-like prepropolypeptide



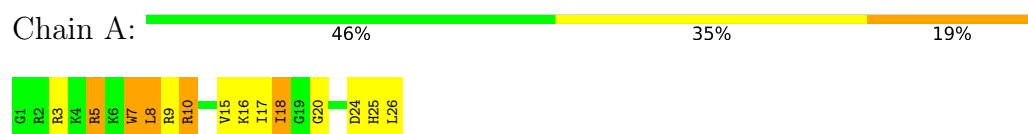
4.2.86 Score per residue for model 86

- Molecule 1: Pleurocidin-like prepropolypeptide



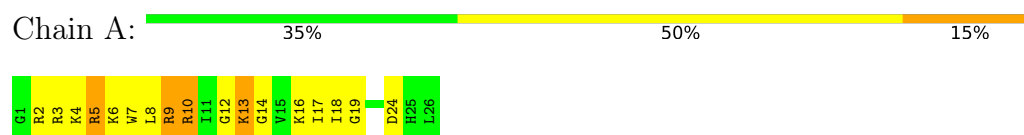
4.2.87 Score per residue for model 87

- Molecule 1: Pleurocidin-like prepropolypeptide



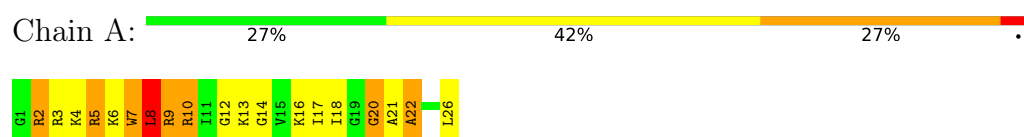
4.2.88 Score per residue for model 88

- Molecule 1: Pleurocidin-like prepropolypeptide



4.2.89 Score per residue for model 89

- Molecule 1: Pleurocidin-like prepropolypeptide



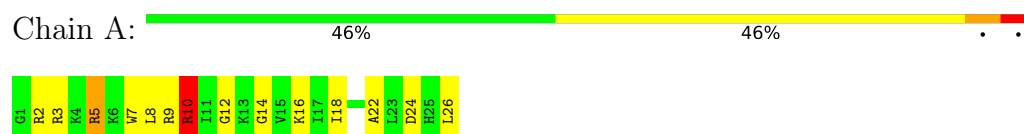
4.2.90 Score per residue for model 90

- Molecule 1: Pleurocidin-like prepropolypeptide



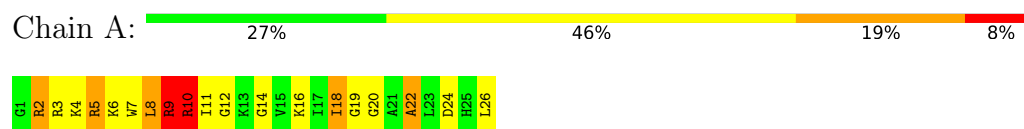
4.2.91 Score per residue for model 91

- Molecule 1: Pleurocidin-like prepropolypeptide



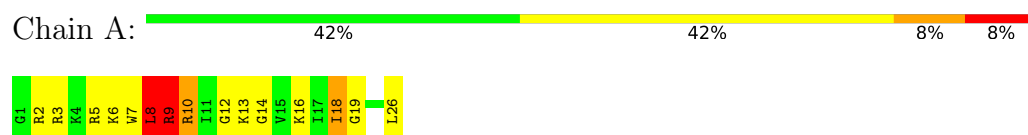
4.2.92 Score per residue for model 92

- Molecule 1: Pleurocidin-like prepropolypeptide



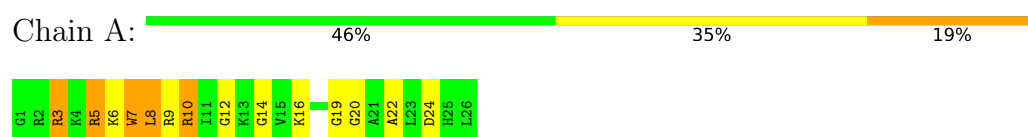
4.2.93 Score per residue for model 93

- Molecule 1: Pleurocidin-like prepropolypeptide



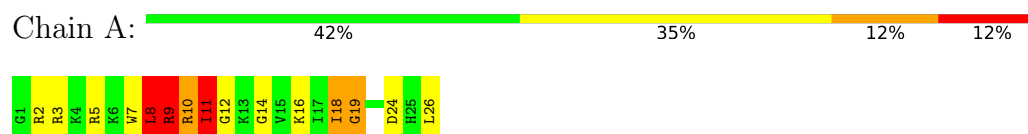
4.2.94 Score per residue for model 94

- Molecule 1: Pleurocidin-like prepropolypeptide



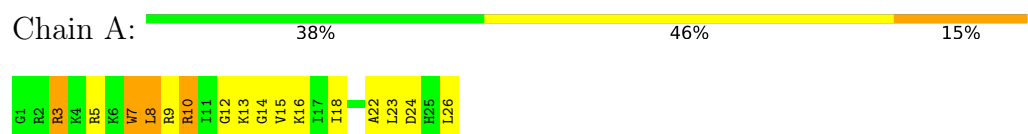
4.2.95 Score per residue for model 95

- Molecule 1: Pleurocidin-like prepropolypeptide



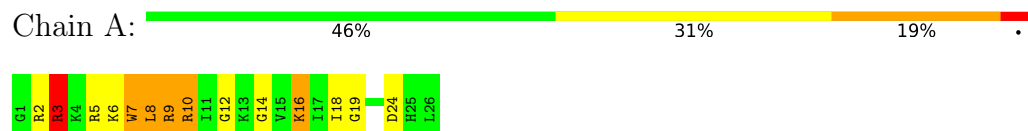
4.2.96 Score per residue for model 96

- Molecule 1: Pleurocidin-like prepropolypeptide



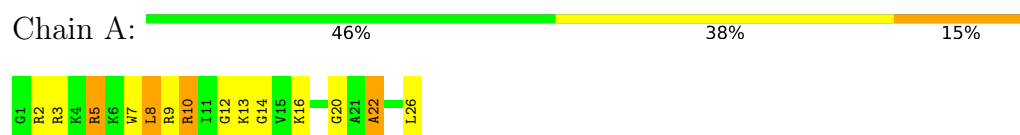
4.2.97 Score per residue for model 97

- Molecule 1: Pleurocidin-like prepropolypeptide



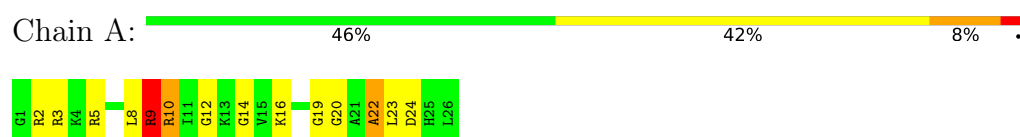
4.2.98 Score per residue for model 98

- Molecule 1: Pleurocidin-like prepropolypeptide



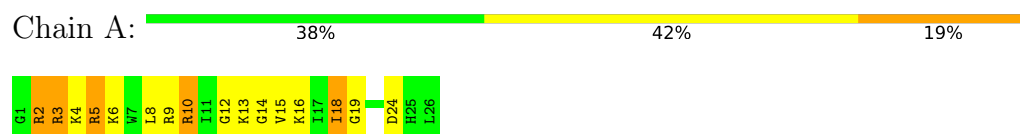
4.2.99 Score per residue for model 99

- Molecule 1: Pleurocidin-like prepropolypeptide



4.2.100 Score per residue for model 100

- Molecule 1: Pleurocidin-like prepropolypeptide



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	157
Number of shifts mapped to atoms	157
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	39%

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	0.81±0.01	0±0/210 (0.0± 0.0%)	1.07±0.04	0±0/275 (0.0± 0.1%)
All	All	0.81	0/21000 (0.0%)	1.07	8/27500 (0.0%)

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	4.4±0.8
All	All	0	437

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	11	ILE	N-CA-C	-6.59	107.45	113.71	12	8

There are no chirality outliers.

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	5	ARG	Sidechain	91
1	A	2	ARG	Sidechain	90
1	A	9	ARG	Sidechain	88
1	A	3	ARG	Sidechain	84
1	A	10	ARG	Sidechain	84

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	208	240	240	12±3
All	All	20800	24000	24000	1200

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:LEU:H	1:A:8:LEU:HD13	0.84	1.32	58	1
1:A:8:LEU:H	1:A:8:LEU:HD22	0.70	1.47	65	3
1:A:2:ARG:HH22	1:A:6:LYS:HZ3	0.67	1.30	56	1
1:A:8:LEU:HD23	1:A:8:LEU:H	0.65	1.51	61	24
1:A:17:ILE:HG23	1:A:18:ILE:H	0.63	1.53	17	4
1:A:8:LEU:N	1:A:8:LEU:HD13	0.63	2.07	92	3
1:A:8:LEU:N	1:A:8:LEU:HD23	0.63	2.09	16	12
1:A:18:ILE:HG23	1:A:18:ILE:O	0.63	1.93	57	9
1:A:2:ARG:NE	1:A:2:ARG:N	0.60	2.49	53	2
1:A:12:GLY:O	1:A:16:LYS:N	0.60	2.35	5	96
1:A:8:LEU:HD23	1:A:8:LEU:N	0.60	2.12	61	9
1:A:17:ILE:HG23	1:A:18:ILE:N	0.59	2.11	17	14
1:A:7:TRP:CE2	1:A:9:ARG:NH2	0.59	2.71	88	2
1:A:6:LYS:NZ	1:A:10:ARG:NH2	0.59	2.51	44	2
1:A:10:ARG:C	1:A:12:GLY:H	0.58	2.06	15	2
1:A:2:ARG:NE	1:A:2:ARG:H	0.58	1.96	53	1
1:A:9:ARG:NH2	1:A:16:LYS:NZ	0.57	2.52	3	1
1:A:9:ARG:HE	1:A:9:ARG:N	0.56	1.98	11	1
1:A:9:ARG:HE	1:A:9:ARG:H	0.56	1.42	11	2
1:A:2:ARG:HE	1:A:2:ARG:H	0.56	1.42	55	1
1:A:9:ARG:NE	1:A:9:ARG:N	0.56	2.53	72	1
1:A:7:TRP:CZ2	1:A:9:ARG:NH2	0.56	2.74	88	1
1:A:2:ARG:H	1:A:2:ARG:NE	0.55	2.00	55	1
1:A:8:LEU:H	1:A:8:LEU:CD2	0.55	2.15	50	19
1:A:12:GLY:C	1:A:14:GLY:N	0.55	2.64	48	97
1:A:23:LEU:HD12	1:A:23:LEU:N	0.54	2.18	44	11
1:A:26:LEU:HD12	1:A:26:LEU:N	0.54	2.18	92	36

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:ARG:N	1:A:9:ARG:HE	0.54	2.00	72	1
1:A:20:GLY:C	1:A:22:ALA:H	0.53	2.11	89	10
1:A:5:ARG:O	1:A:7:TRP:N	0.53	2.42	40	7
1:A:5:ARG:CD	1:A:5:ARG:N	0.53	2.72	24	7
1:A:7:TRP:NE1	1:A:9:ARG:HH22	0.53	2.02	79	1
1:A:26:LEU:HD23	1:A:26:LEU:N	0.52	2.20	50	1
1:A:20:GLY:O	1:A:24:ASP:N	0.52	2.42	61	1
1:A:6:LYS:N	1:A:6:LYS:CD	0.52	2.73	3	6
1:A:2:ARG:O	1:A:4:LYS:N	0.52	2.43	55	9
1:A:18:ILE:HG23	1:A:19:GLY:N	0.52	2.18	9	7
1:A:12:GLY:O	1:A:14:GLY:N	0.52	2.43	5	48
1:A:17:ILE:O	1:A:18:ILE:HG22	0.52	2.04	25	1
1:A:4:LYS:O	1:A:6:LYS:N	0.52	2.43	41	22
1:A:1:GLY:N	1:A:3:ARG:NH1	0.52	2.58	42	1
1:A:23:LEU:CD2	1:A:23:LEU:N	0.52	2.73	72	11
1:A:26:LEU:N	1:A:26:LEU:CD2	0.52	2.73	3	12
1:A:26:LEU:N	1:A:26:LEU:HD23	0.51	2.20	3	3
1:A:15:VAL:O	1:A:19:GLY:N	0.51	2.44	19	13
1:A:23:LEU:N	1:A:23:LEU:CD1	0.51	2.73	96	11
1:A:1:GLY:O	1:A:3:ARG:N	0.51	2.43	70	5
1:A:6:LYS:O	1:A:7:TRP:CG	0.51	2.63	62	21
1:A:2:ARG:N	1:A:2:ARG:CD	0.51	2.73	43	5
1:A:7:TRP:CG	1:A:7:TRP:O	0.51	2.64	22	9
1:A:19:GLY:O	1:A:21:ALA:N	0.51	2.43	18	5
1:A:9:ARG:O	1:A:11:ILE:N	0.51	2.44	15	2
1:A:26:LEU:N	1:A:26:LEU:CD1	0.50	2.74	92	35
1:A:7:TRP:CZ3	1:A:10:ARG:NH2	0.50	2.79	71	1
1:A:16:LYS:C	1:A:18:ILE:N	0.50	2.69	87	27
1:A:10:ARG:O	1:A:12:GLY:N	0.50	2.44	14	2
1:A:20:GLY:O	1:A:22:ALA:N	0.50	2.44	84	6
1:A:5:ARG:O	1:A:7:TRP:CD1	0.50	2.65	37	2
1:A:7:TRP:O	1:A:7:TRP:CD1	0.50	2.65	31	18
1:A:6:LYS:O	1:A:7:TRP:CD1	0.50	2.65	92	10
1:A:24:ASP:C	1:A:25:HIS:CG	0.50	2.90	32	3
1:A:7:TRP:O	1:A:8:LEU:C	0.50	2.55	66	4
1:A:24:ASP:O	1:A:25:HIS:CG	0.50	2.65	42	3
1:A:8:LEU:HD12	1:A:9:ARG:N	0.50	2.22	20	1
1:A:6:LYS:O	1:A:7:TRP:CD2	0.50	2.65	40	3
1:A:16:LYS:C	1:A:18:ILE:H	0.49	2.15	37	34
1:A:16:LYS:O	1:A:18:ILE:N	0.49	2.45	87	6
1:A:8:LEU:HD12	1:A:8:LEU:H	0.49	1.67	33	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LYS:O	1:A:10:ARG:NE	0.49	2.45	72	1
1:A:18:ILE:O	1:A:20:GLY:N	0.49	2.46	2	2
1:A:14:GLY:O	1:A:19:GLY:N	0.49	2.45	10	4
1:A:2:ARG:NE	1:A:6:LYS:NZ	0.49	2.61	12	1
1:A:8:LEU:HD13	1:A:8:LEU:N	0.49	2.13	58	1
1:A:24:ASP:O	1:A:26:LEU:N	0.49	2.45	58	2
1:A:3:ARG:NE	1:A:3:ARG:H	0.49	2.06	42	1
1:A:22:ALA:O	1:A:25:HIS:NE2	0.49	2.45	7	1
1:A:20:GLY:C	1:A:22:ALA:N	0.49	2.71	16	16
1:A:26:LEU:N	1:A:26:LEU:HD12	0.49	2.23	16	1
1:A:21:ALA:O	1:A:22:ALA:CB	0.49	2.61	89	1
1:A:7:TRP:O	1:A:7:TRP:CE3	0.49	2.66	6	3
1:A:21:ALA:O	1:A:22:ALA:HB3	0.49	2.07	89	1
1:A:10:ARG:C	1:A:12:GLY:N	0.48	2.70	14	2
1:A:7:TRP:O	1:A:7:TRP:CD2	0.48	2.66	23	5
1:A:11:ILE:C	1:A:11:ILE:HD12	0.48	2.32	92	2
1:A:7:TRP:C	1:A:9:ARG:N	0.48	2.72	16	4
1:A:26:LEU:N	1:A:26:LEU:HD22	0.48	2.23	29	8
1:A:2:ARG:NH1	1:A:5:ARG:HH22	0.48	2.05	18	1
1:A:24:ASP:OD1	1:A:25:HIS:ND1	0.48	2.45	63	1
1:A:10:ARG:CG	1:A:11:ILE:N	0.48	2.77	20	11
1:A:4:LYS:N	1:A:4:LYS:CD	0.48	2.77	45	3
1:A:7:TRP:NE1	1:A:9:ARG:HH21	0.48	2.06	3	1
1:A:7:TRP:O	1:A:7:TRP:CG	0.48	2.66	4	10
1:A:10:ARG:CG	1:A:11:ILE:H	0.48	2.21	54	6
1:A:7:TRP:O	1:A:9:ARG:N	0.48	2.47	28	2
1:A:4:LYS:C	1:A:6:LYS:H	0.48	2.16	78	1
1:A:3:ARG:HH12	1:A:4:LYS:NZ	0.48	2.07	9	1
1:A:3:ARG:HE	1:A:9:ARG:HH22	0.48	1.50	51	1
1:A:22:ALA:C	1:A:24:ASP:N	0.47	2.71	34	3
1:A:17:ILE:CG2	1:A:18:ILE:H	0.47	2.22	17	1
1:A:17:ILE:O	1:A:18:ILE:CB	0.47	2.62	25	1
1:A:24:ASP:C	1:A:25:HIS:ND1	0.47	2.73	32	2
1:A:8:LEU:N	1:A:8:LEU:CD2	0.47	2.78	74	17
1:A:25:HIS:ND1	1:A:26:LEU:N	0.47	2.63	21	1
1:A:11:ILE:HD12	1:A:12:GLY:N	0.47	2.25	92	4
1:A:25:HIS:ND1	1:A:25:HIS:O	0.47	2.48	16	2
1:A:23:LEU:N	1:A:23:LEU:HD22	0.47	2.25	72	11
1:A:24:ASP:OD1	1:A:24:ASP:N	0.47	2.47	64	1
1:A:3:ARG:N	1:A:3:ARG:CD	0.47	2.77	94	2
1:A:2:ARG:NH1	1:A:2:ARG:O	0.47	2.48	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:LEU:C	1:A:25:HIS:N	0.46	2.73	64	2
1:A:6:LYS:C	1:A:10:ARG:HE	0.46	2.19	49	1
1:A:18:ILE:CG2	1:A:19:GLY:N	0.46	2.78	43	6
1:A:1:GLY:C	1:A:3:ARG:N	0.46	2.72	81	1
1:A:18:ILE:O	1:A:18:ILE:CG2	0.46	2.64	65	5
1:A:25:HIS:ND1	1:A:25:HIS:N	0.46	2.64	16	4
1:A:4:LYS:NZ	1:A:4:LYS:CB	0.46	2.78	70	2
1:A:9:ARG:NE	1:A:9:ARG:H	0.46	2.08	72	1
1:A:2:ARG:C	1:A:4:LYS:N	0.46	2.72	17	3
1:A:17:ILE:CG2	1:A:18:ILE:N	0.46	2.79	20	5
1:A:17:ILE:HG23	1:A:17:ILE:O	0.46	2.10	3	1
1:A:19:GLY:C	1:A:21:ALA:N	0.46	2.72	20	7
1:A:15:VAL:O	1:A:19:GLY:CA	0.45	2.64	23	1
1:A:9:ARG:NE	1:A:9:ARG:CA	0.45	2.79	72	2
1:A:9:ARG:N	1:A:9:ARG:CD	0.45	2.79	90	3
1:A:3:ARG:C	1:A:5:ARG:N	0.45	2.73	45	1
1:A:24:ASP:OD2	1:A:25:HIS:N	0.45	2.50	84	1
1:A:9:ARG:N	1:A:9:ARG:NE	0.45	2.65	11	1
1:A:2:ARG:NH2	1:A:6:LYS:HZ1	0.45	2.08	15	1
1:A:6:LYS:O	1:A:10:ARG:CZ	0.45	2.65	35	3
1:A:2:ARG:NH1	1:A:5:ARG:NH2	0.45	2.65	18	1
1:A:24:ASP:C	1:A:26:LEU:N	0.45	2.72	68	3
1:A:6:LYS:C	1:A:7:TRP:CG	0.45	2.95	41	3
1:A:11:ILE:HD12	1:A:11:ILE:C	0.45	2.37	42	2
1:A:10:ARG:O	1:A:11:ILE:CG1	0.44	2.65	14	1
1:A:13:LYS:O	1:A:17:ILE:CG2	0.44	2.65	5	2
1:A:12:GLY:C	1:A:14:GLY:H	0.44	2.21	68	55
1:A:8:LEU:H	1:A:8:LEU:CD1	0.44	2.25	39	15
1:A:9:ARG:CD	1:A:9:ARG:C	0.44	2.91	40	23
1:A:26:LEU:HD12	1:A:26:LEU:C	0.44	2.38	72	2
1:A:8:LEU:CD1	1:A:8:LEU:H	0.43	2.26	29	6
1:A:8:LEU:H	1:A:8:LEU:HD12	0.43	1.72	29	5
1:A:8:LEU:HD22	1:A:8:LEU:N	0.43	2.23	65	2
1:A:2:ARG:N	1:A:8:LEU:CD2	0.43	2.81	70	1
1:A:2:ARG:C	1:A:4:LYS:H	0.43	2.21	81	2
1:A:8:LEU:H	1:A:8:LEU:HD23	0.43	1.73	42	2
1:A:3:ARG:C	1:A:5:ARG:H	0.43	2.21	45	1
1:A:6:LYS:C	1:A:8:LEU:N	0.43	2.76	85	2
1:A:18:ILE:C	1:A:20:GLY:N	0.43	2.76	55	1
1:A:5:ARG:O	1:A:6:LYS:C	0.43	2.61	7	1
1:A:24:ASP:OD1	1:A:25:HIS:N	0.43	2.51	53	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LYS:C	1:A:7:TRP:CD1	0.43	2.97	62	5
1:A:8:LEU:CD2	1:A:8:LEU:H	0.43	2.27	79	5
1:A:26:LEU:C	1:A:26:LEU:HD23	0.43	2.39	37	3
1:A:7:TRP:C	1:A:9:ARG:H	0.43	2.22	8	14
1:A:6:LYS:HZ3	1:A:10:ARG:NH2	0.43	2.10	73	1
1:A:4:LYS:C	1:A:6:LYS:N	0.43	2.77	78	2
1:A:2:ARG:NH2	1:A:6:LYS:HZ3	0.43	2.06	56	1
1:A:9:ARG:O	1:A:10:ARG:C	0.42	2.62	65	13
1:A:13:LYS:NZ	1:A:13:LYS:CB	0.42	2.82	17	2
1:A:11:ILE:CD1	1:A:11:ILE:H	0.42	2.27	43	1
1:A:16:LYS:O	1:A:17:ILE:C	0.42	2.62	81	4
1:A:8:LEU:CD2	1:A:8:LEU:N	0.42	2.81	43	2
1:A:17:ILE:O	1:A:18:ILE:C	0.42	2.62	3	3
1:A:12:GLY:O	1:A:15:VAL:N	0.42	2.52	5	3
1:A:17:ILE:O	1:A:18:ILE:CG2	0.42	2.66	25	1
1:A:25:HIS:C	1:A:25:HIS:ND1	0.42	2.78	59	1
1:A:12:GLY:O	1:A:13:LYS:C	0.42	2.62	48	3
1:A:2:ARG:NE	1:A:2:ARG:CA	0.42	2.81	53	1
1:A:23:LEU:C	1:A:25:HIS:H	0.42	2.22	1	2
1:A:19:GLY:C	1:A:21:ALA:H	0.42	2.22	20	1
1:A:6:LYS:CD	1:A:6:LYS:H	0.42	2.28	33	1
1:A:18:ILE:O	1:A:18:ILE:HG23	0.42	2.13	23	1
1:A:24:ASP:O	1:A:25:HIS:ND1	0.42	2.53	42	1
1:A:2:ARG:HE	1:A:2:ARG:N	0.42	2.07	55	1
1:A:8:LEU:CD1	1:A:9:ARG:H	0.41	2.28	78	1
1:A:10:ARG:CZ	1:A:10:ARG:CB	0.41	2.98	91	1
1:A:15:VAL:O	1:A:16:LYS:C	0.41	2.63	63	2
1:A:26:LEU:C	1:A:26:LEU:CD1	0.41	2.93	72	6
1:A:4:LYS:O	1:A:5:ARG:O	0.41	2.37	40	2
1:A:25:HIS:C	1:A:25:HIS:HD1	0.41	2.23	59	1
1:A:24:ASP:O	1:A:24:ASP:CG	0.41	2.63	34	2
1:A:23:LEU:HD23	1:A:23:LEU:O	0.41	2.14	43	1
1:A:6:LYS:NZ	1:A:10:ARG:HH22	0.41	2.12	73	1
1:A:16:LYS:C	1:A:16:LYS:CD	0.41	2.93	97	1
1:A:9:ARG:C	1:A:9:ARG:CD	0.41	2.92	56	2
1:A:8:LEU:O	1:A:9:ARG:CB	0.41	2.68	74	1
1:A:24:ASP:C	1:A:26:LEU:H	0.41	2.23	68	1
1:A:9:ARG:O	1:A:10:ARG:O	0.41	2.39	65	2
1:A:25:HIS:O	1:A:25:HIS:CD2	0.41	2.74	32	1
1:A:26:LEU:C	1:A:26:LEU:CD2	0.41	2.94	87	2
1:A:6:LYS:C	1:A:8:LEU:H	0.41	2.22	85	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ILE:C	1:A:11:ILE:CD1	0.41	2.94	42	3
1:A:22:ALA:C	1:A:24:ASP:H	0.41	2.24	79	1
1:A:15:VAL:HG23	1:A:16:LYS:N	0.41	2.30	100	1
1:A:23:LEU:O	1:A:24:ASP:CG	0.41	2.64	19	4
1:A:25:HIS:O	1:A:25:HIS:CG	0.41	2.74	8	1
1:A:18:ILE:C	1:A:20:GLY:H	0.41	2.23	17	1
1:A:1:GLY:O	1:A:2:ARG:O	0.41	2.39	78	2
1:A:1:GLY:C	1:A:3:ARG:H	0.41	2.23	84	2
1:A:9:ARG:HH22	1:A:17:ILE:CA	0.41	2.29	74	1
1:A:7:TRP:O	1:A:8:LEU:O	0.41	2.39	87	3
1:A:24:ASP:O	1:A:25:HIS:O	0.40	2.39	21	2
1:A:8:LEU:N	1:A:8:LEU:HD22	0.40	2.28	92	1
1:A:13:LYS:CB	1:A:13:LYS:NZ	0.40	2.83	31	1
1:A:15:VAL:O	1:A:19:GLY:C	0.40	2.64	60	1
1:A:26:LEU:CD1	1:A:26:LEU:C	0.40	2.94	85	1
1:A:8:LEU:C	1:A:8:LEU:CD2	0.40	2.95	58	1
1:A:20:GLY:O	1:A:24:ASP:OD1	0.40	2.39	60	1
1:A:17:ILE:O	1:A:18:ILE:O	0.40	2.39	8	1
1:A:3:ARG:NE	1:A:3:ARG:N	0.40	2.70	42	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	24/26 (92%)	10±2 (41±8%)	8±2 (31±9%)	7±2 (28±9%)	0	1
All	All	2400/2600 (92%)	985 (41%)	753 (31%)	662 (28%)	0	1

All 20 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	10	ARG	88
1	A	18	ILE	76
1	A	24	ASP	76

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Mol	Chain	Res	Type	Models (Total)
1	A	7	TRP	54
1	A	5	ARG	53
1	A	8	LEU	47
1	A	9	ARG	40
1	A	19	GLY	38
1	A	2	ARG	29
1	A	22	ALA	27
1	A	20	GLY	26
1	A	13	LYS	23
1	A	25	HIS	20
1	A	3	ARG	20
1	A	6	LYS	13
1	A	17	ILE	12
1	A	21	ALA	11
1	A	4	LYS	6
1	A	11	ILE	2
1	A	23	LEU	1

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	19/19 (100%)	17±1 (92±5%)	2±1 (8±5%)	13	60
All	All	1900/1900 (100%)	1747 (92%)	153 (8%)	13	60

All 15 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	8	LEU	78
1	A	9	ARG	18
1	A	26	LEU	14
1	A	11	ILE	8
1	A	6	LYS	7
1	A	23	LEU	6
1	A	13	LYS	5
1	A	4	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	10	ARG	4
1	A	2	ARG	2
1	A	25	HIS	2
1	A	16	LYS	2
1	A	18	ILE	1
1	A	17	ILE	1
1	A	3	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 39% for the well-defined parts and 39% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *WF1a-1-chemicalshift.php*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	157
Number of shifts mapped to atoms	157
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

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

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 39%, i.e. 157 atoms were assigned a chemical shift out of a possible 402. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	52/135 (39%)	52/57 (91%)	0/52 (0%)	0/26 (0%)
Sidechain	105/248 (42%)	105/160 (66%)	0/69 (0%)	0/19 (0%)
Aromatic	0/19 (0%)	0/10 (0%)	0/7 (0%)	0/2 (0%)
Overall	157/402 (39%)	157/227 (69%)	0/128 (0%)	0/47 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 39%, i.e. 157 atoms were assigned a chemical shift out of a possible 402. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	52/135 (39%)	52/57 (91%)	0/52 (0%)	0/26 (0%)
Sidechain	105/248 (42%)	105/160 (66%)	0/69 (0%)	0/19 (0%)
Aromatic	0/19 (0%)	0/10 (0%)	0/7 (0%)	0/2 (0%)
Overall	157/402 (39%)	157/227 (69%)	0/128 (0%)	0/47 (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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

