



Full wwPDB NMR Structure Validation Report ⓘ

Mar 3, 2022 – 08:39 PM EST

PDB ID : 2HYN
Title : Complete ensemble of NMR structures of unphosphorylated human phospholamban pentamer
Authors : Potluri, S.; Yan, A.K.; Chou, J.J.; Donald, B.R.; Bailey-Kellogg, C.
Deposited on : 2006-08-07

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 : 2.27
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

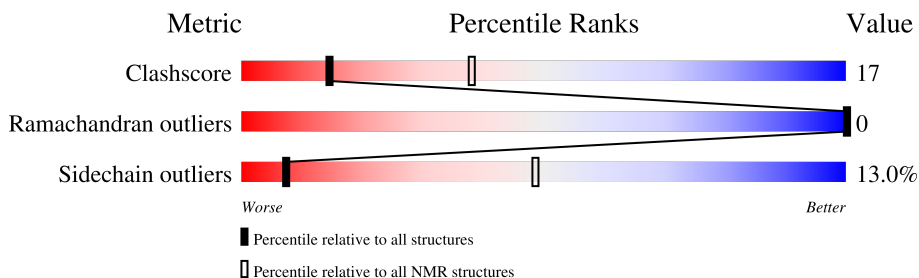
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 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	52	63% (Green) 37% (Yellow)
1	B	52	63% (Green) 37% (Yellow)
1	C	52	63% (Green) 37% (Yellow)
1	D	52	63% (Green) 37% (Yellow)
1	E	52	63% (Green) 37% (Yellow)

2 Ensemble composition and analysis i

This entry contains 184 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 139 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:1-A:52 (52)	0.02	139
2	B:1-B:52 (52)	0.02	139
3	C:1-C:52 (52)	0.02	139
4	D:1-D:52 (52)	0.02	139
5	E:1-E:52 (52)	0.02	139

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 19 clusters. No single-model clusters were found.

Cluster number	Models
1	26, 31, 36, 44, 46, 48, 58, 60, 81, 90, 99, 104, 107, 110, 119, 128, 130, 132, 137, 148, 176, 180
2	7, 40, 41, 42, 57, 78, 87, 93, 95, 117, 123, 136, 144, 146, 149, 158, 160, 161, 179
3	68, 72, 85, 86, 97, 102, 105, 108, 114, 116, 118, 121, 139, 140, 154, 166, 172
4	4, 16, 21, 30, 47, 62, 66, 73, 74, 76, 89, 109, 115, 124, 152
5	12, 29, 113, 129, 133, 134, 159, 162, 171, 173, 177, 178, 181, 183
6	2, 8, 14, 20, 52, 53, 83, 112, 122, 142, 145, 151, 164, 168
7	32, 55, 64, 103, 106, 131, 153, 165, 167, 174, 175, 182, 184
8	27, 28, 43, 61, 75, 77, 82, 88, 91, 125, 127, 141, 150
9	13, 17, 34, 35, 65, 96, 120, 157, 163, 169
10	11, 18, 22, 24, 33, 39, 69, 79, 126
11	1, 15, 49, 63, 70, 143, 156
12	23, 37, 59, 100, 101, 111
13	6, 9, 80, 92, 98, 135
14	84, 94, 138, 170
15	5, 54, 56, 71
16	10, 38, 51, 155
17	3, 25, 67
18	45, 147

19	19, 50
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3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 4494 atoms, of which 2375 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cardiac phospholamban.

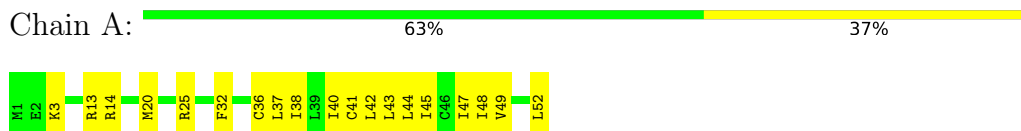
Mol	Chain	Residues	Atoms					Trace	
1	A	52	Total	C	H	N	O	S	0
			899	276	475	73	69	6	
1	B	52	Total	C	H	N	O	S	0
			899	276	475	73	69	6	
1	C	52	Total	C	H	N	O	S	0
			899	276	475	73	69	6	
1	D	52	Total	C	H	N	O	S	0
			899	276	475	73	69	6	
1	E	52	Total	C	H	N	O	S	0
			898	276	475	73	68	6	

4 Residue-property plots [i](#)

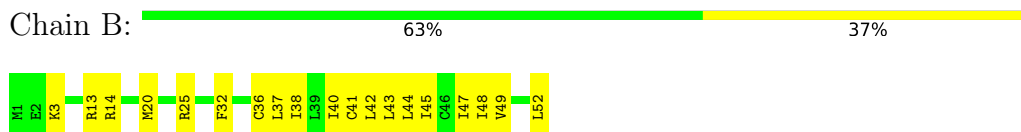
4.1 Average score per residue in the NMR ensemble

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.

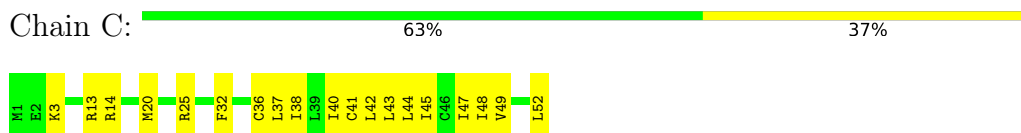
- Molecule 1: Cardiac phospholamban



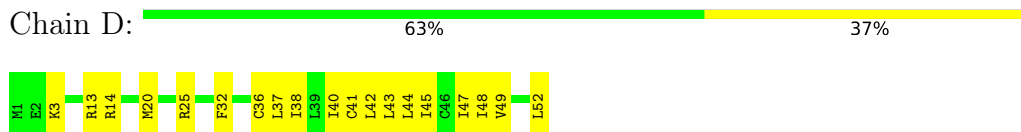
- Molecule 1: Cardiac phospholamban



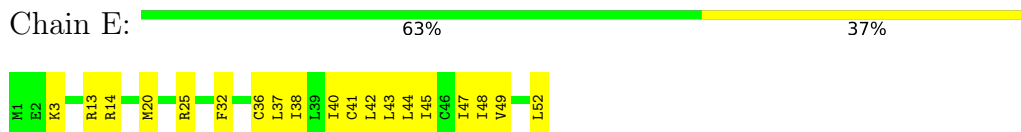
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



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: Cardiac phospholamban

Chain A:  65% 29% 6%



- Molecule 1: Cardiac phospholamban

Chain B:  65% 29% 6%



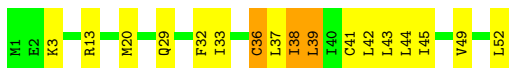
- Molecule 1: Cardiac phospholamban

Chain C:  65% 29% 6%



- Molecule 1: Cardiac phospholamban

Chain D:  67% 27% 6%



- Molecule 1: Cardiac phospholamban

Chain E:  65% 29% 6%



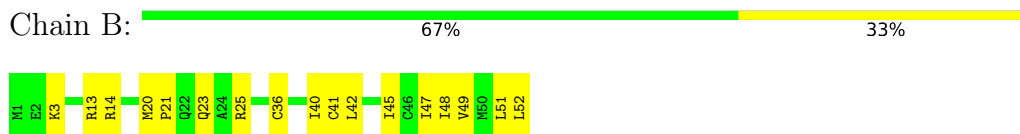
4.2.2 Score per residue for model 2

- Molecule 1: Cardiac phospholamban

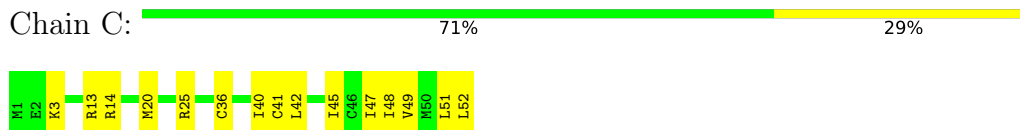
Chain A:  71% 29%



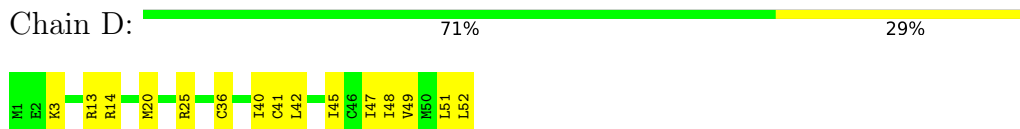
- Molecule 1: Cardiac phospholamban



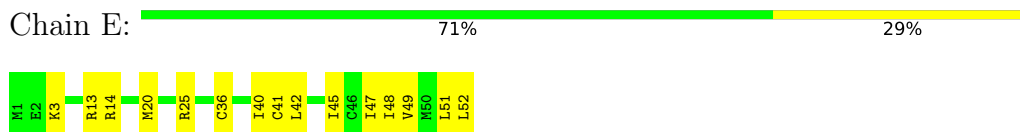
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

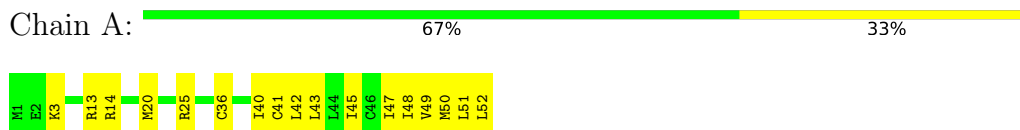


- Molecule 1: Cardiac phospholamban

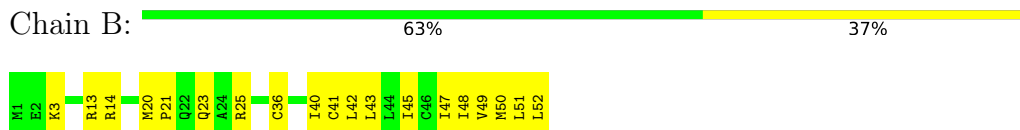


4.2.3 Score per residue for model 3

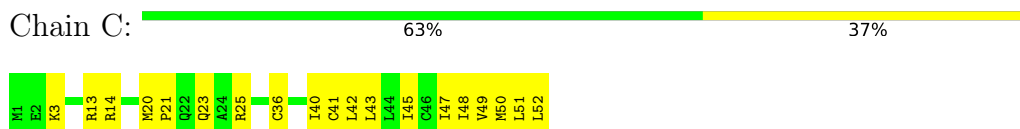
- Molecule 1: Cardiac phospholamban



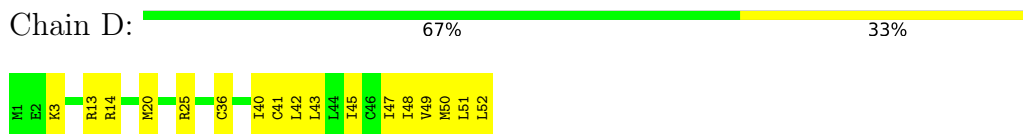
- Molecule 1: Cardiac phospholamban



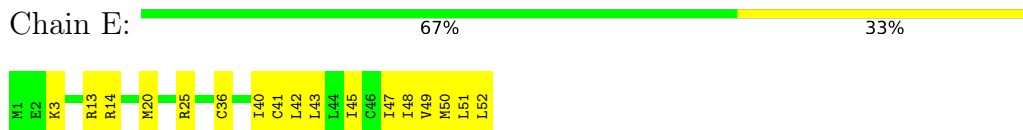
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

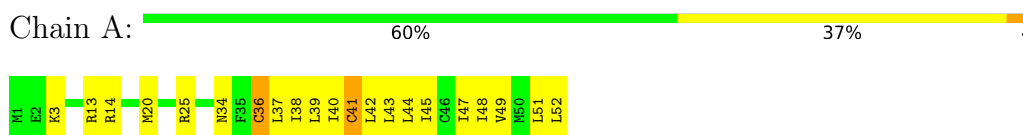


- Molecule 1: Cardiac phospholamban



4.2.4 Score per residue for model 4

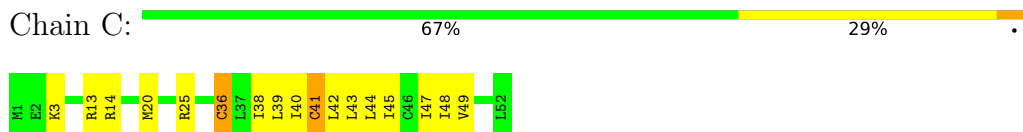
- Molecule 1: Cardiac phospholamban



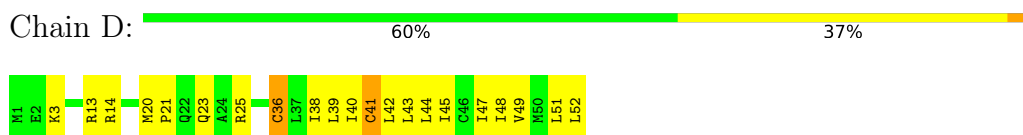
- Molecule 1: Cardiac phospholamban



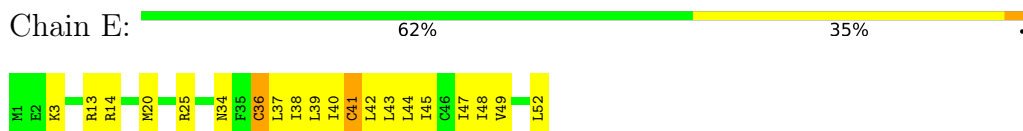
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

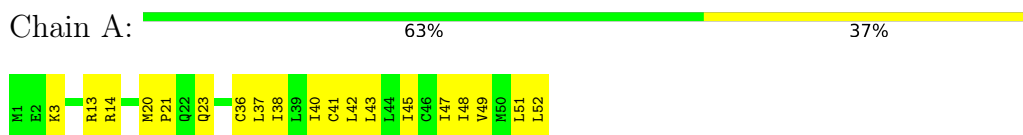


- Molecule 1: Cardiac phospholamban

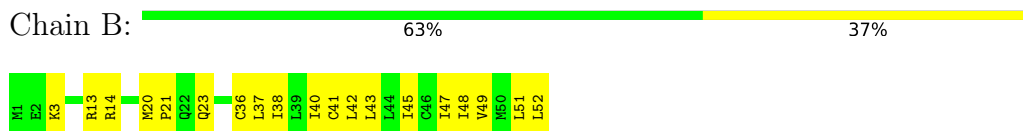


4.2.5 Score per residue for model 5

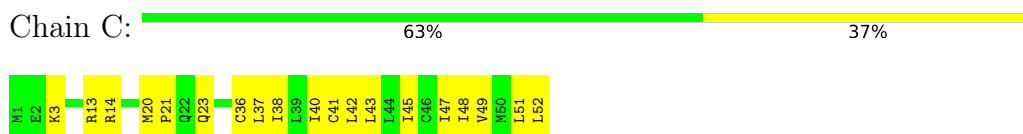
- Molecule 1: Cardiac phospholamban



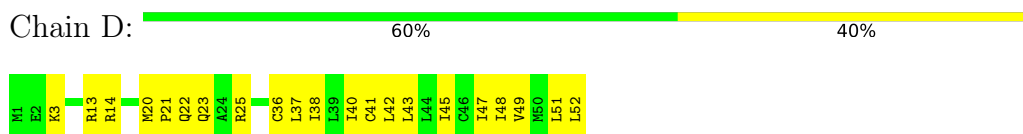
- Molecule 1: Cardiac phospholamban



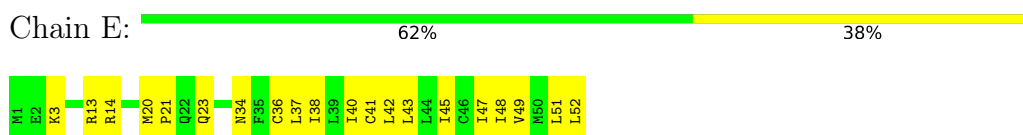
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

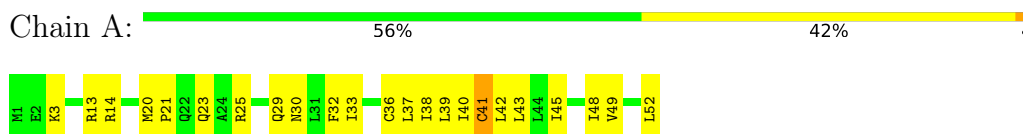


- Molecule 1: Cardiac phospholamban



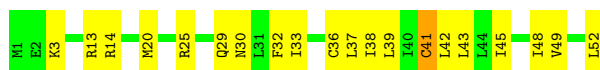
4.2.6 Score per residue for model 6

- Molecule 1: Cardiac phospholamban

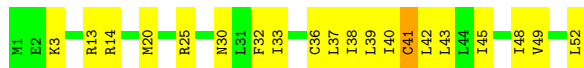


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

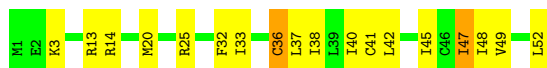


4.2.7 Score per residue for model 7

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

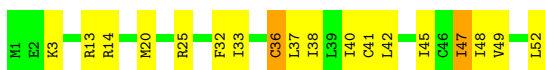


- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



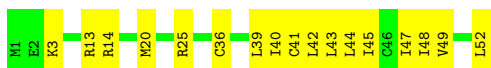


- Molecule 1: Cardiac phospholamban



4.2.8 Score per residue for model 8

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

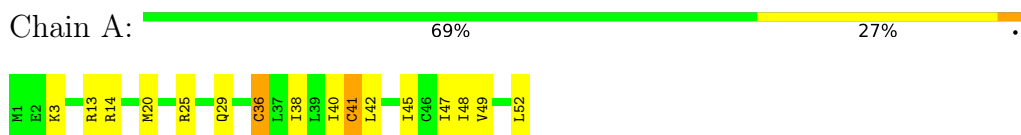


- Molecule 1: Cardiac phospholamban

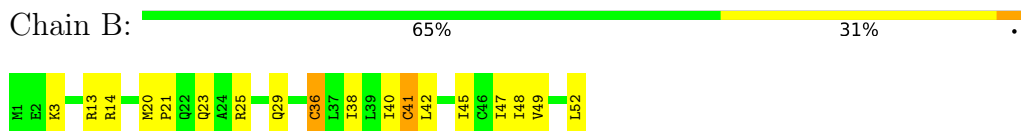


4.2.9 Score per residue for model 9

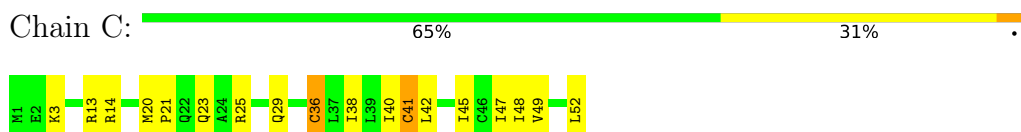
- Molecule 1: Cardiac phospholamban



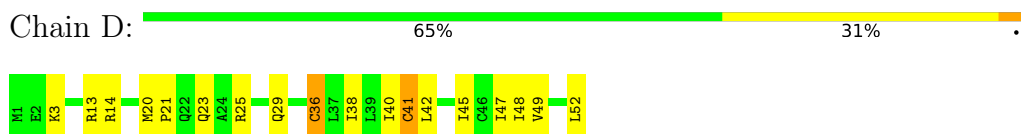
- Molecule 1: Cardiac phospholamban



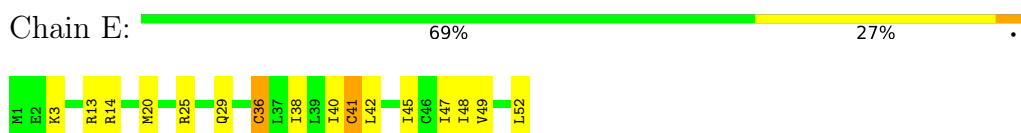
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

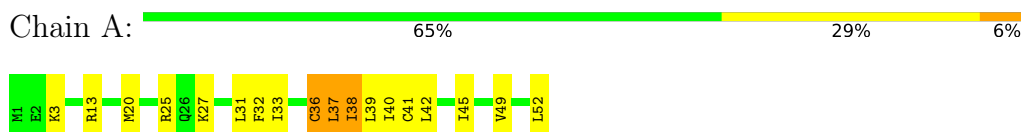


- Molecule 1: Cardiac phospholamban



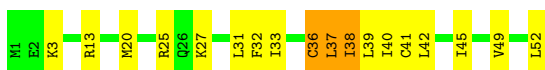
4.2.10 Score per residue for model 10

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

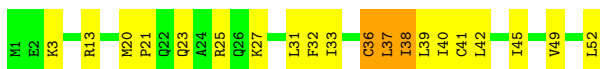




- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.11 Score per residue for model 11

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

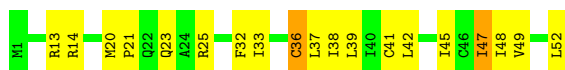


- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



4.2.12 Score per residue for model 12

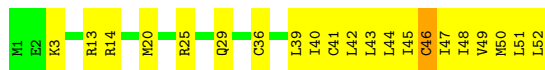
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- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

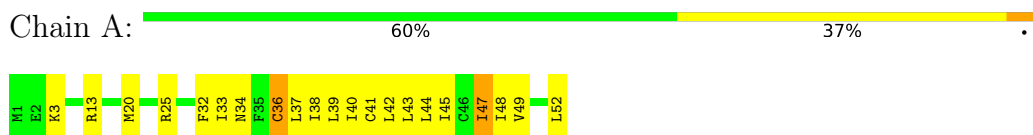


- Molecule 1: Cardiac phospholamban

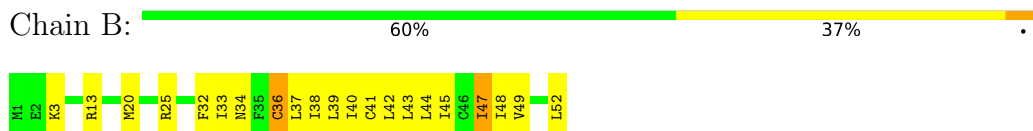


4.2.13 Score per residue for model 13

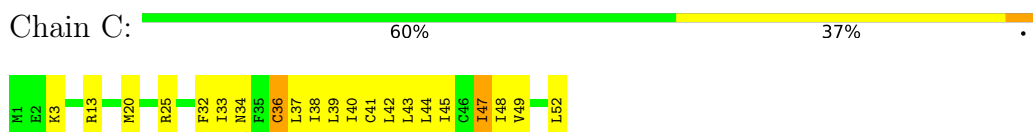
- Molecule 1: Cardiac phospholamban



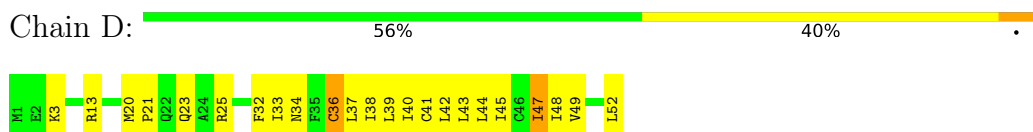
- Molecule 1: Cardiac phospholamban



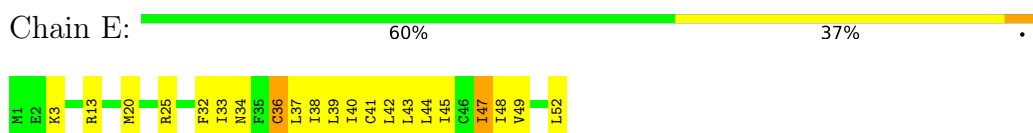
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

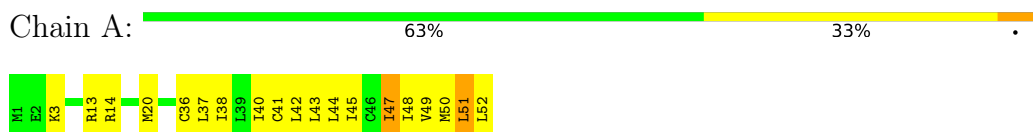


- Molecule 1: Cardiac phospholamban



4.2.14 Score per residue for model 14

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.15 Score per residue for model 15

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

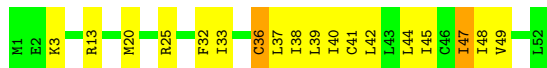


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



4.2.16 Score per residue for model 16

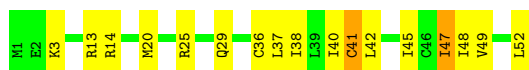
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

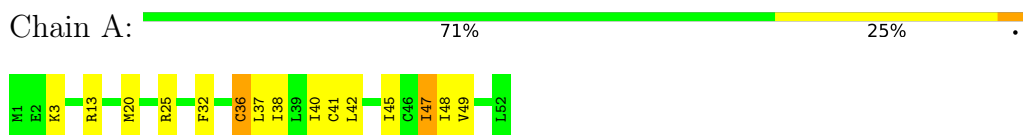


- Molecule 1: Cardiac phospholamban

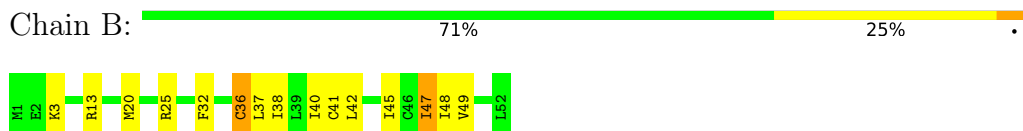


4.2.17 Score per residue for model 17

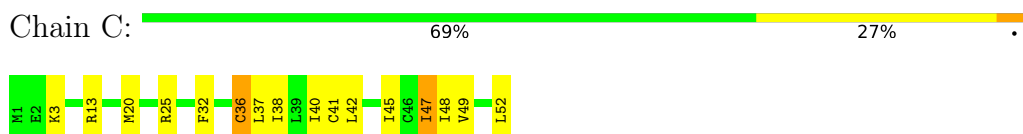
- Molecule 1: Cardiac phospholamban



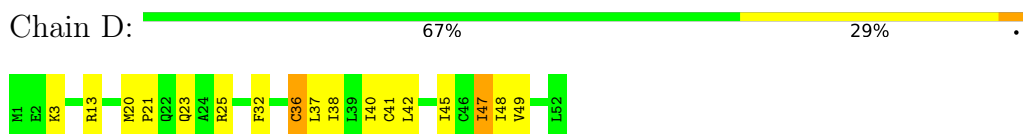
- Molecule 1: Cardiac phospholamban



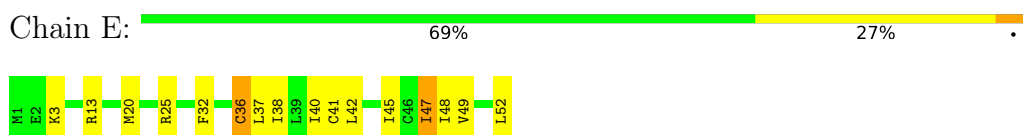
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

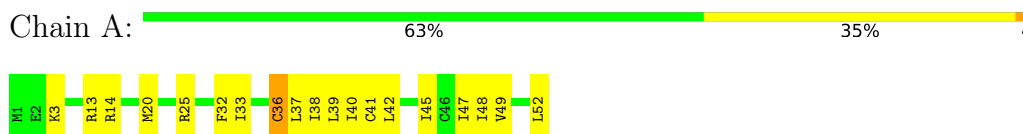


- Molecule 1: Cardiac phospholamban



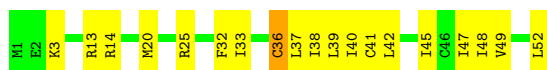
4.2.18 Score per residue for model 18

- Molecule 1: Cardiac phospholamban

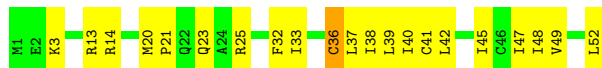


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.19 Score per residue for model 19

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

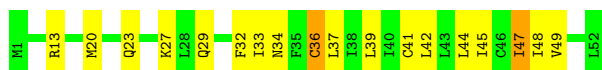


- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



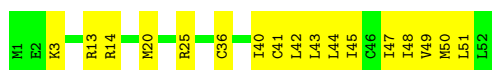


- Molecule 1: Cardiac phospholamban



4.2.20 Score per residue for model 20

- Molecule 1: Cardiac phospholamban



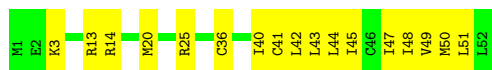
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

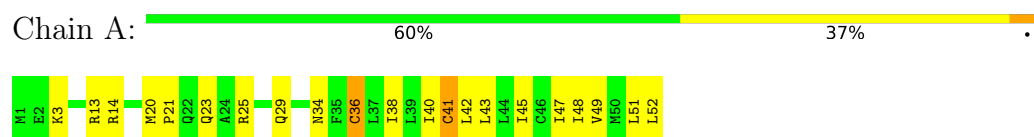


- Molecule 1: Cardiac phospholamban

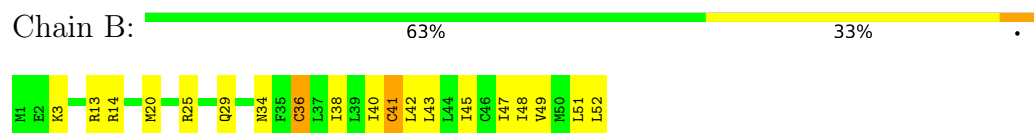


4.2.21 Score per residue for model 21

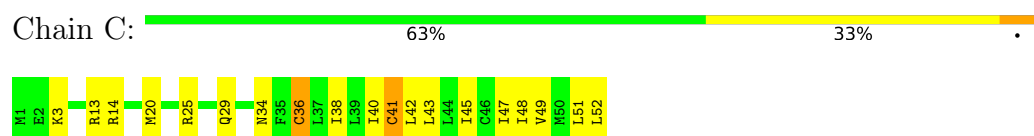
- Molecule 1: Cardiac phospholamban



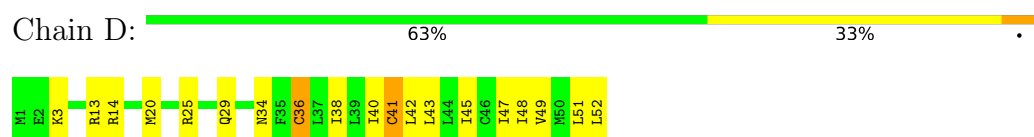
- Molecule 1: Cardiac phospholamban



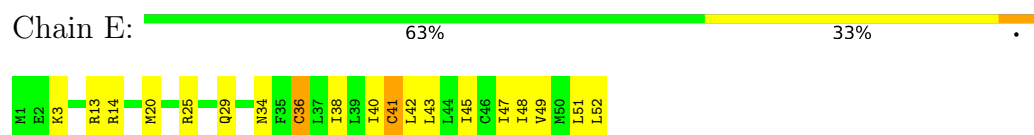
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

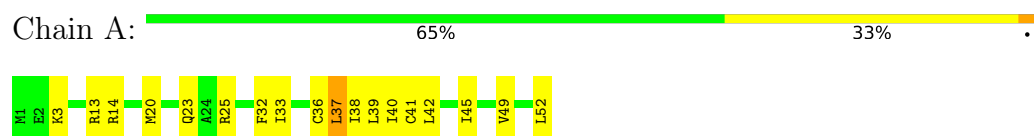


- Molecule 1: Cardiac phospholamban



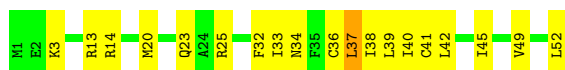
4.2.22 Score per residue for model 22

- Molecule 1: Cardiac phospholamban

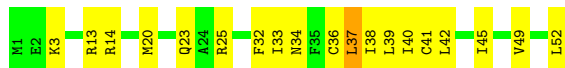


- Molecule 1: Cardiac phospholamban

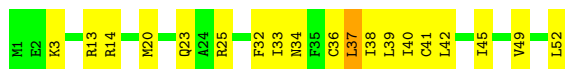




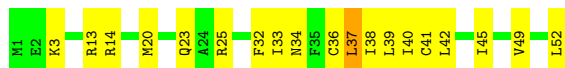
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

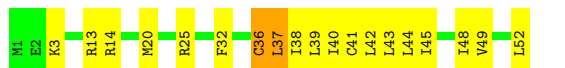


- Molecule 1: Cardiac phospholamban



4.2.23 Score per residue for model 23

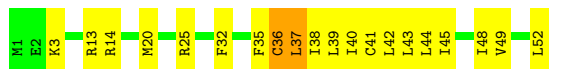
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

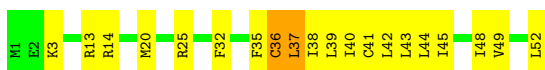


- Molecule 1: Cardiac phospholamban

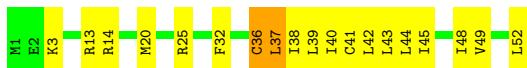


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



4.2.24 Score per residue for model 24

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



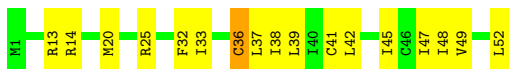
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

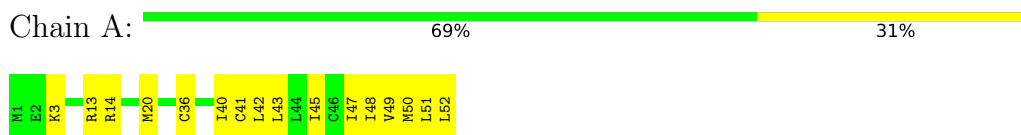


- Molecule 1: Cardiac phospholamban

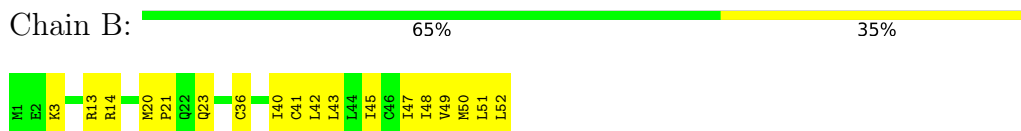


4.2.25 Score per residue for model 25

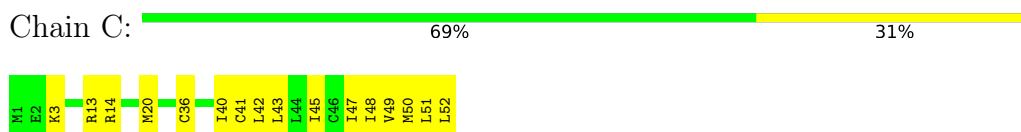
- Molecule 1: Cardiac phospholamban



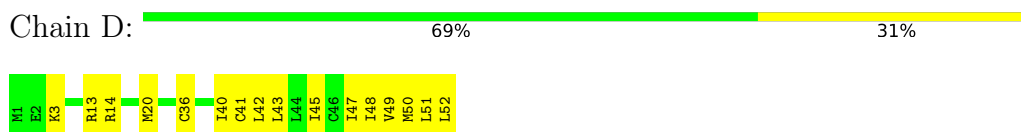
- Molecule 1: Cardiac phospholamban



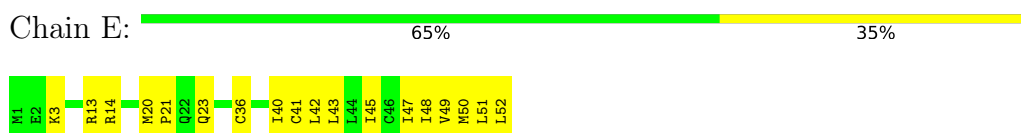
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

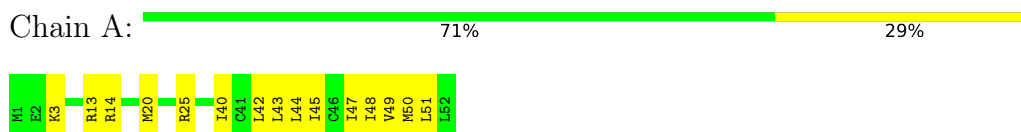


- Molecule 1: Cardiac phospholamban



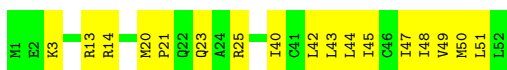
4.2.26 Score per residue for model 26

- Molecule 1: Cardiac phospholamban

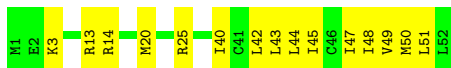


- Molecule 1: Cardiac phospholamban





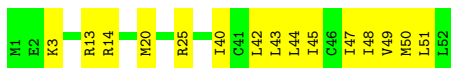
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

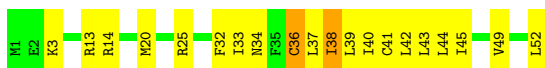


4.2.27 Score per residue for model 27

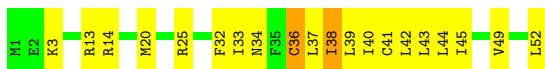
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

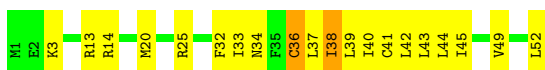


- Molecule 1: Cardiac phospholamban

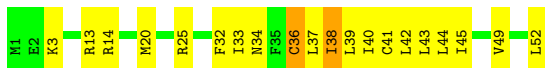


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

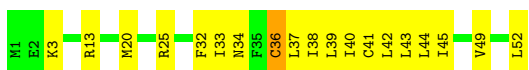


4.2.28 Score per residue for model 28

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



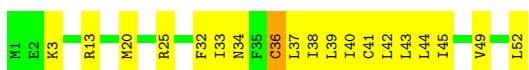
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

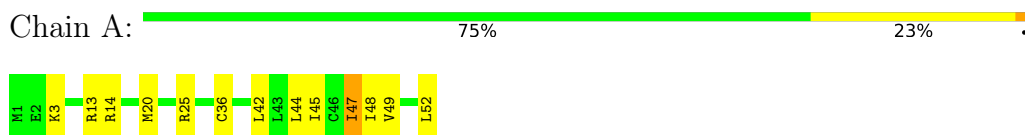


- Molecule 1: Cardiac phospholamban

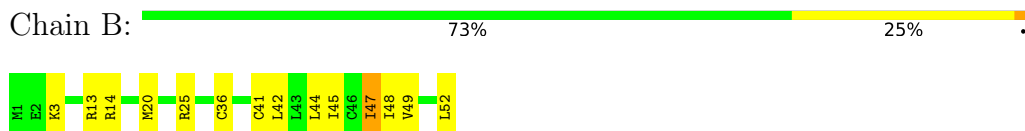


4.2.29 Score per residue for model 29

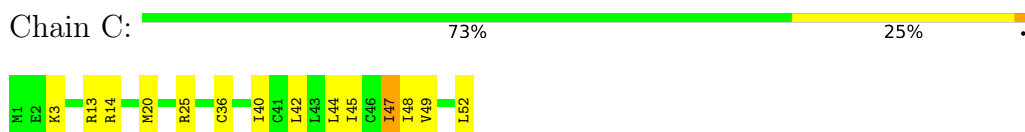
- Molecule 1: Cardiac phospholamban



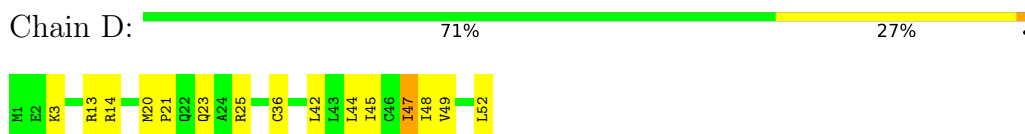
- Molecule 1: Cardiac phospholamban



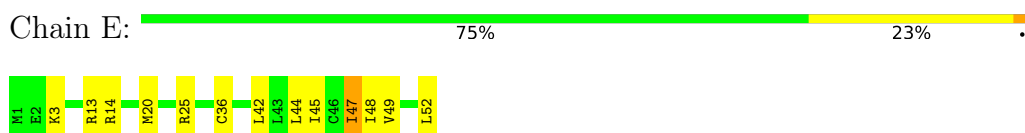
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

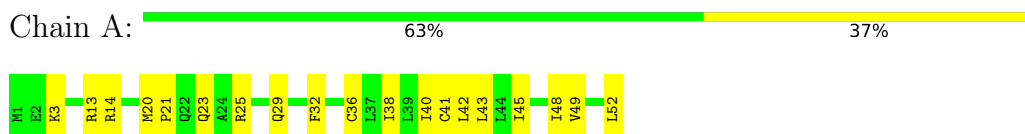


- Molecule 1: Cardiac phospholamban



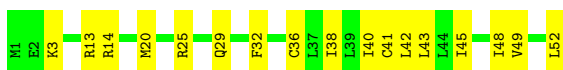
4.2.30 Score per residue for model 30

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

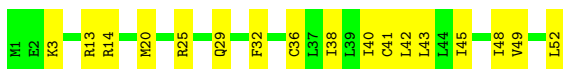




- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.31 Score per residue for model 31

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



4.2.32 Score per residue for model 32

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



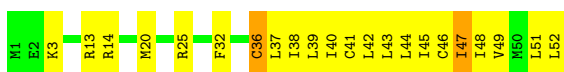
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

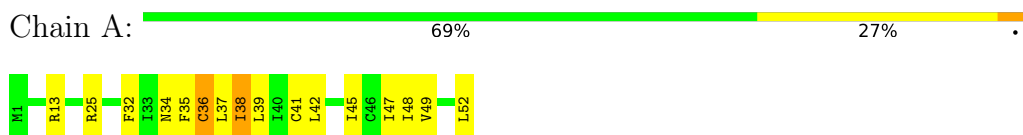


- Molecule 1: Cardiac phospholamban

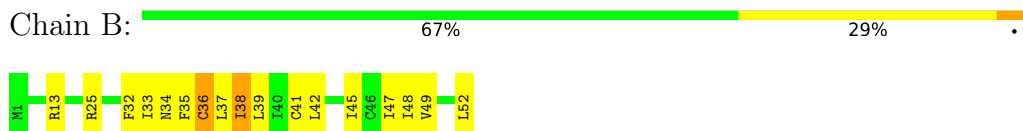


4.2.33 Score per residue for model 33

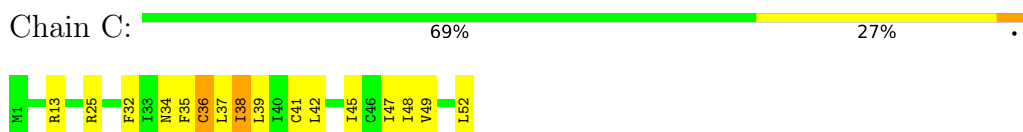
- Molecule 1: Cardiac phospholamban



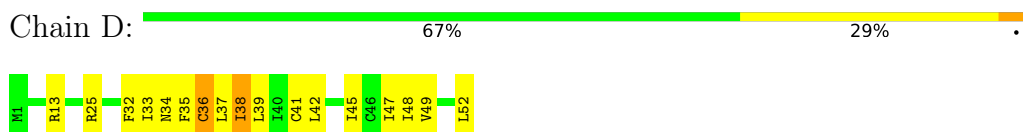
- Molecule 1: Cardiac phospholamban



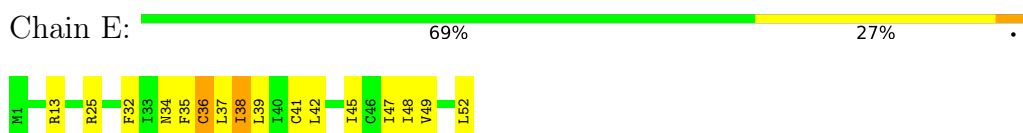
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

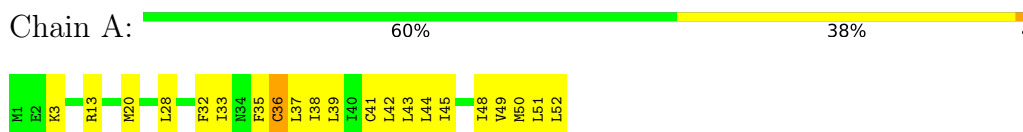


- Molecule 1: Cardiac phospholamban



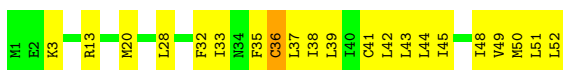
4.2.34 Score per residue for model 34

- Molecule 1: Cardiac phospholamban

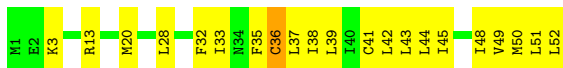


- Molecule 1: Cardiac phospholamban

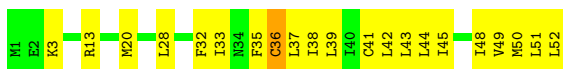




- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

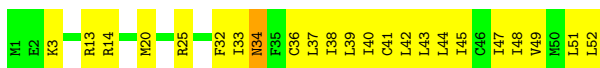


4.2.35 Score per residue for model 35

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

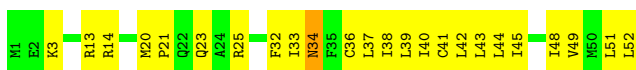


- Molecule 1: Cardiac phospholamban

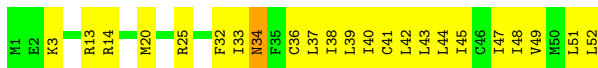


- Molecule 1: Cardiac phospholamban



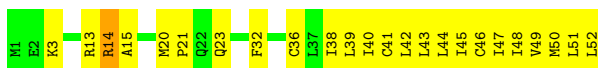


- Molecule 1: Cardiac phospholamban

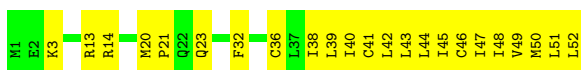


4.2.36 Score per residue for model 36

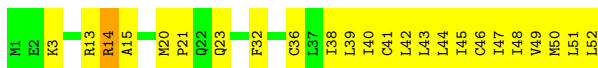
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

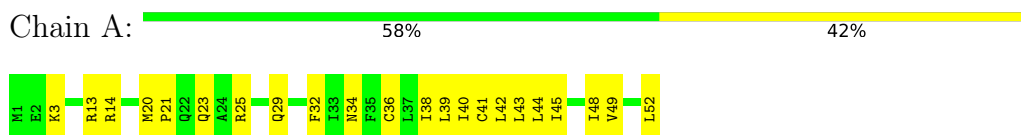


- Molecule 1: Cardiac phospholamban

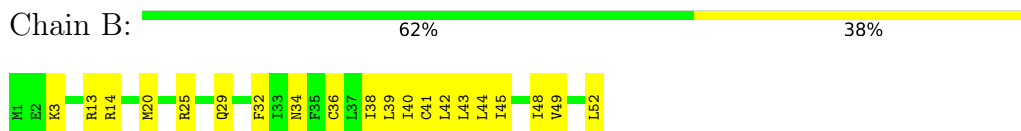


4.2.37 Score per residue for model 37

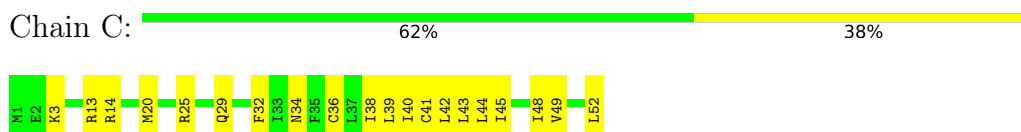
- Molecule 1: Cardiac phospholamban



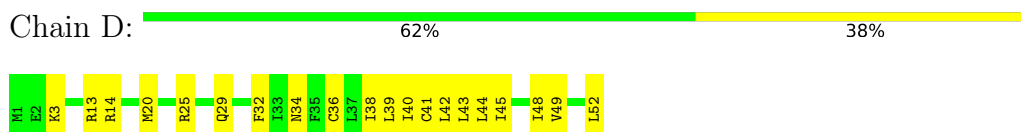
- Molecule 1: Cardiac phospholamban



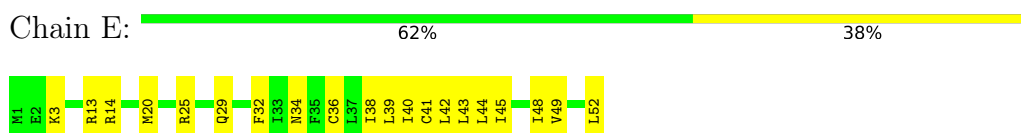
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

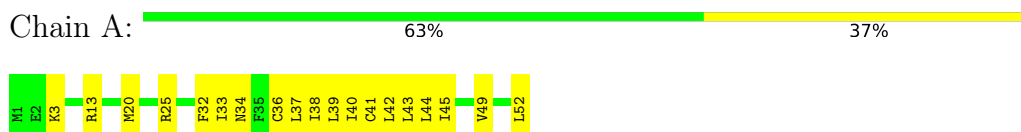


- Molecule 1: Cardiac phospholamban



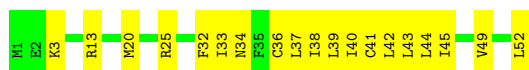
4.2.38 Score per residue for model 38

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

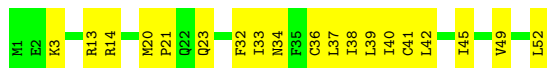


- Molecule 1: Cardiac phospholamban



4.2.39 Score per residue for model 39

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



4.2.40 Score per residue for model 40

- Molecule 1: Cardiac phospholamban



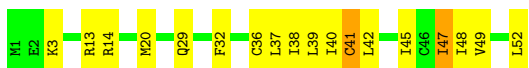
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

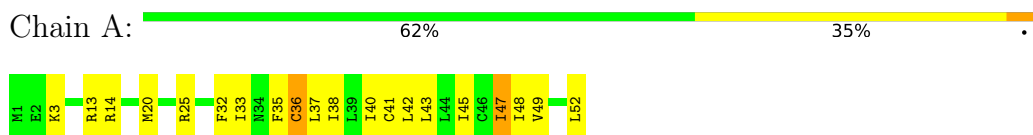


- Molecule 1: Cardiac phospholamban

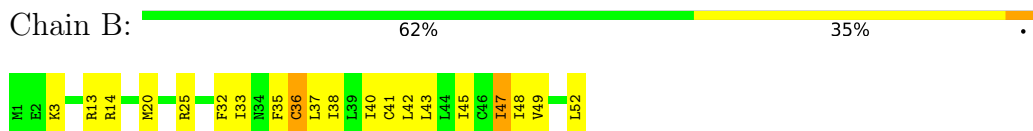


4.2.41 Score per residue for model 41

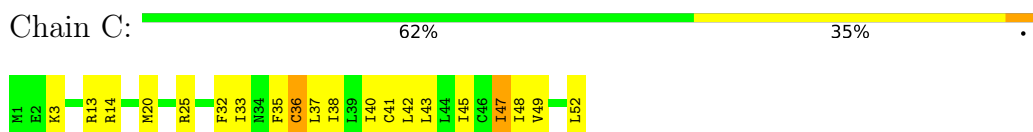
- Molecule 1: Cardiac phospholamban



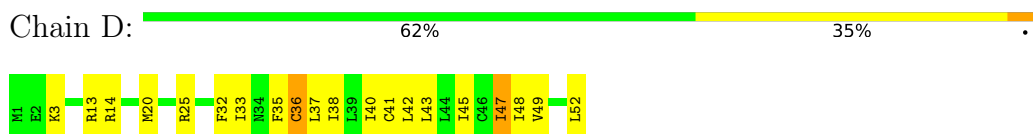
- Molecule 1: Cardiac phospholamban



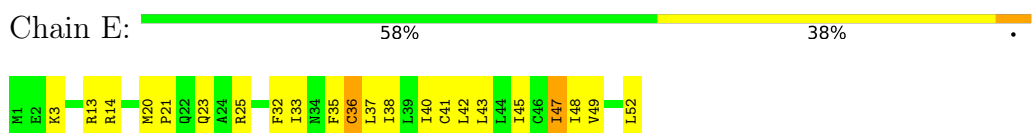
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

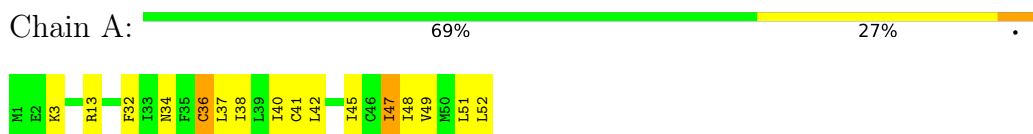


- Molecule 1: Cardiac phospholamban



4.2.42 Score per residue for model 42

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

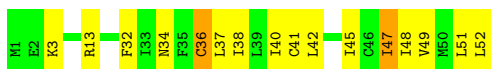




- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

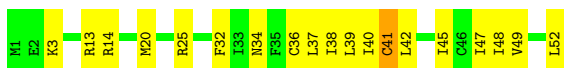


4.2.43 Score per residue for model 43

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

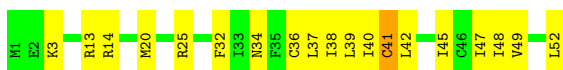


- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

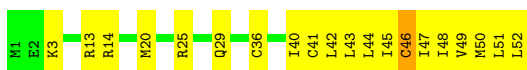


4.2.44 Score per residue for model 44

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

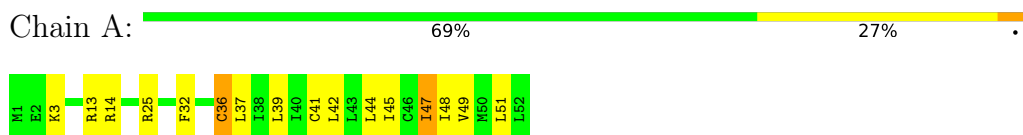


- Molecule 1: Cardiac phospholamban

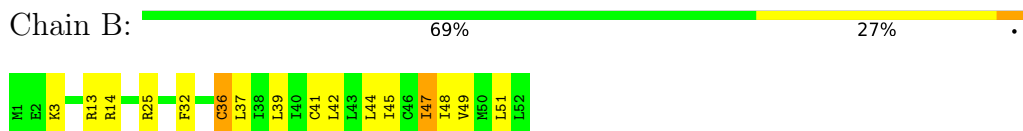


4.2.45 Score per residue for model 45

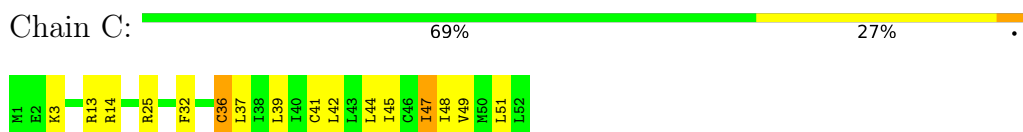
- Molecule 1: Cardiac phospholamban



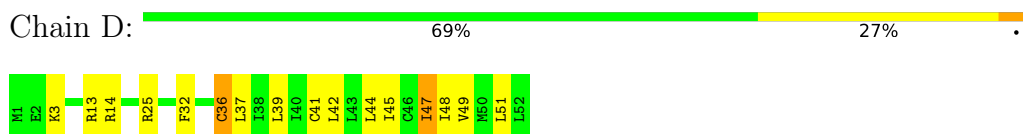
- Molecule 1: Cardiac phospholamban



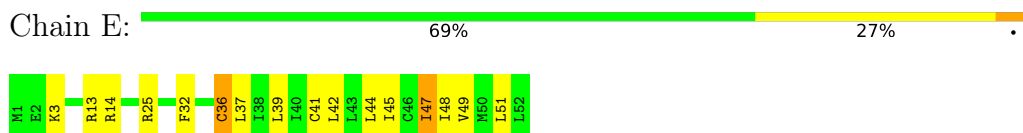
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

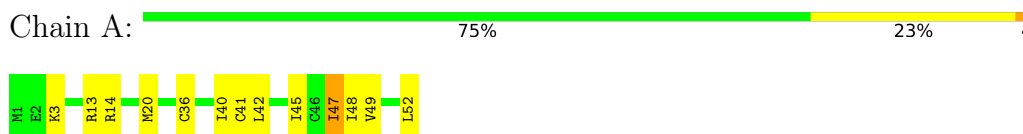


- Molecule 1: Cardiac phospholamban



4.2.46 Score per residue for model 46

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

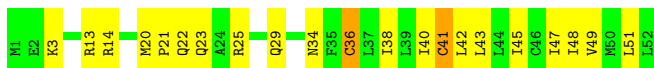


- Molecule 1: Cardiac phospholamban

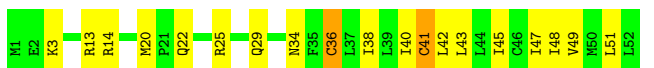


4.2.47 Score per residue for model 47

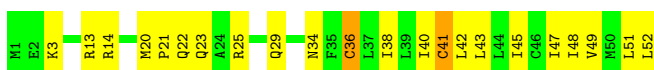
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

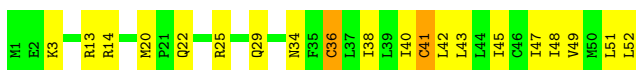


- Molecule 1: Cardiac phospholamban

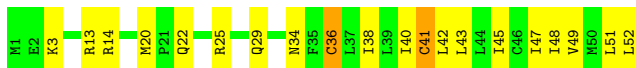


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

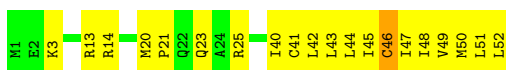


4.2.48 Score per residue for model 48

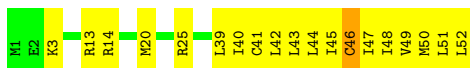
- Molecule 1: Cardiac phospholamban



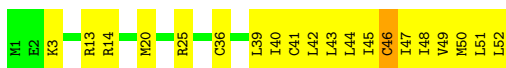
- Molecule 1: Cardiac phospholamban



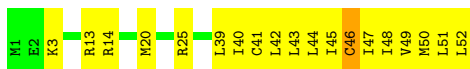
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

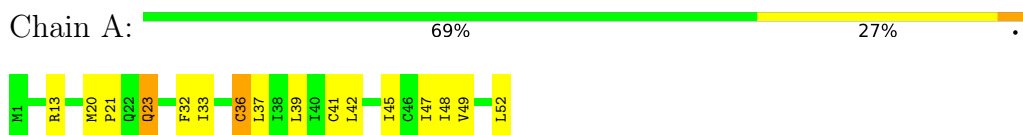


- Molecule 1: Cardiac phospholamban

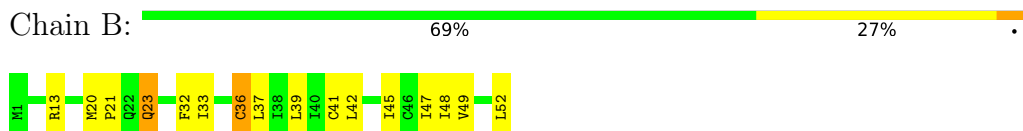


4.2.49 Score per residue for model 49

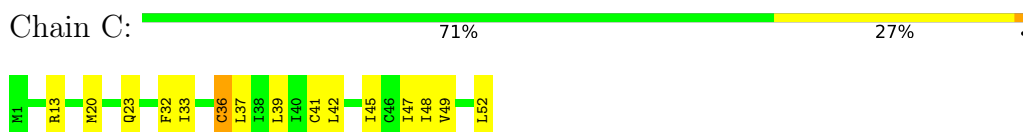
- Molecule 1: Cardiac phospholamban



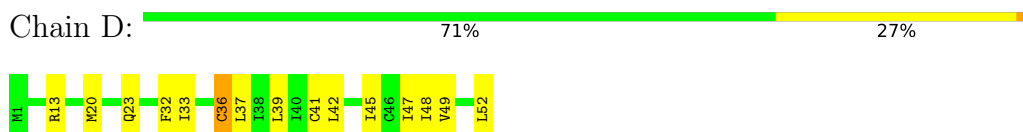
- Molecule 1: Cardiac phospholamban



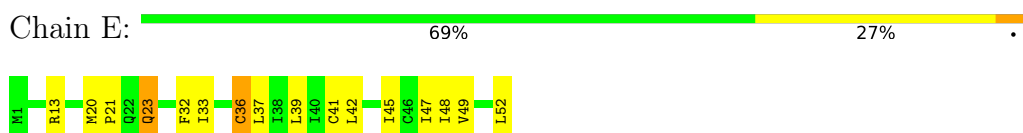
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

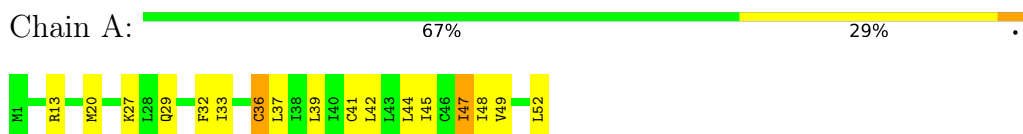


- Molecule 1: Cardiac phospholamban



4.2.50 Score per residue for model 50

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

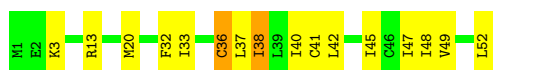


4.2.51 Score per residue for model 51

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

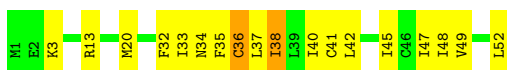


- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

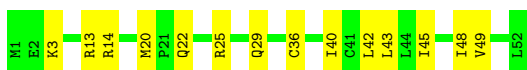


4.2.52 Score per residue for model 52

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

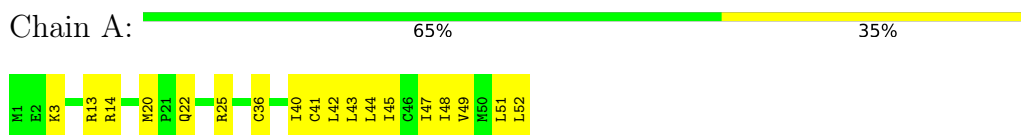


- Molecule 1: Cardiac phospholamban

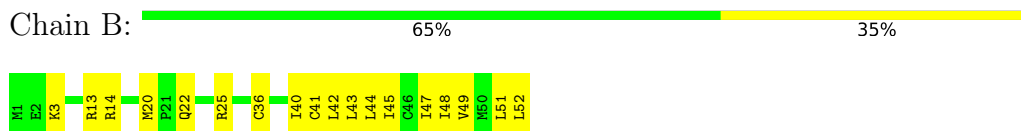


4.2.53 Score per residue for model 53

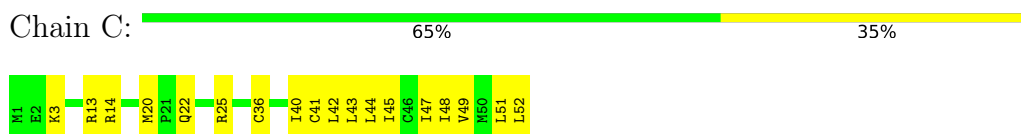
- Molecule 1: Cardiac phospholamban



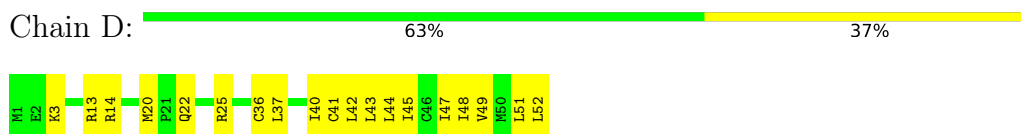
- Molecule 1: Cardiac phospholamban



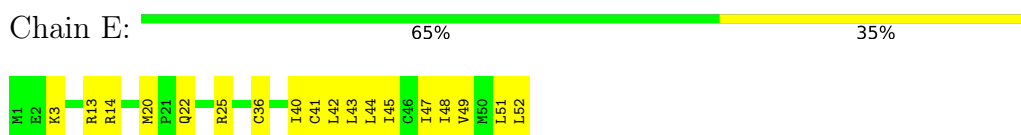
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

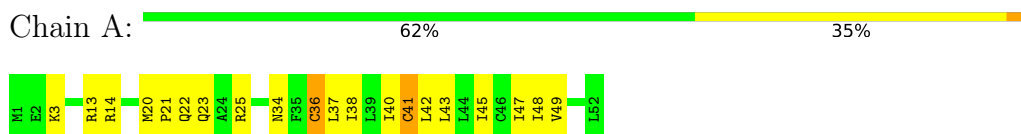


- Molecule 1: Cardiac phospholamban



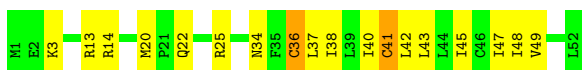
4.2.54 Score per residue for model 54

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

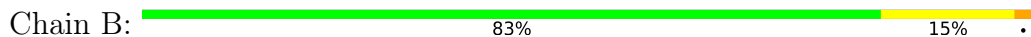


4.2.55 Score per residue for model 55

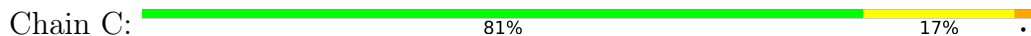
- Molecule 1: Cardiac phospholamban



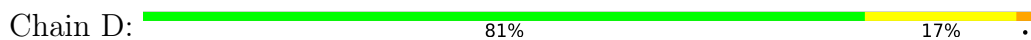
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



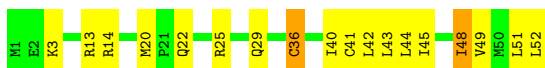


- Molecule 1: Cardiac phospholamban

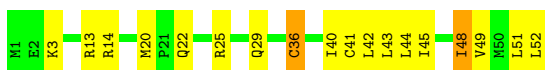


4.2.56 Score per residue for model 56

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



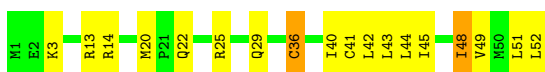
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

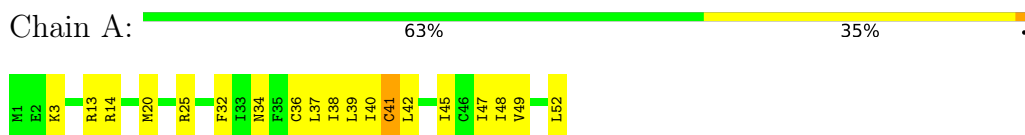


- Molecule 1: Cardiac phospholamban

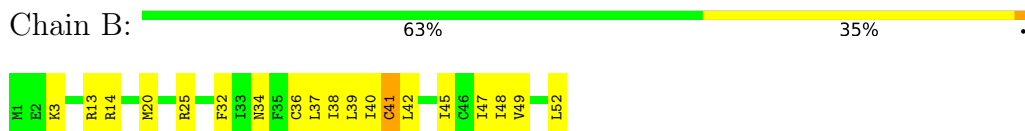


4.2.57 Score per residue for model 57

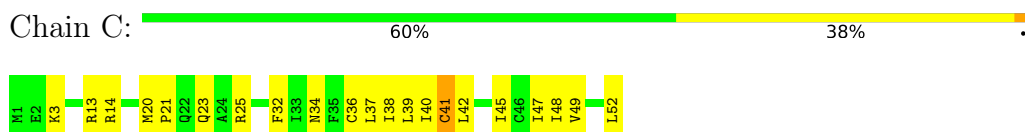
- Molecule 1: Cardiac phospholamban



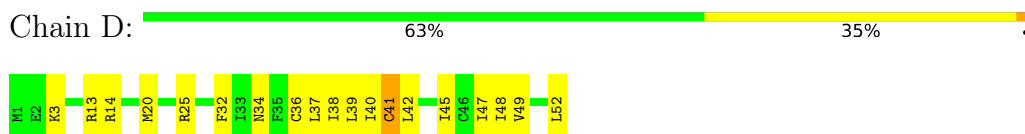
- Molecule 1: Cardiac phospholamban



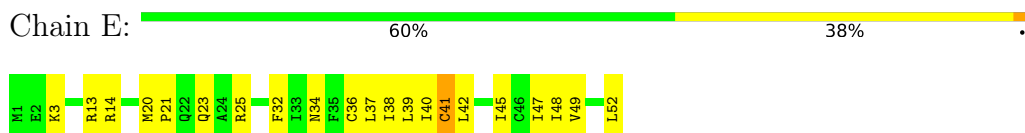
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

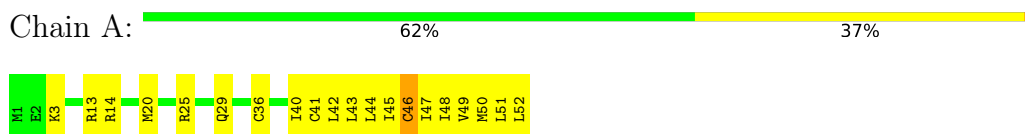


- Molecule 1: Cardiac phospholamban



4.2.58 Score per residue for model 58

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

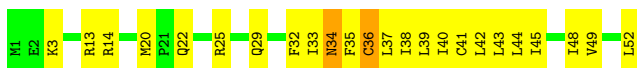


4.2.59 Score per residue for model 59

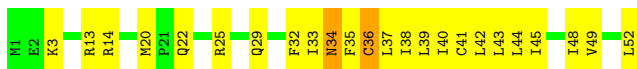
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

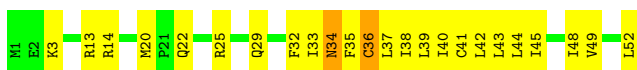


- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



4.2.60 Score per residue for model 60

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

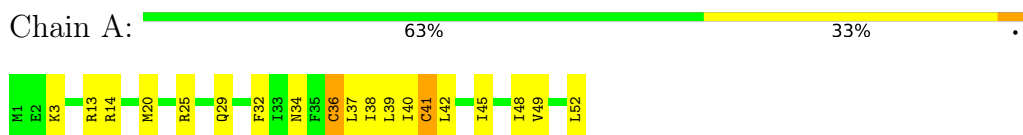


- Molecule 1: Cardiac phospholamban

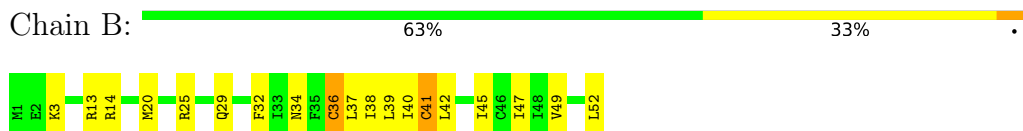


4.2.61 Score per residue for model 61

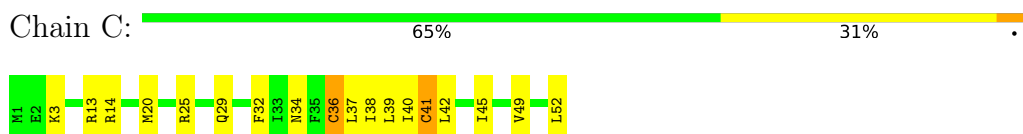
- Molecule 1: Cardiac phospholamban



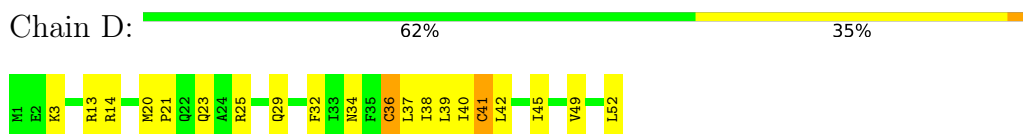
- Molecule 1: Cardiac phospholamban



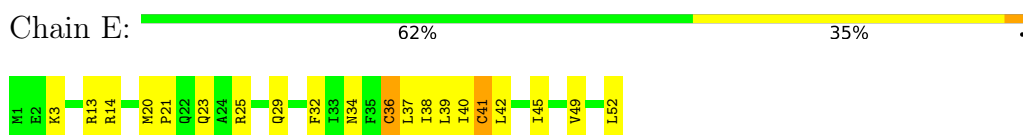
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

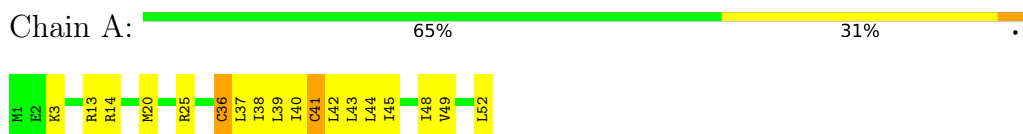


- Molecule 1: Cardiac phospholamban



4.2.62 Score per residue for model 62

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

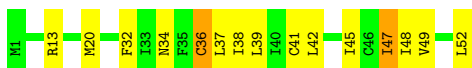


4.2.63 Score per residue for model 63

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

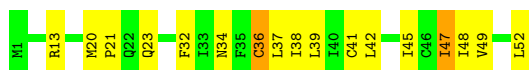


- Molecule 1: Cardiac phospholamban

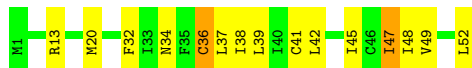


- Molecule 1: Cardiac phospholamban



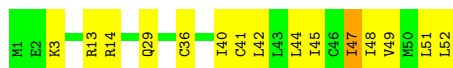


- Molecule 1: Cardiac phospholamban



4.2.64 Score per residue for model 64

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

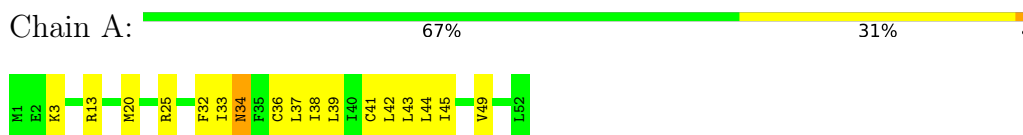


- Molecule 1: Cardiac phospholamban

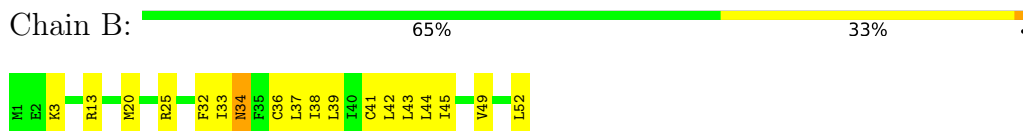


4.2.65 Score per residue for model 65

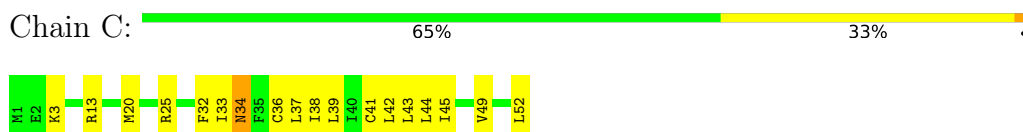
- Molecule 1: Cardiac phospholamban



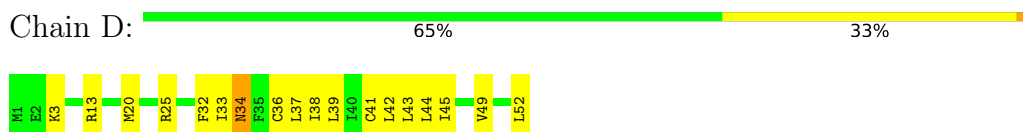
- Molecule 1: Cardiac phospholamban



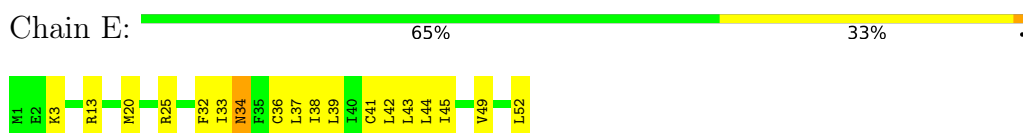
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

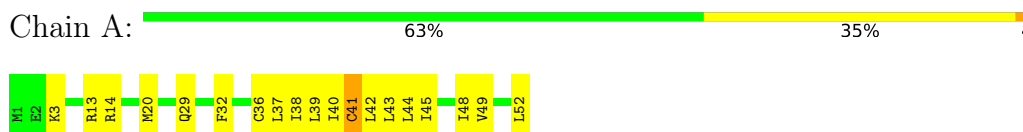


- Molecule 1: Cardiac phospholamban



4.2.66 Score per residue for model 66

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.67 Score per residue for model 67

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



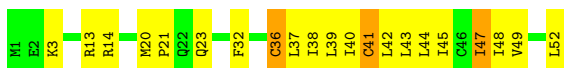


- Molecule 1: Cardiac phospholamban

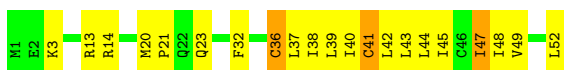


4.2.68 Score per residue for model 68

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

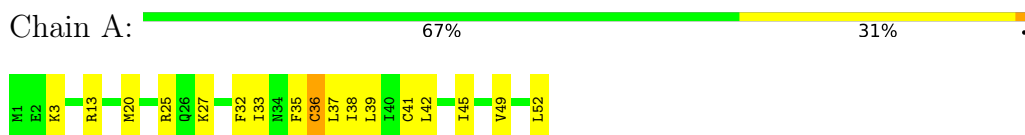


- Molecule 1: Cardiac phospholamban

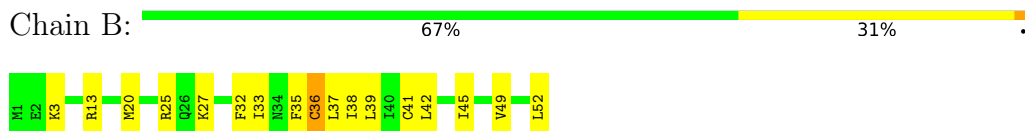


4.2.69 Score per residue for model 69

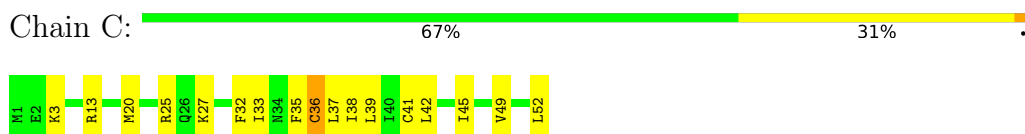
- Molecule 1: Cardiac phospholamban



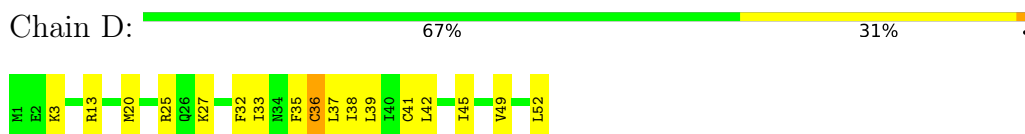
- Molecule 1: Cardiac phospholamban



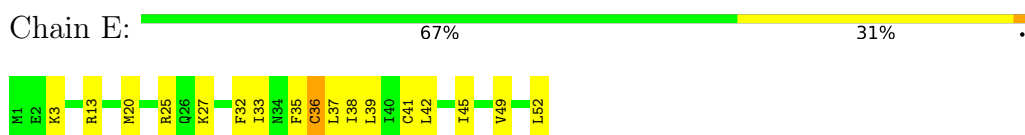
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

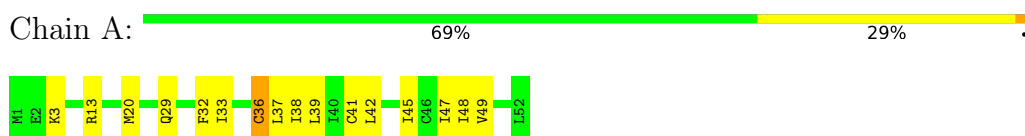


- Molecule 1: Cardiac phospholamban



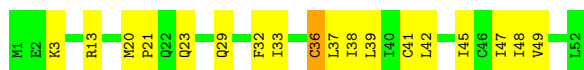
4.2.70 Score per residue for model 70

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

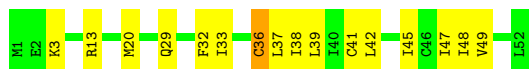




- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.71 Score per residue for model 71

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

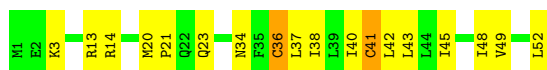


- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

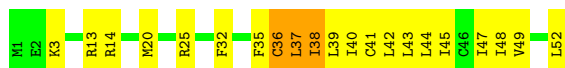
Chain E: 65% 31%



4.2.72 Score per residue for model 72

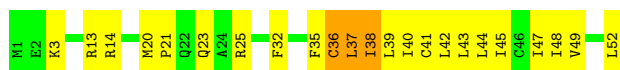
- Molecule 1: Cardiac phospholamban

Chain A: 60% 35% 6%



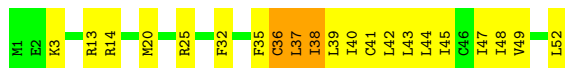
- Molecule 1: Cardiac phospholamban

Chain B: 56% 38% 6%



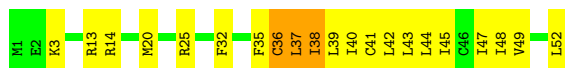
- Molecule 1: Cardiac phospholamban

Chain C: 60% 35% 6%



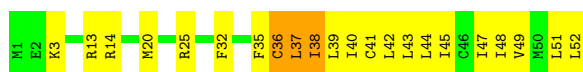
- Molecule 1: Cardiac phospholamban

Chain D: 60% 35% 6%



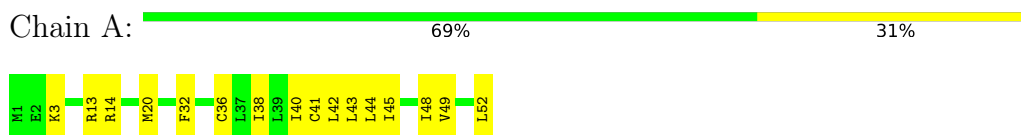
- Molecule 1: Cardiac phospholamban

Chain E: 58% 37% 6%

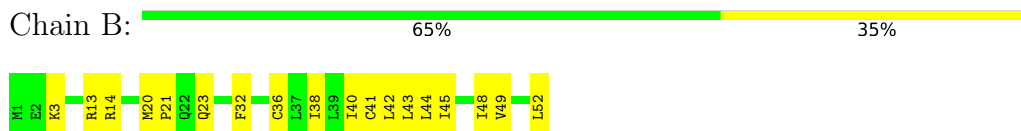


4.2.73 Score per residue for model 73

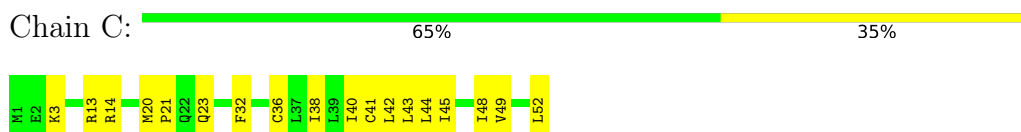
- Molecule 1: Cardiac phospholamban



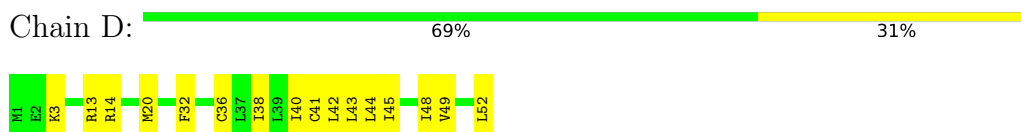
- Molecule 1: Cardiac phospholamban



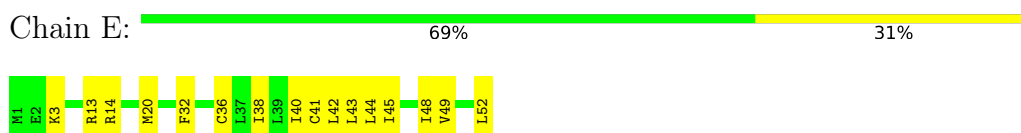
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

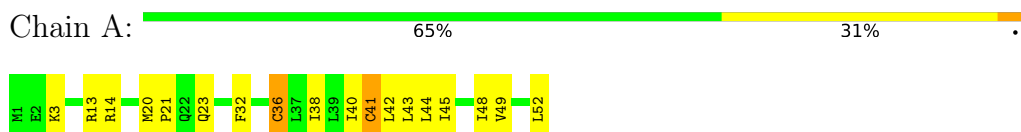


- Molecule 1: Cardiac phospholamban



4.2.74 Score per residue for model 74

- Molecule 1: Cardiac phospholamban

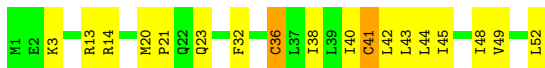


- Molecule 1: Cardiac phospholamban





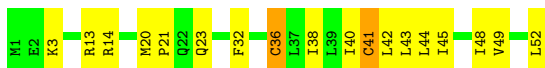
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.75 Score per residue for model 75

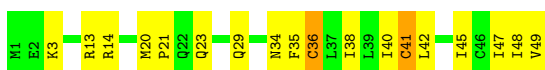
- Molecule 1: Cardiac phospholamban



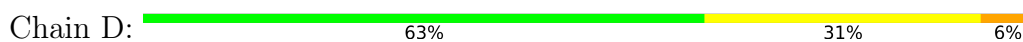
- Molecule 1: Cardiac phospholamban

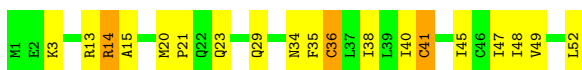


- Molecule 1: Cardiac phospholamban

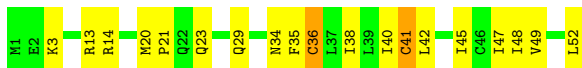


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

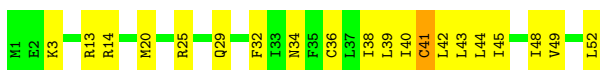


4.2.76 Score per residue for model 76

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

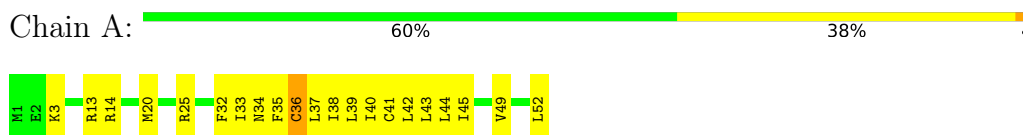


- Molecule 1: Cardiac phospholamban

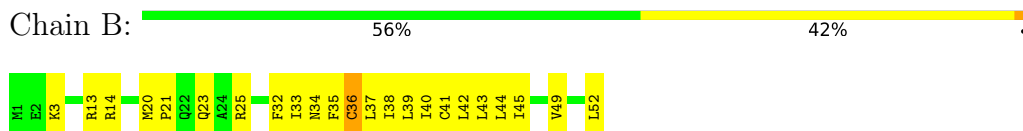


4.2.77 Score per residue for model 77

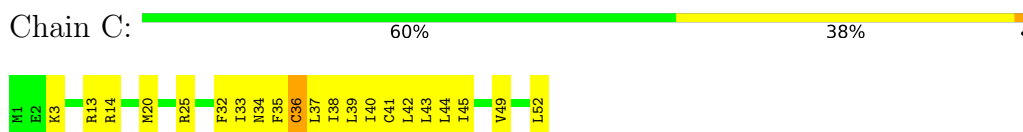
- Molecule 1: Cardiac phospholamban



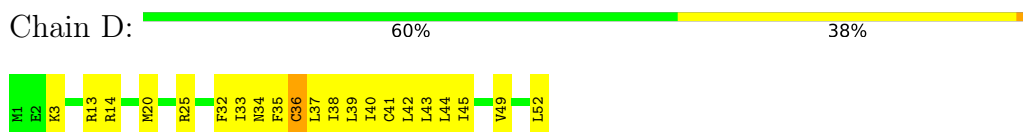
- Molecule 1: Cardiac phospholamban



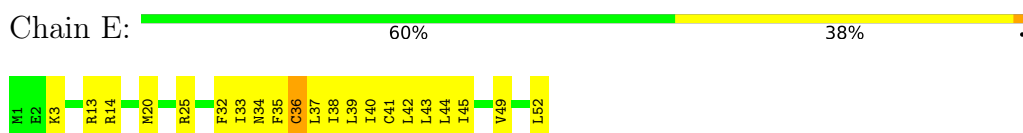
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

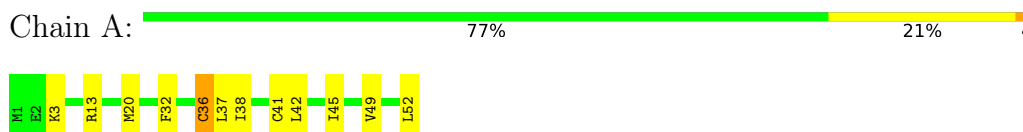


- Molecule 1: Cardiac phospholamban

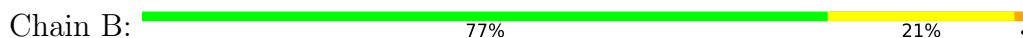


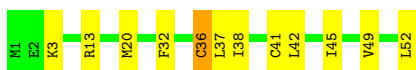
4.2.78 Score per residue for model 78

- Molecule 1: Cardiac phospholamban

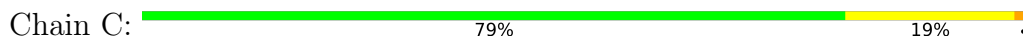


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

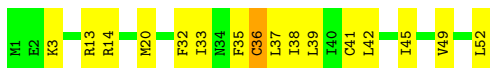


- Molecule 1: Cardiac phospholamban

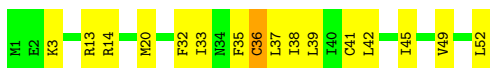


4.2.79 Score per residue for model 79

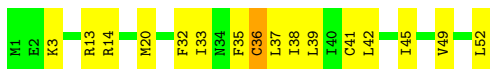
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

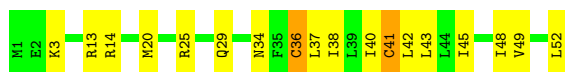


4.2.80 Score per residue for model 80

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



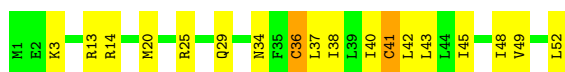
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

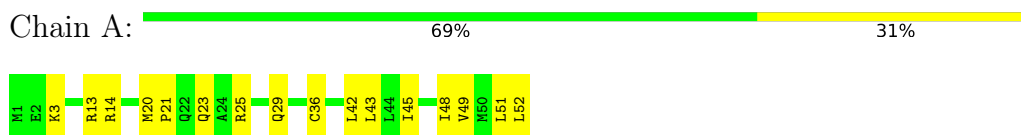


- Molecule 1: Cardiac phospholamban

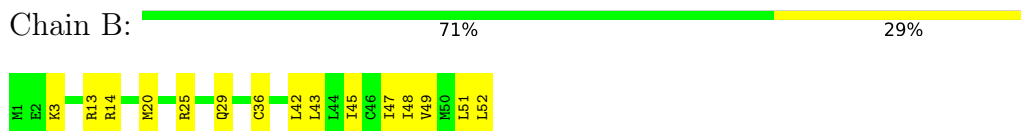


4.2.81 Score per residue for model 81

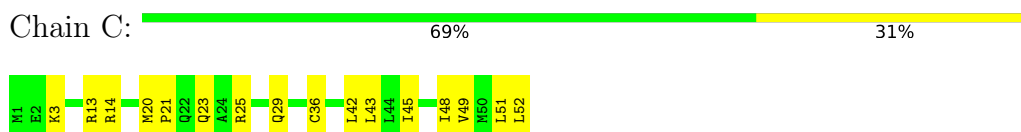
- Molecule 1: Cardiac phospholamban



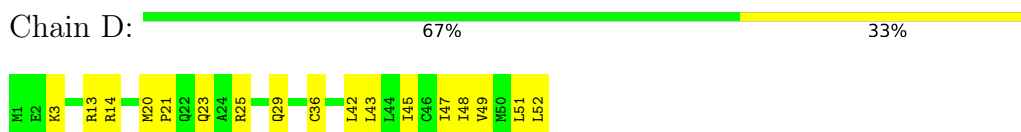
- Molecule 1: Cardiac phospholamban



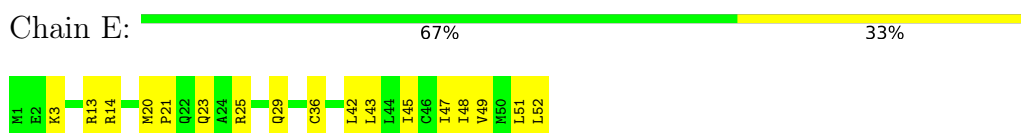
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

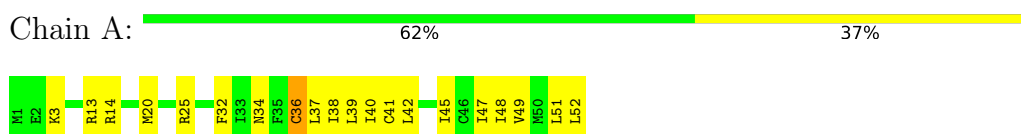


- Molecule 1: Cardiac phospholamban



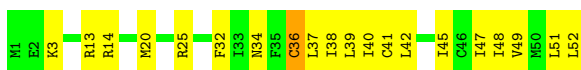
4.2.82 Score per residue for model 82

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.83 Score per residue for model 83

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



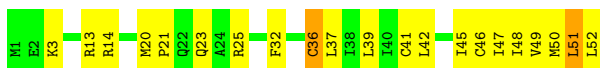


- Molecule 1: Cardiac phospholamban



4.2.84 Score per residue for model 84

- Molecule 1: Cardiac phospholamban



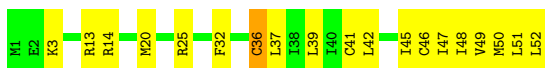
- Molecule 1: Cardiac phospholamban



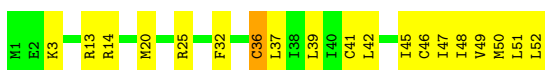
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

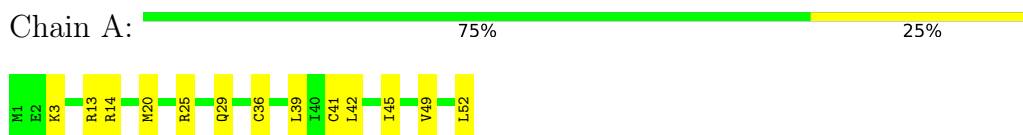


- Molecule 1: Cardiac phospholamban

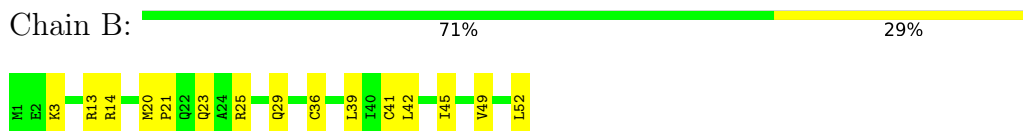


4.2.85 Score per residue for model 85

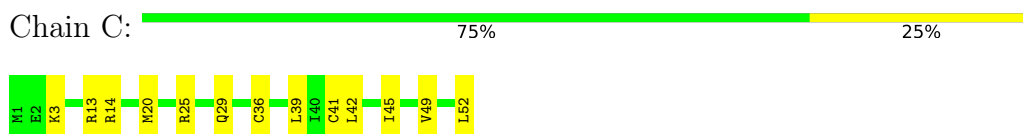
- Molecule 1: Cardiac phospholamban



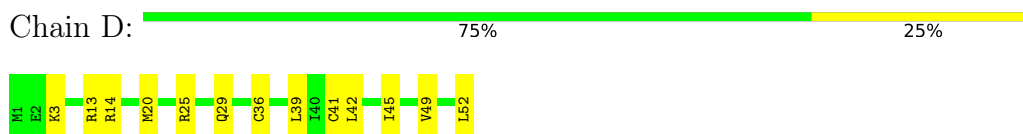
- Molecule 1: Cardiac phospholamban



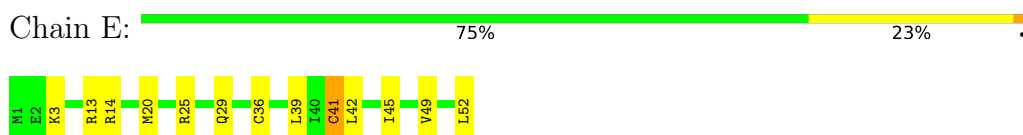
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

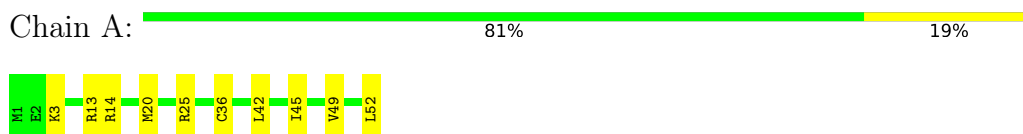


- Molecule 1: Cardiac phospholamban

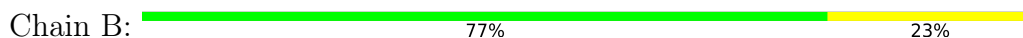


4.2.86 Score per residue for model 86

- Molecule 1: Cardiac phospholamban

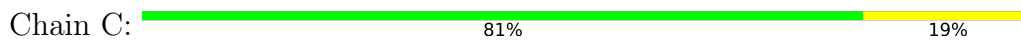


- Molecule 1: Cardiac phospholamban

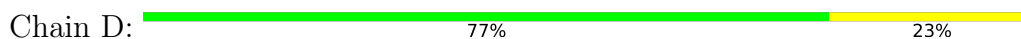




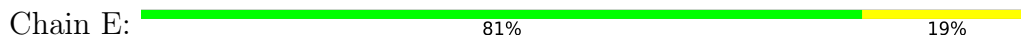
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

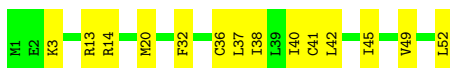


4.2.87 Score per residue for model 87

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

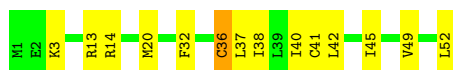


- Molecule 1: Cardiac phospholamban

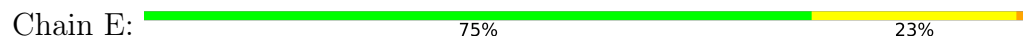


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



4.2.88 Score per residue for model 88

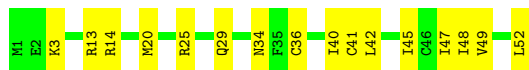
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

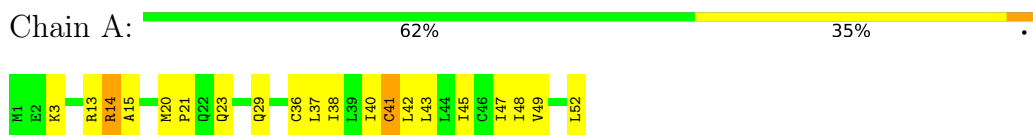


- Molecule 1: Cardiac phospholamban

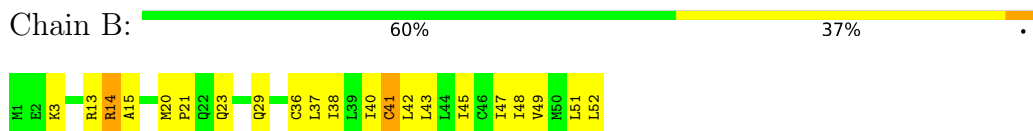


4.2.89 Score per residue for model 89

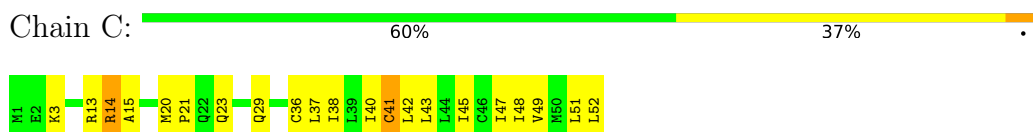
- Molecule 1: Cardiac phospholamban



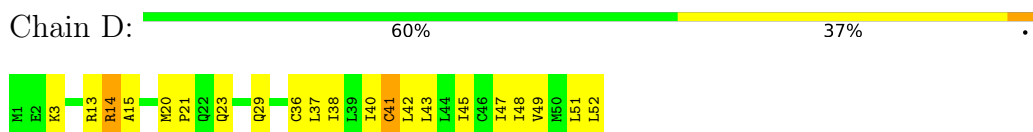
- Molecule 1: Cardiac phospholamban



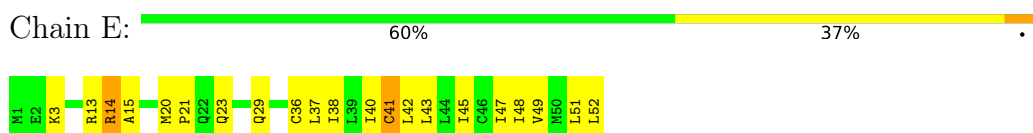
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

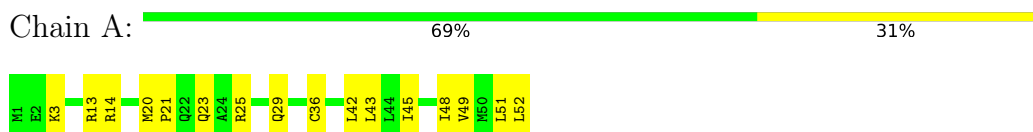


- Molecule 1: Cardiac phospholamban



4.2.90 Score per residue for model 90

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

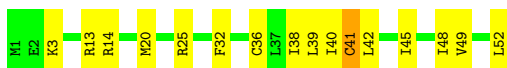


4.2.91 Score per residue for model 91

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

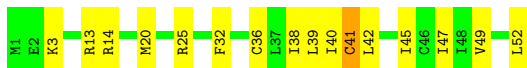


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

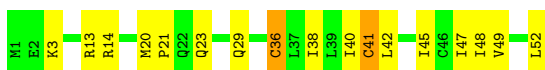


4.2.92 Score per residue for model 92

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



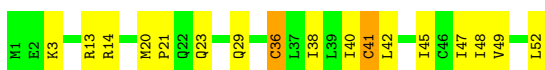
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

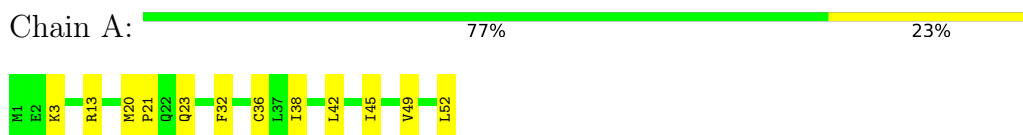


- Molecule 1: Cardiac phospholamban

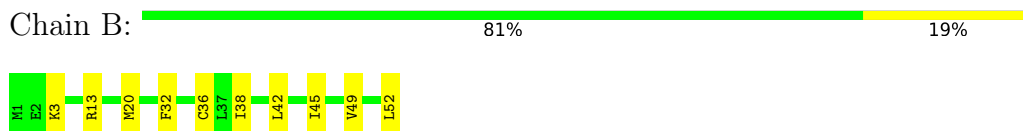


4.2.93 Score per residue for model 93

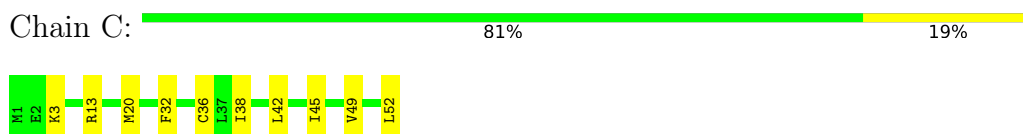
- Molecule 1: Cardiac phospholamban



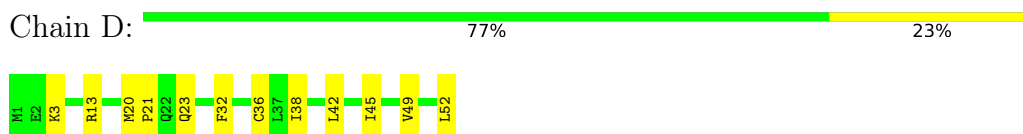
- Molecule 1: Cardiac phospholamban



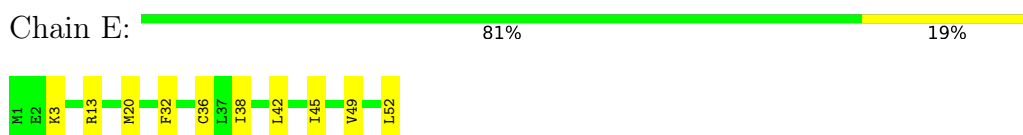
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

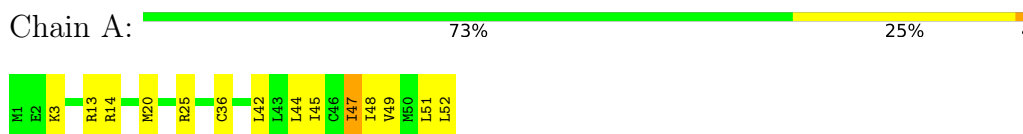


- Molecule 1: Cardiac phospholamban



4.2.94 Score per residue for model 94

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

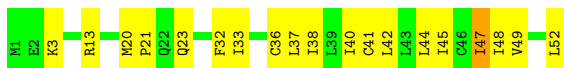


- Molecule 1: Cardiac phospholamban

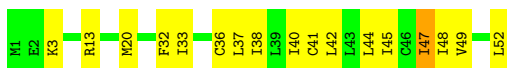


4.2.95 Score per residue for model 95

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

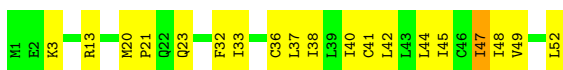


- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

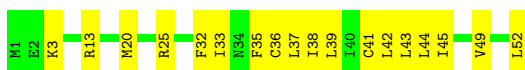


4.2.96 Score per residue for model 96

- Molecule 1: Cardiac phospholamban



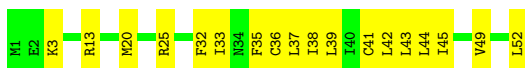
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

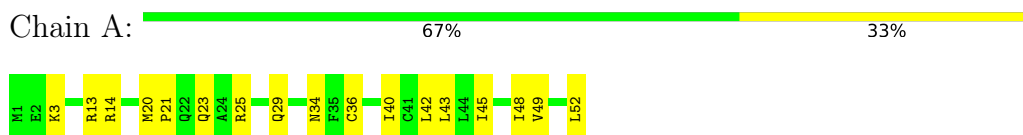


- Molecule 1: Cardiac phospholamban

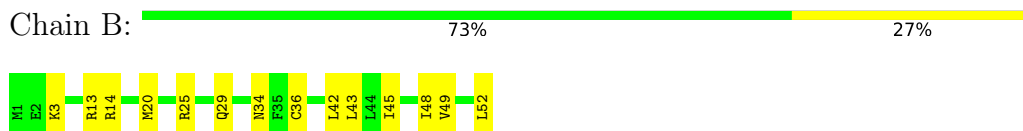


4.2.97 Score per residue for model 97

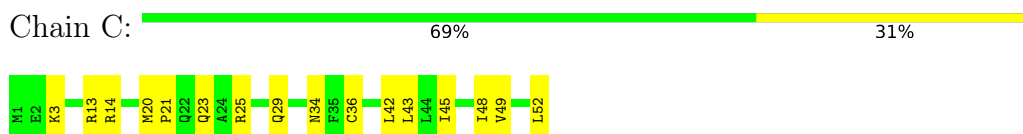
- Molecule 1: Cardiac phospholamban



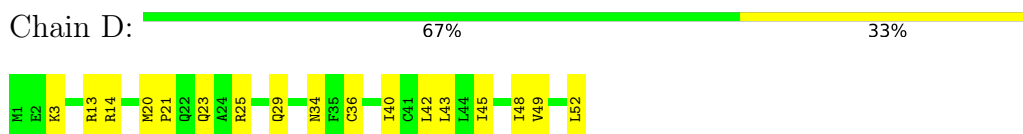
- Molecule 1: Cardiac phospholamban



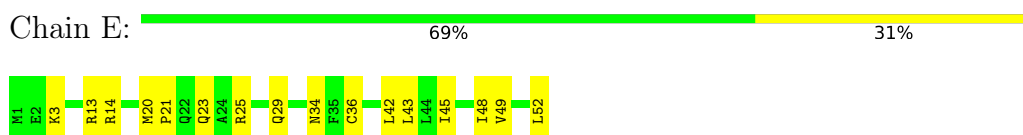
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

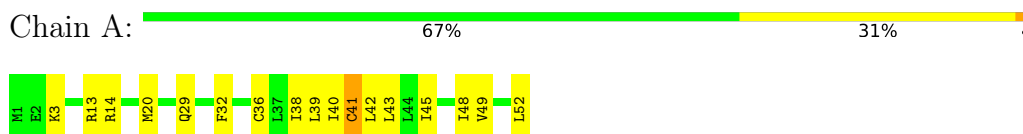


- Molecule 1: Cardiac phospholamban



4.2.98 Score per residue for model 98

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.99 Score per residue for model 99

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



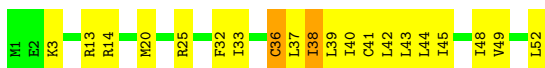


- Molecule 1: Cardiac phospholamban



4.2.100 Score per residue for model 100

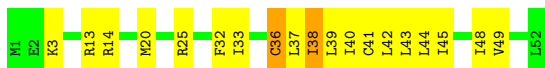
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

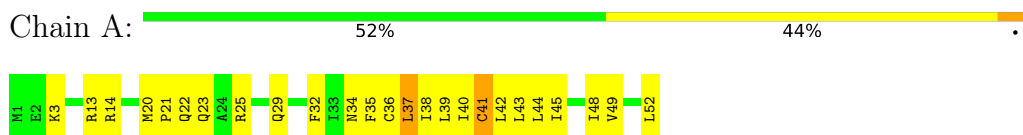


- Molecule 1: Cardiac phospholamban

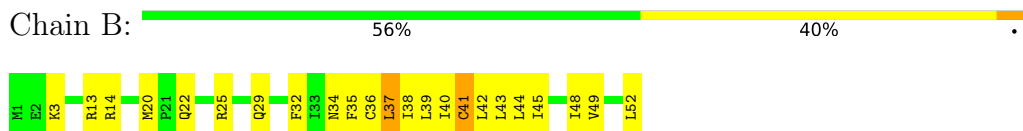


4.2.101 Score per residue for model 101

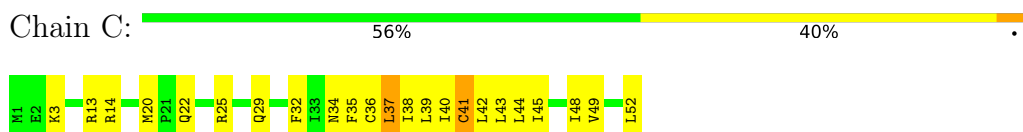
- Molecule 1: Cardiac phospholamban



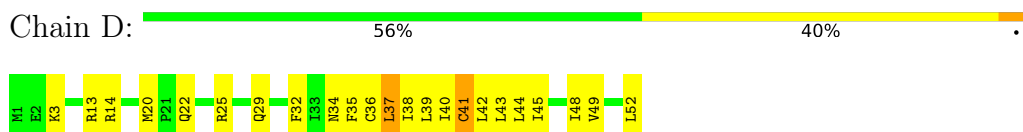
- Molecule 1: Cardiac phospholamban



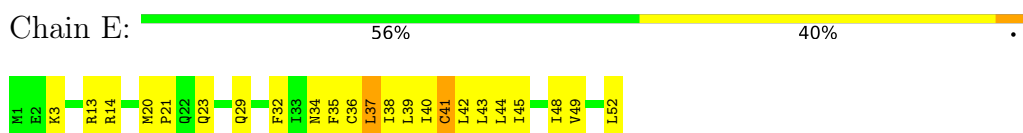
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

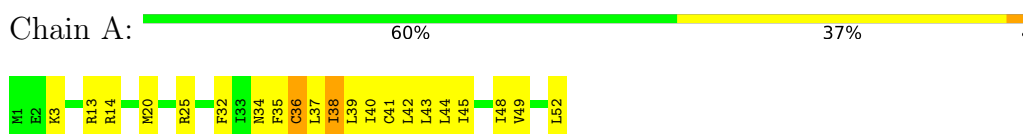


- Molecule 1: Cardiac phospholamban



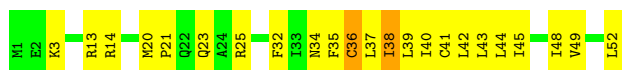
4.2.102 Score per residue for model 102

- Molecule 1: Cardiac phospholamban

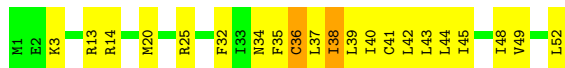


- Molecule 1: Cardiac phospholamban

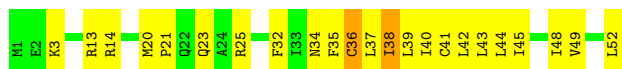




- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.103 Score per residue for model 103

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

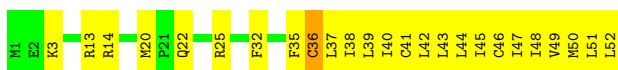


- Molecule 1: Cardiac phospholamban

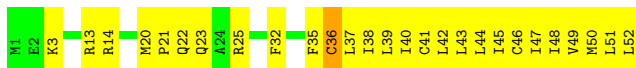


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



4.2.104 Score per residue for model 104

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

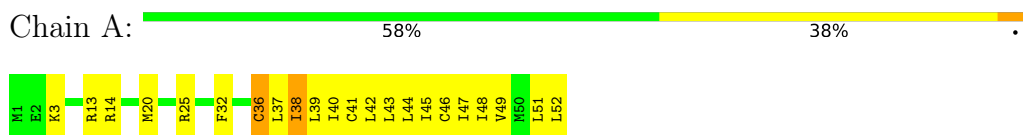


- Molecule 1: Cardiac phospholamban

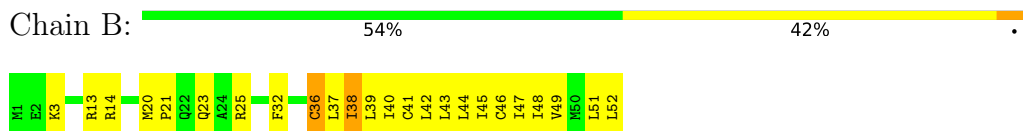


4.2.105 Score per residue for model 105

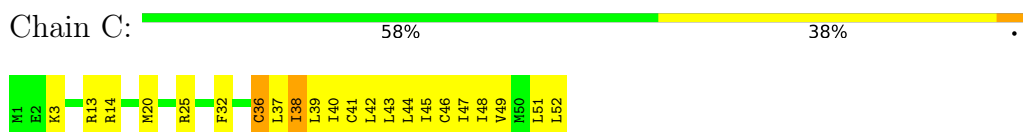
- Molecule 1: Cardiac phospholamban



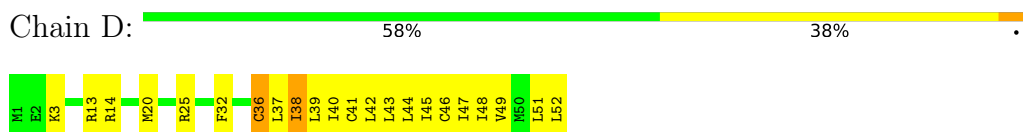
- Molecule 1: Cardiac phospholamban



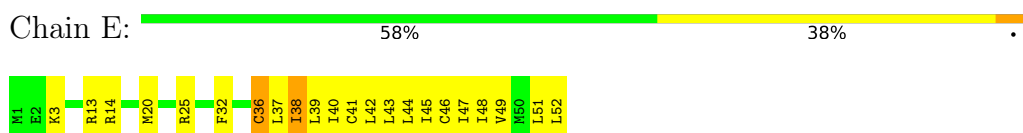
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

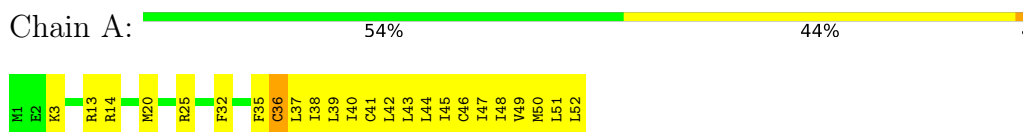


- Molecule 1: Cardiac phospholamban



4.2.106 Score per residue for model 106

- Molecule 1: Cardiac phospholamban

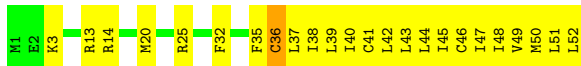


- Molecule 1: Cardiac phospholamban





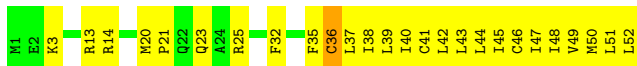
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

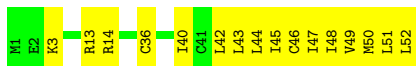


4.2.107 Score per residue for model 107

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

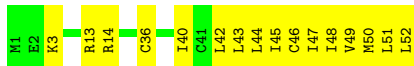


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

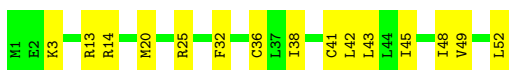


4.2.108 Score per residue for model 108

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

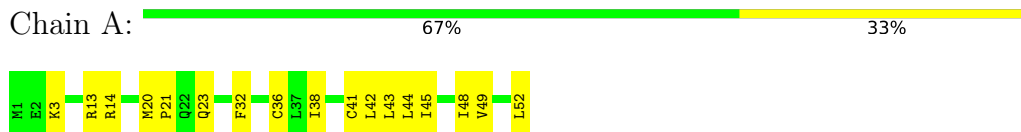


- Molecule 1: Cardiac phospholamban

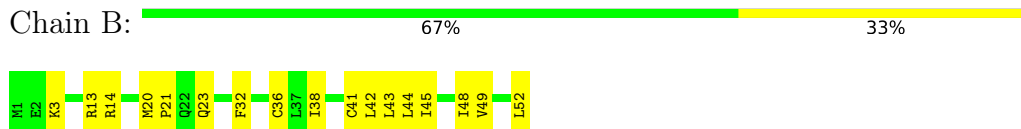


4.2.109 Score per residue for model 109

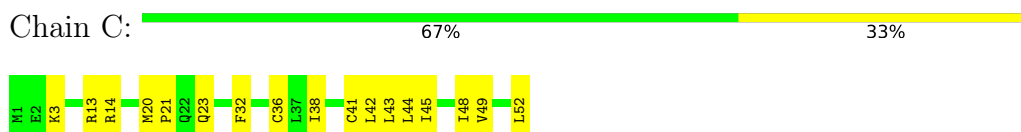
- Molecule 1: Cardiac phospholamban



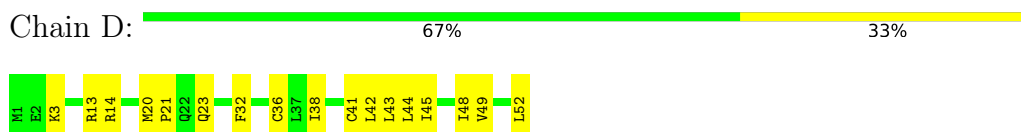
- Molecule 1: Cardiac phospholamban



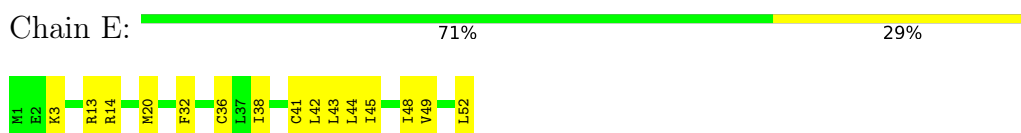
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

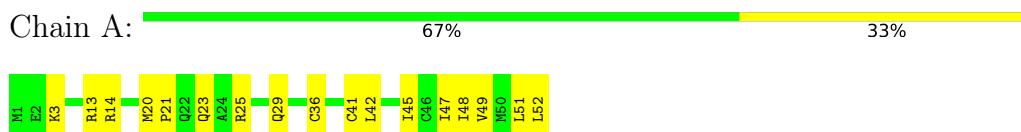


- Molecule 1: Cardiac phospholamban



4.2.110 Score per residue for model 110

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.111 Score per residue for model 111

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



4.2.112 Score per residue for model 112

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

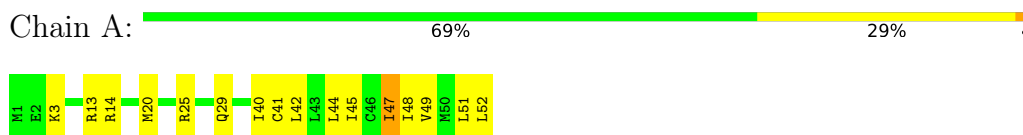


- Molecule 1: Cardiac phospholamban

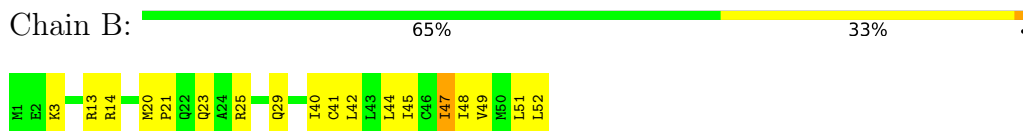


4.2.113 Score per residue for model 113

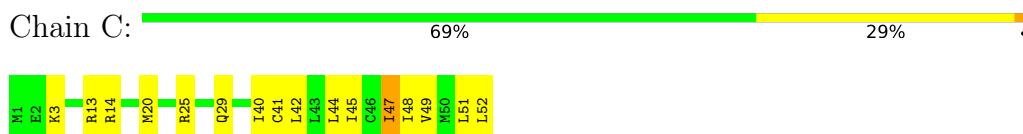
- Molecule 1: Cardiac phospholamban



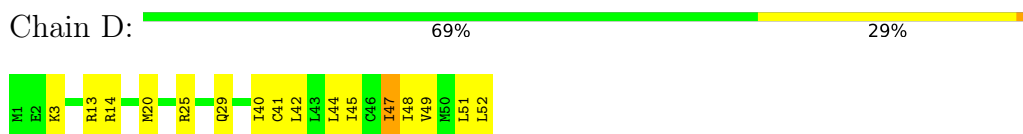
- Molecule 1: Cardiac phospholamban



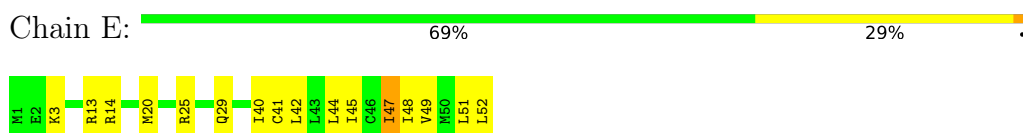
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

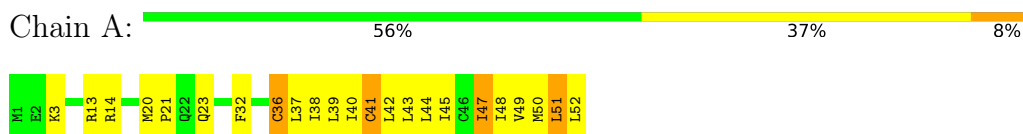


- Molecule 1: Cardiac phospholamban



4.2.114 Score per residue for model 114

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





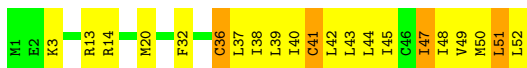
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

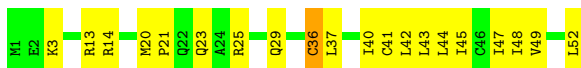


- Molecule 1: Cardiac phospholamban



4.2.115 Score per residue for model 115

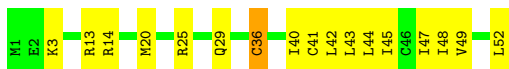
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

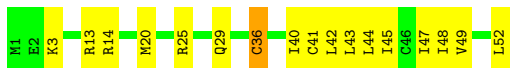


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



4.2.116 Score per residue for model 116

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

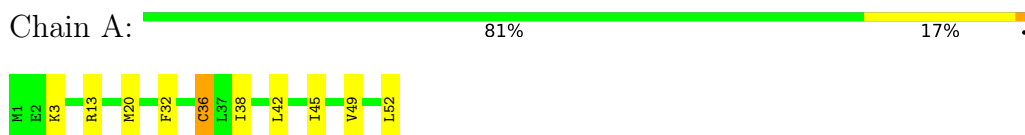


- Molecule 1: Cardiac phospholamban

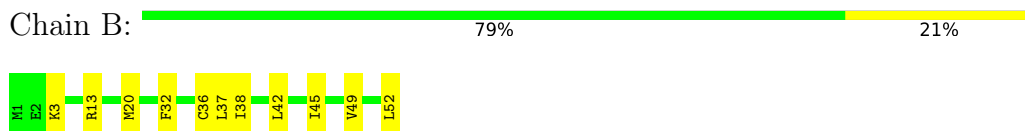


4.2.117 Score per residue for model 117

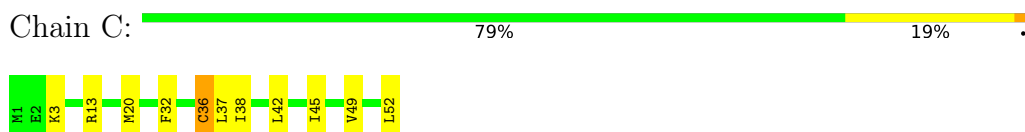
- Molecule 1: Cardiac phospholamban



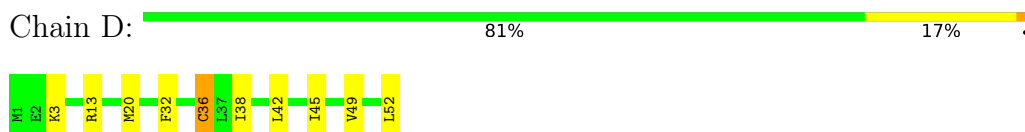
- Molecule 1: Cardiac phospholamban



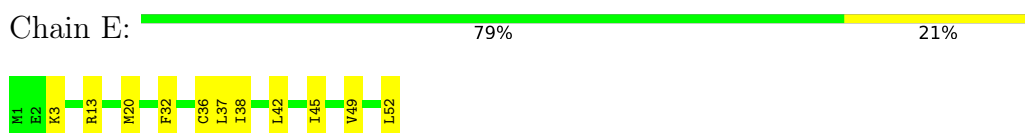
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

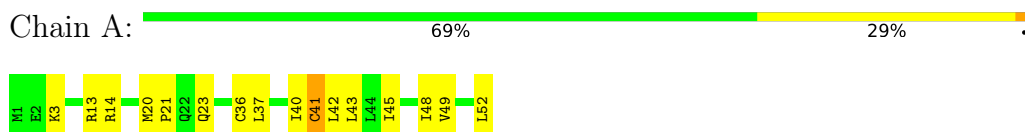


- Molecule 1: Cardiac phospholamban



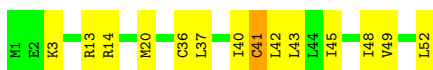
4.2.118 Score per residue for model 118

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.119 Score per residue for model 119

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

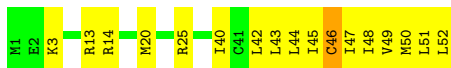


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

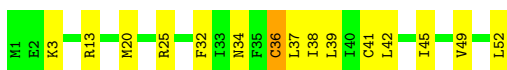


4.2.120 Score per residue for model 120

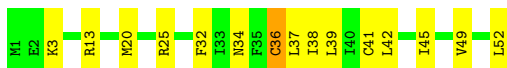
- Molecule 1: Cardiac phospholamban



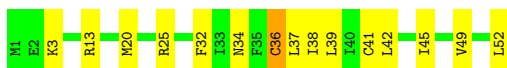
- Molecule 1: Cardiac phospholamban



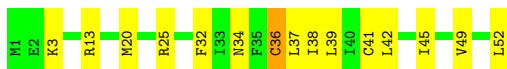
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

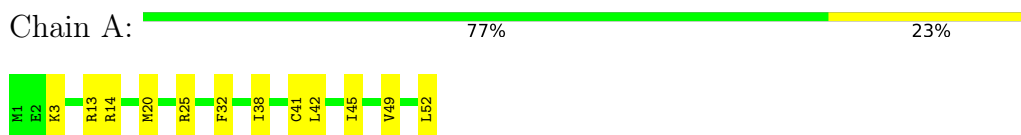


- Molecule 1: Cardiac phospholamban

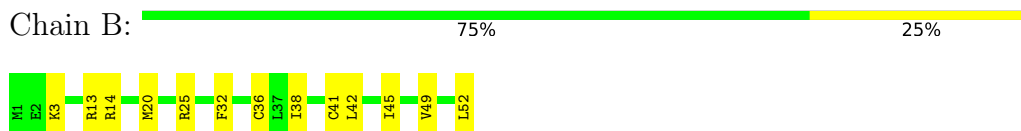


4.2.121 Score per residue for model 121

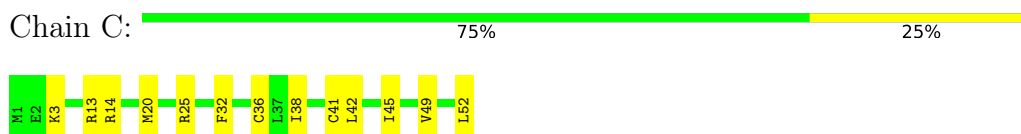
- Molecule 1: Cardiac phospholamban



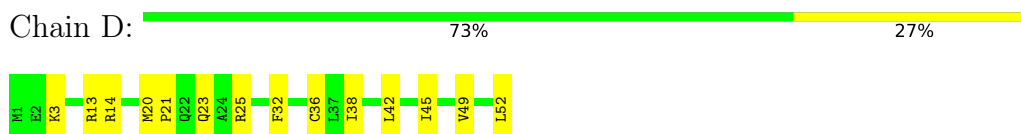
- Molecule 1: Cardiac phospholamban



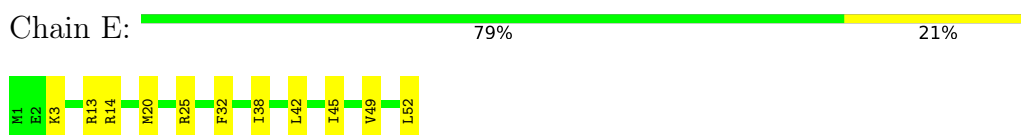
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

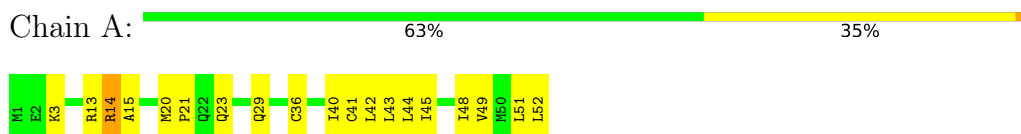


- Molecule 1: Cardiac phospholamban



4.2.122 Score per residue for model 122

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

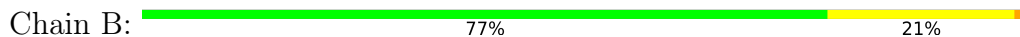


4.2.123 Score per residue for model 123

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



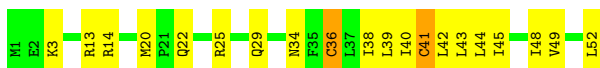


- Molecule 1: Cardiac phospholamban

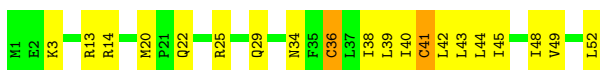


4.2.124 Score per residue for model 124

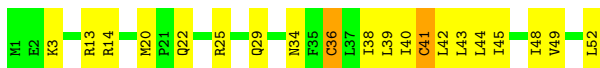
- Molecule 1: Cardiac phospholamban



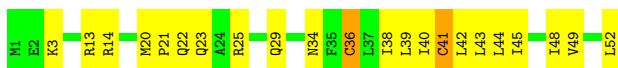
- Molecule 1: Cardiac phospholamban



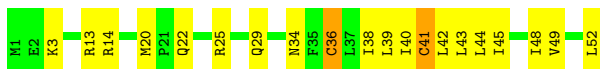
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

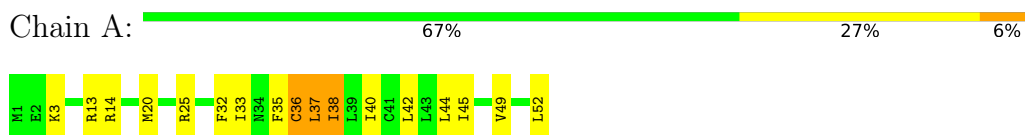


- Molecule 1: Cardiac phospholamban

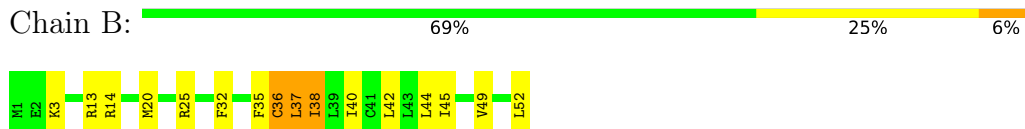


4.2.125 Score per residue for model 125

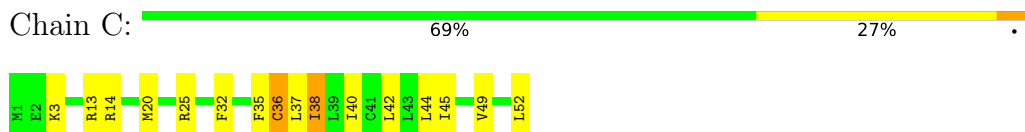
- Molecule 1: Cardiac phospholamban



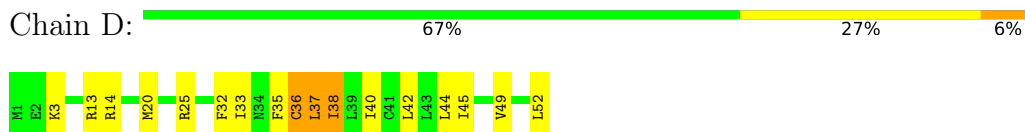
- Molecule 1: Cardiac phospholamban



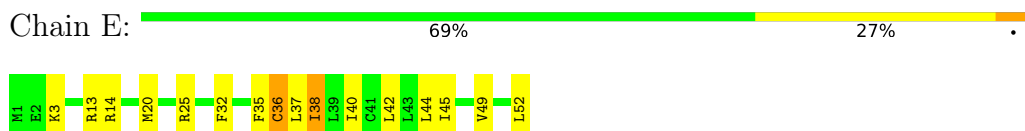
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

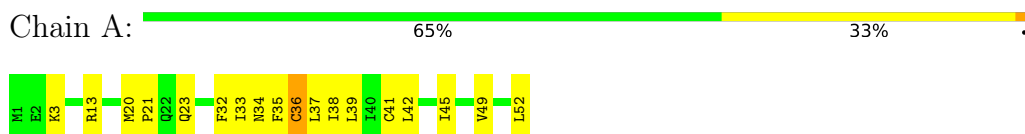


- Molecule 1: Cardiac phospholamban



4.2.126 Score per residue for model 126

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.127 Score per residue for model 127

- Molecule 1: Cardiac phospholamban



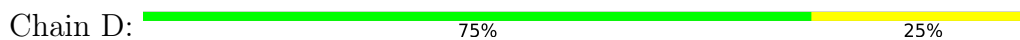
- Molecule 1: Cardiac phospholamban

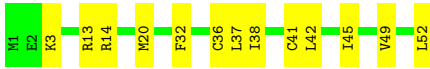


- Molecule 1: Cardiac phospholamban



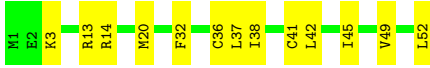
- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

Chain E: 75% 25%



4.2.128 Score per residue for model 128

- Molecule 1: Cardiac phospholamban

Chain A: 69% 29%



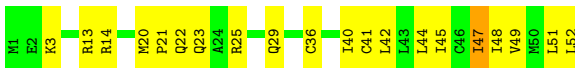
- Molecule 1: Cardiac phospholamban

Chain B: 65% 33%



- Molecule 1: Cardiac phospholamban

Chain C: 62% 37%



- Molecule 1: Cardiac phospholamban

Chain D: 62% 37%



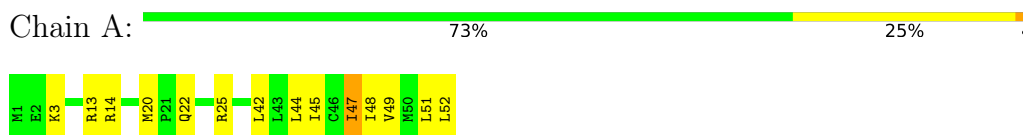
- Molecule 1: Cardiac phospholamban

Chain E: 65% 33%

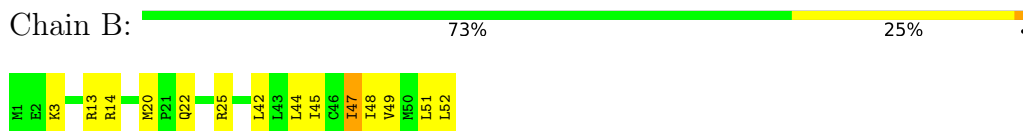


4.2.129 Score per residue for model 129

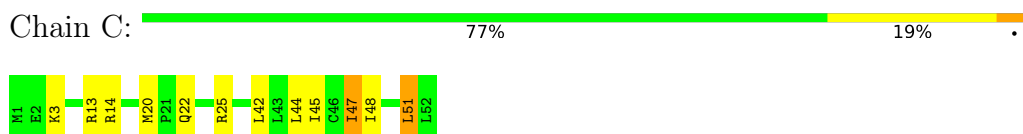
- Molecule 1: Cardiac phospholamban



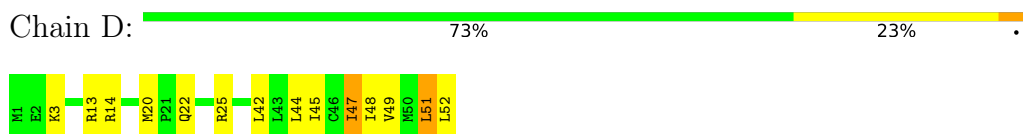
- Molecule 1: Cardiac phospholamban



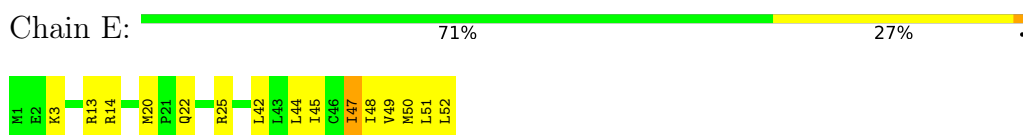
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

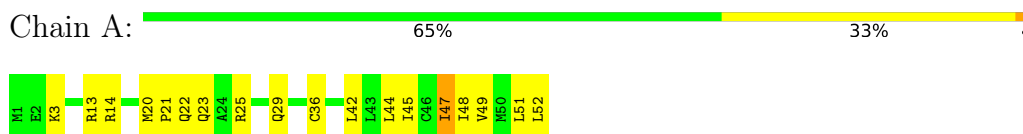


- Molecule 1: Cardiac phospholamban



4.2.130 Score per residue for model 130

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.131 Score per residue for model 131

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

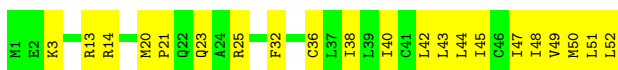


4.2.132 Score per residue for model 132

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

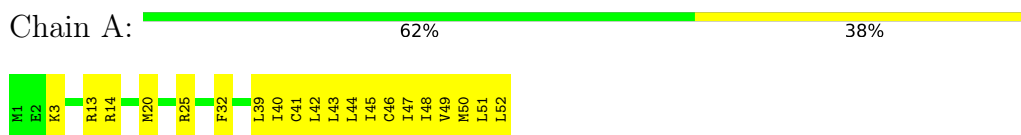


- Molecule 1: Cardiac phospholamban

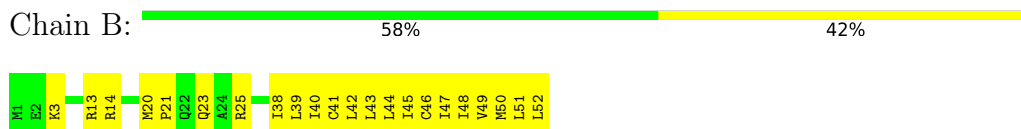


4.2.133 Score per residue for model 133

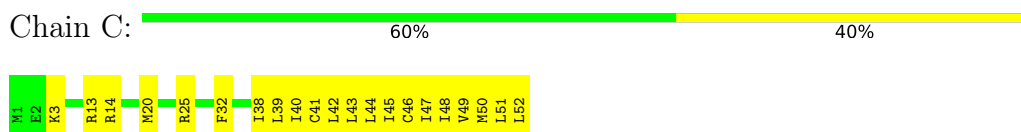
- Molecule 1: Cardiac phospholamban



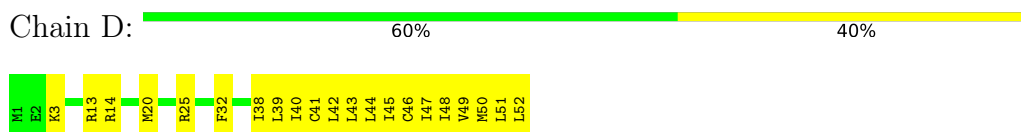
- Molecule 1: Cardiac phospholamban



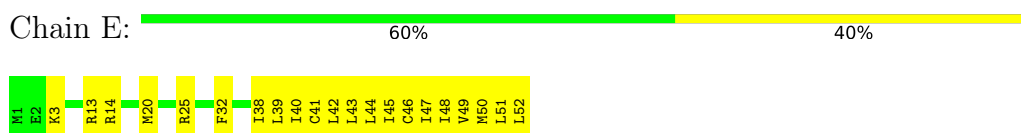
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

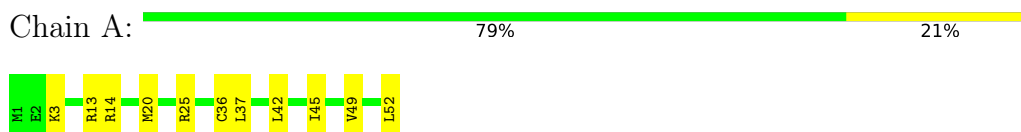


- Molecule 1: Cardiac phospholamban

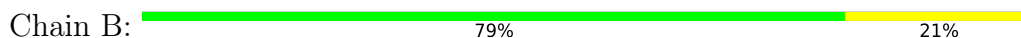


4.2.134 Score per residue for model 134

- Molecule 1: Cardiac phospholamban

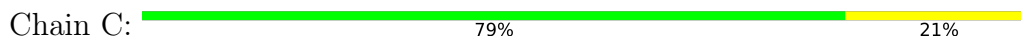


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

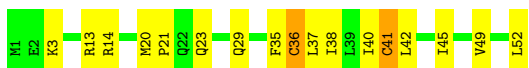


4.2.135 Score per residue for model 135

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

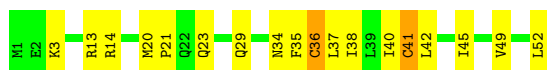


- Molecule 1: Cardiac phospholamban



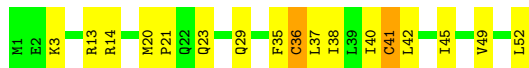
- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

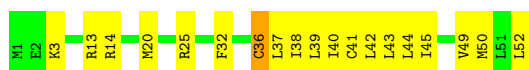
Chain E:



4.2.136 Score per residue for model 136

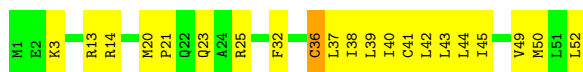
- Molecule 1: Cardiac phospholamban

Chain A:



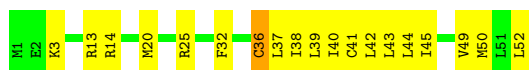
- Molecule 1: Cardiac phospholamban

Chain B:



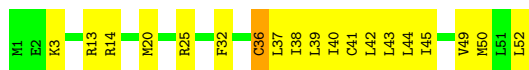
- Molecule 1: Cardiac phospholamban

Chain C:



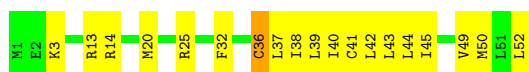
- Molecule 1: Cardiac phospholamban

Chain D:



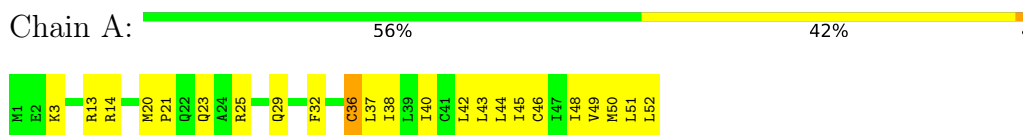
- Molecule 1: Cardiac phospholamban

Chain E:

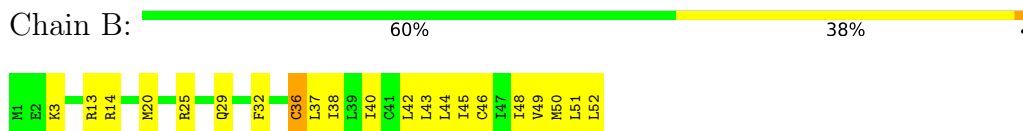


4.2.137 Score per residue for model 137

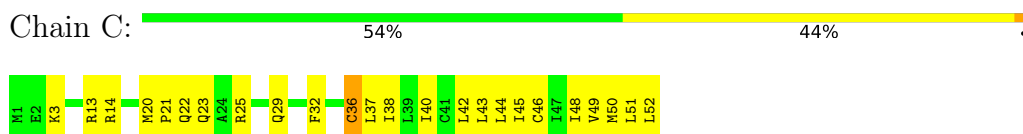
- Molecule 1: Cardiac phospholamban



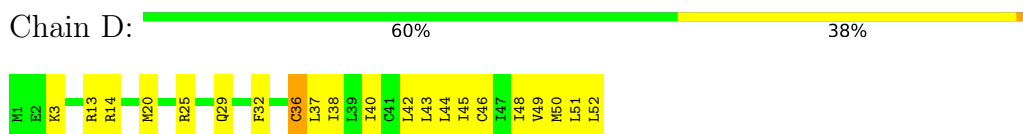
- Molecule 1: Cardiac phospholamban



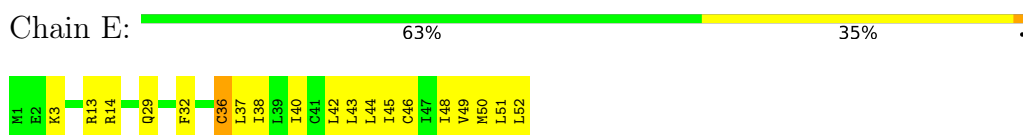
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

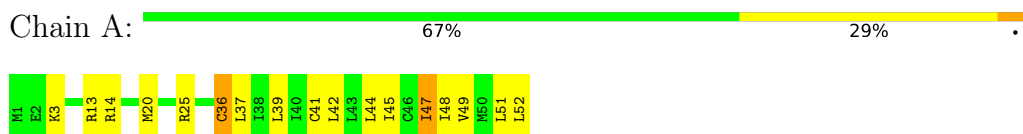


- Molecule 1: Cardiac phospholamban



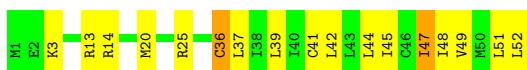
4.2.138 Score per residue for model 138

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

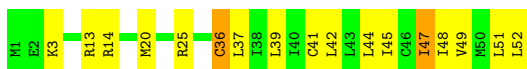




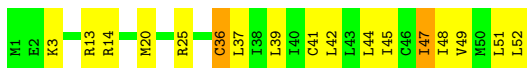
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.139 Score per residue for model 139 (medoid)

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

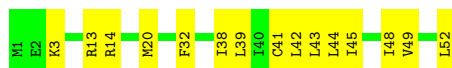
Chain E: 65% 35%



4.2.140 Score per residue for model 140

- Molecule 1: Cardiac phospholamban

Chain A: 71% 29%



- Molecule 1: Cardiac phospholamban

Chain B: 73% 27%



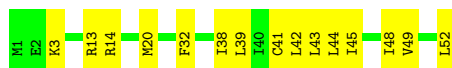
- Molecule 1: Cardiac phospholamban

Chain C: 71% 29%



- Molecule 1: Cardiac phospholamban

Chain D: 71% 29%



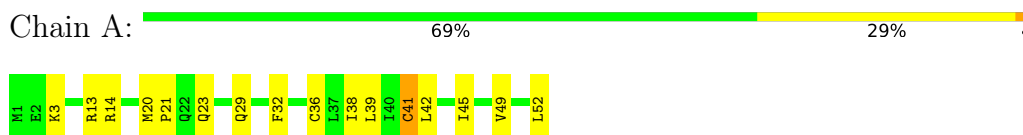
- Molecule 1: Cardiac phospholamban

Chain E: 73% 27%

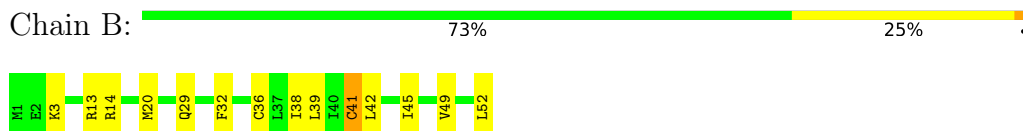


4.2.141 Score per residue for model 141

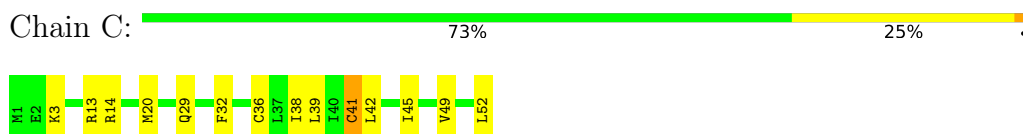
- Molecule 1: Cardiac phospholamban



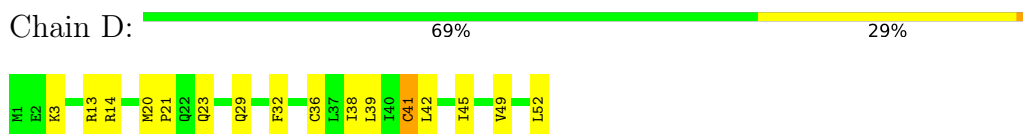
- Molecule 1: Cardiac phospholamban



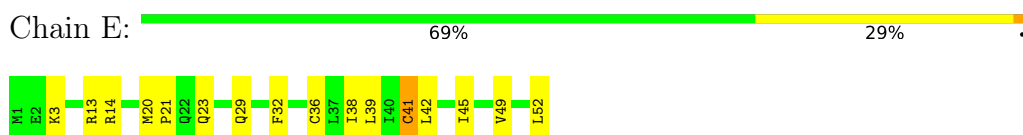
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

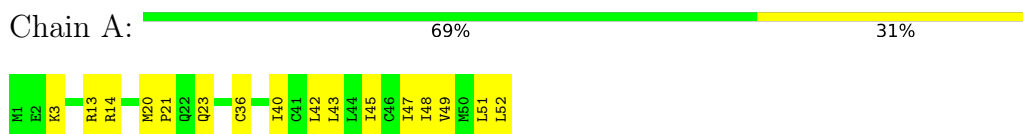


- Molecule 1: Cardiac phospholamban



4.2.142 Score per residue for model 142

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

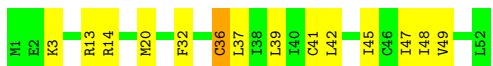


- Molecule 1: Cardiac phospholamban



4.2.143 Score per residue for model 143

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

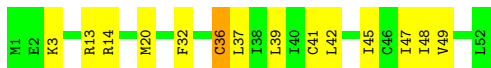


- Molecule 1: Cardiac phospholamban



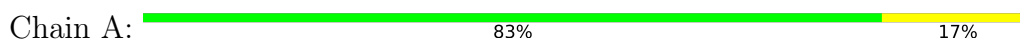


- Molecule 1: Cardiac phospholamban

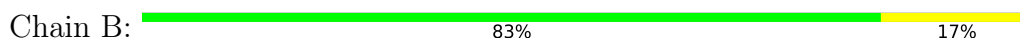


4.2.144 Score per residue for model 144

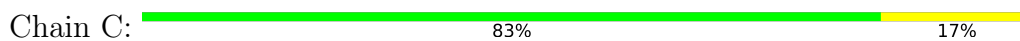
- Molecule 1: Cardiac phospholamban



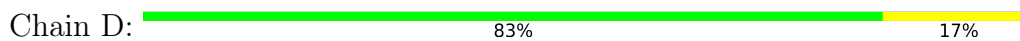
- Molecule 1: Cardiac phospholamban



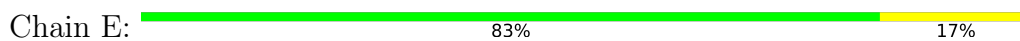
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

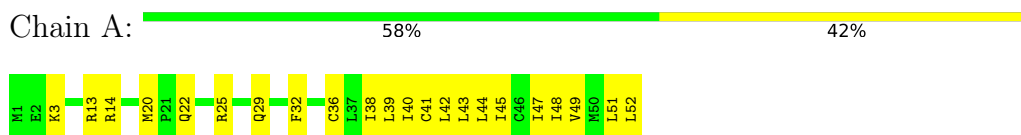


- Molecule 1: Cardiac phospholamban

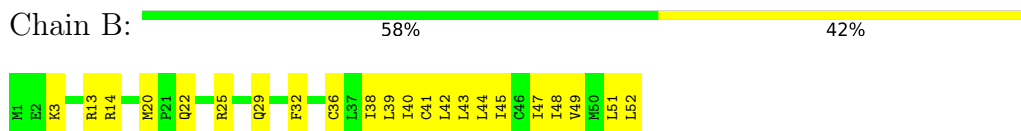


4.2.145 Score per residue for model 145

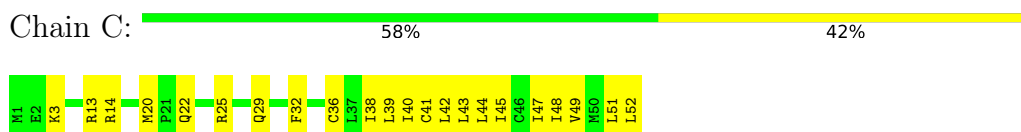
- Molecule 1: Cardiac phospholamban



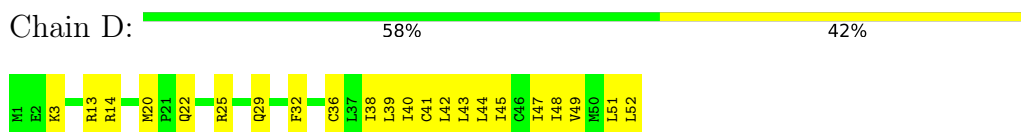
- Molecule 1: Cardiac phospholamban



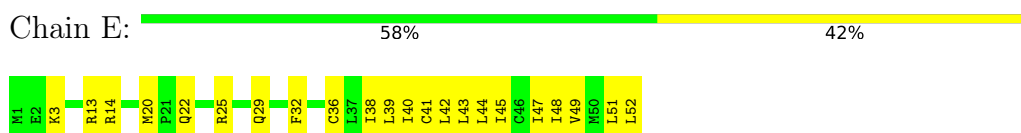
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

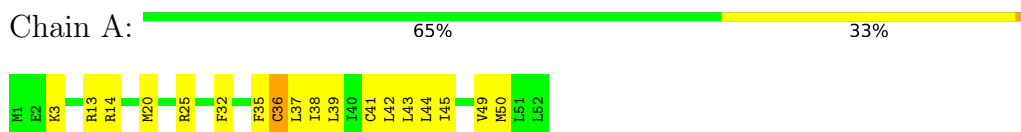


- Molecule 1: Cardiac phospholamban



4.2.146 Score per residue for model 146

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

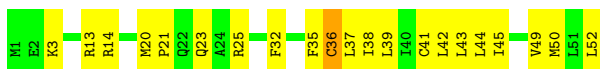




- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.147 Score per residue for model 147

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



4.2.148 Score per residue for model 148

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



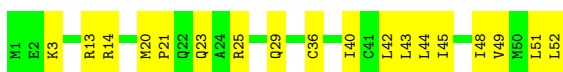
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

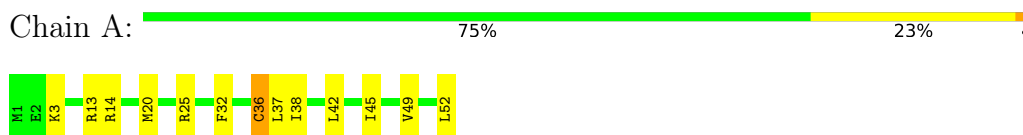


- Molecule 1: Cardiac phospholamban

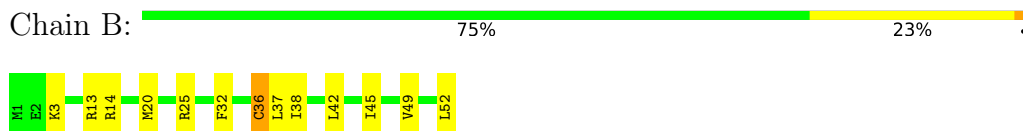


4.2.149 Score per residue for model 149

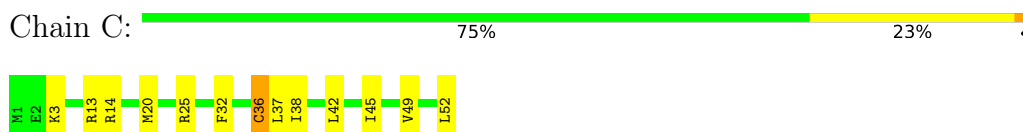
- Molecule 1: Cardiac phospholamban



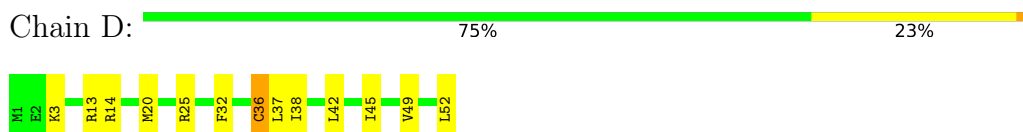
- Molecule 1: Cardiac phospholamban



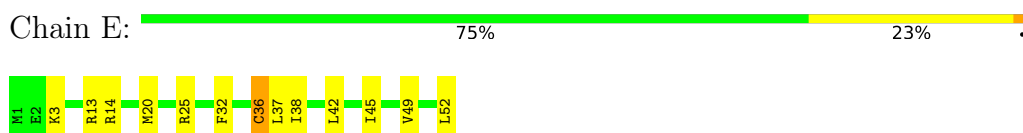
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

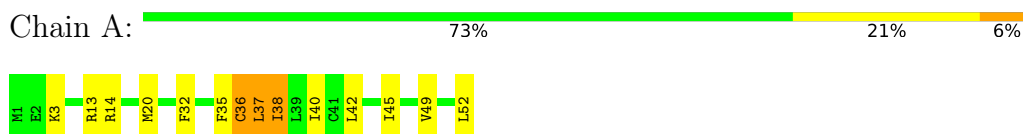


- Molecule 1: Cardiac phospholamban



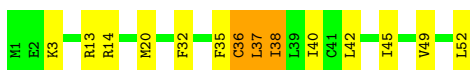
4.2.150 Score per residue for model 150

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

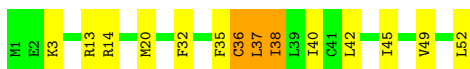




- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.151 Score per residue for model 151

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



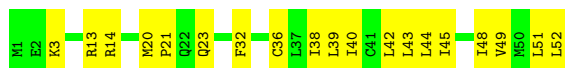


- Molecule 1: Cardiac phospholamban



4.2.152 Score per residue for model 152

- Molecule 1: Cardiac phospholamban



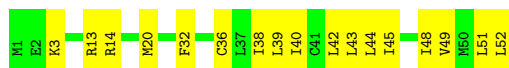
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

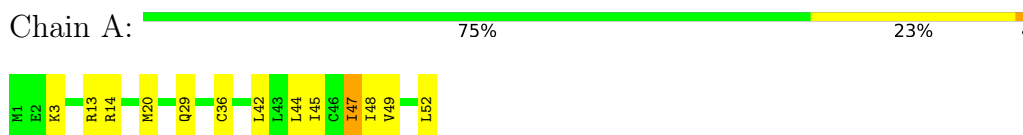


- Molecule 1: Cardiac phospholamban

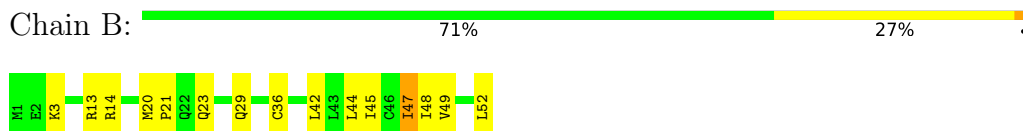


4.2.153 Score per residue for model 153

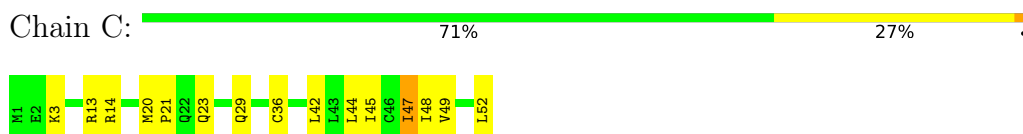
- Molecule 1: Cardiac phospholamban



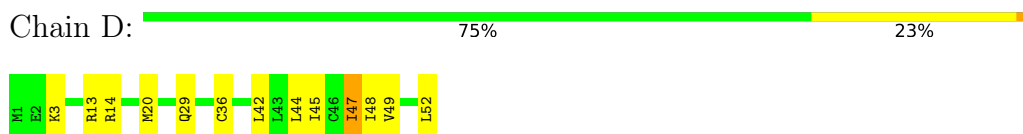
- Molecule 1: Cardiac phospholamban



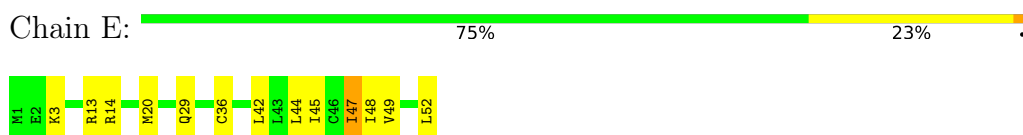
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

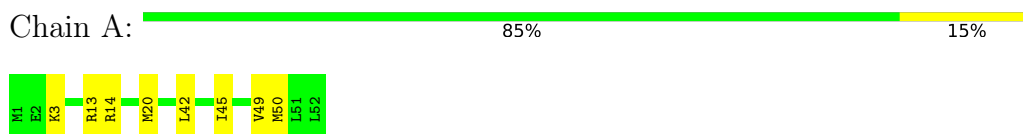


- Molecule 1: Cardiac phospholamban

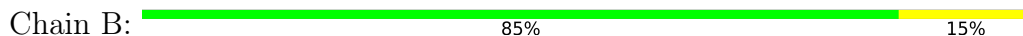


4.2.154 Score per residue for model 154

- Molecule 1: Cardiac phospholamban

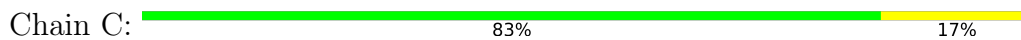


- Molecule 1: Cardiac phospholamban

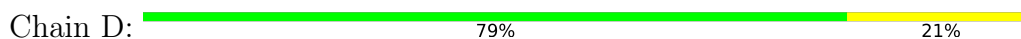




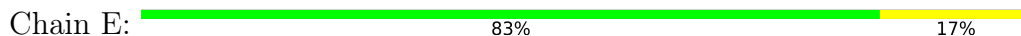
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.155 Score per residue for model 155

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

Chain E: 77% 21% .



4.2.156 Score per residue for model 156

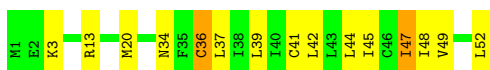
- Molecule 1: Cardiac phospholamban

Chain A: 71% 25% .



- Molecule 1: Cardiac phospholamban

Chain B: 71% 25% .



- Molecule 1: Cardiac phospholamban

Chain C: 71% 25% .



- Molecule 1: Cardiac phospholamban

Chain D: 71% 25% .



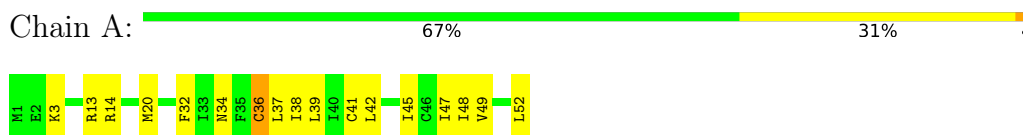
- Molecule 1: Cardiac phospholamban

Chain E: 71% 25% .

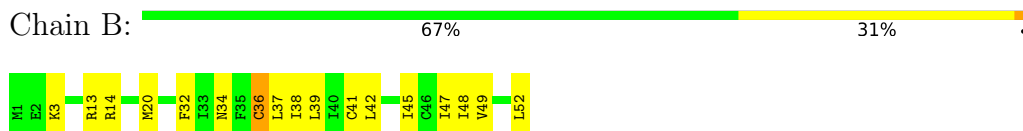


4.2.157 Score per residue for model 157

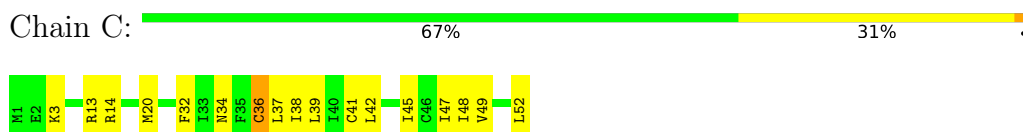
- Molecule 1: Cardiac phospholamban



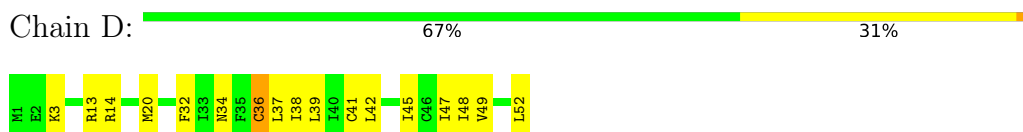
- Molecule 1: Cardiac phospholamban



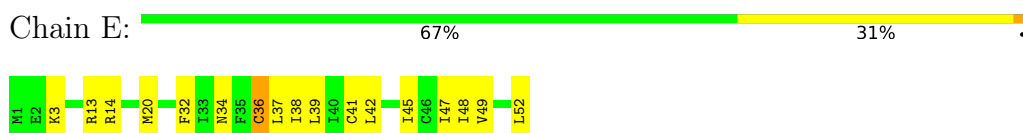
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

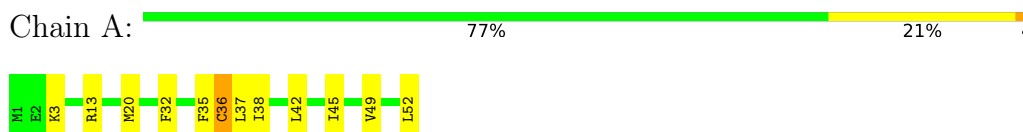


- Molecule 1: Cardiac phospholamban

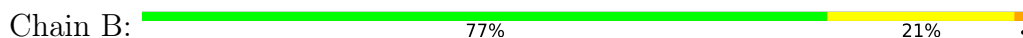


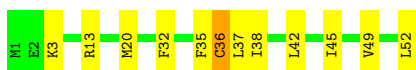
4.2.158 Score per residue for model 158

- Molecule 1: Cardiac phospholamban

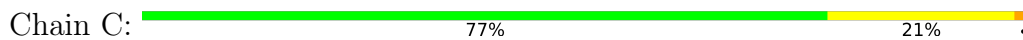


- Molecule 1: Cardiac phospholamban

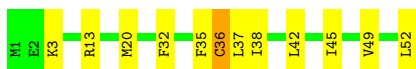
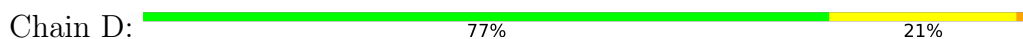




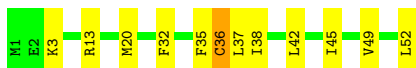
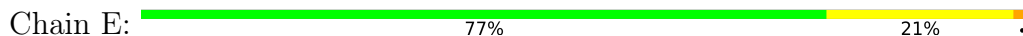
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.159 Score per residue for model 159

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

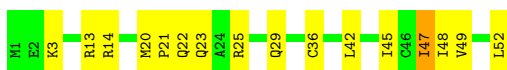


- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

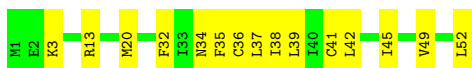
Chain E: 69% 29%



4.2.160 Score per residue for model 160

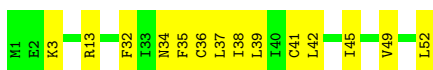
- Molecule 1: Cardiac phospholamban

Chain A: 71% 29%



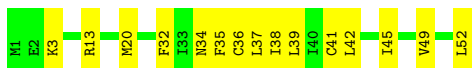
- Molecule 1: Cardiac phospholamban

Chain B: 73% 27%



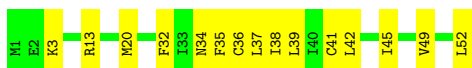
- Molecule 1: Cardiac phospholamban

Chain C: 71% 29%



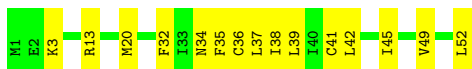
- Molecule 1: Cardiac phospholamban

Chain D: 71% 29%



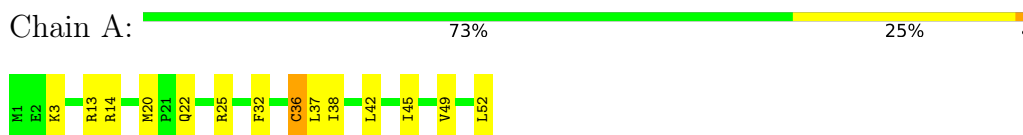
- Molecule 1: Cardiac phospholamban

Chain E: 71% 29%

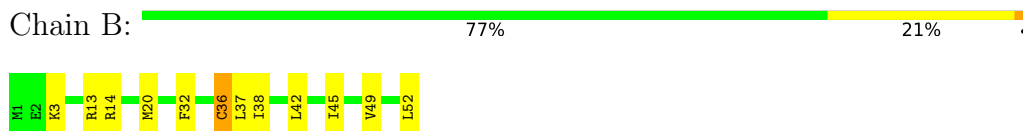


4.2.161 Score per residue for model 161

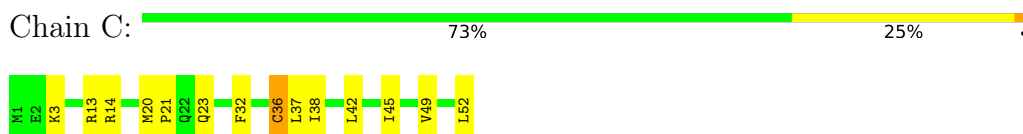
- Molecule 1: Cardiac phospholamban



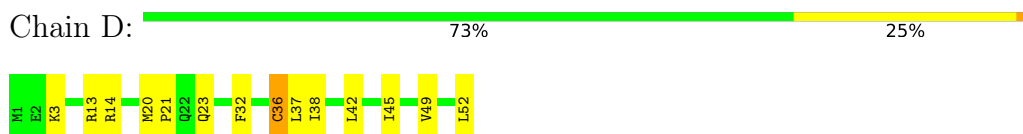
- Molecule 1: Cardiac phospholamban



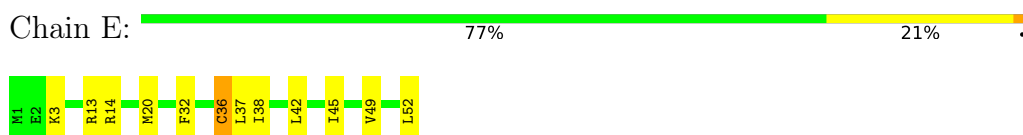
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

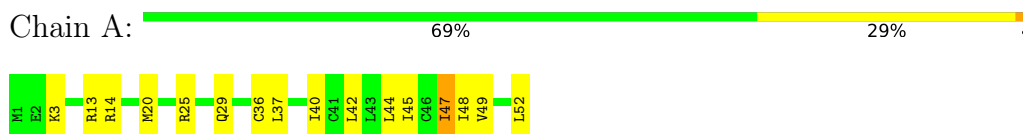


- Molecule 1: Cardiac phospholamban



4.2.162 Score per residue for model 162

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.163 Score per residue for model 163

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

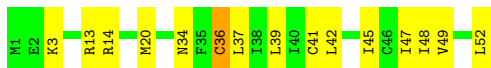


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



4.2.164 Score per residue for model 164

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

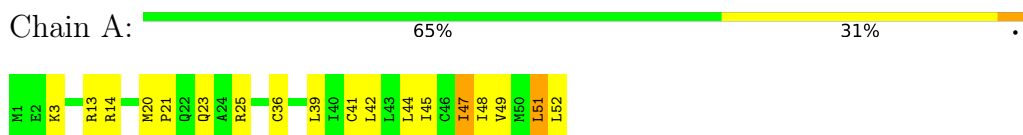


- Molecule 1: Cardiac phospholamban

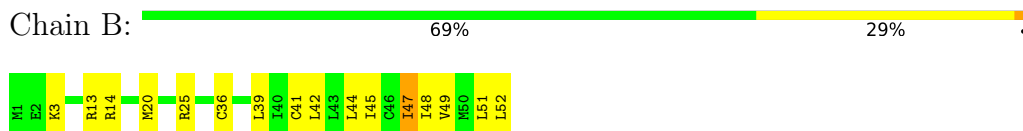


4.2.165 Score per residue for model 165

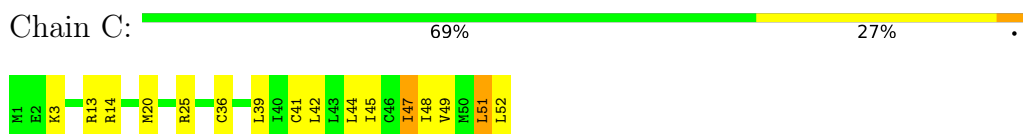
- Molecule 1: Cardiac phospholamban



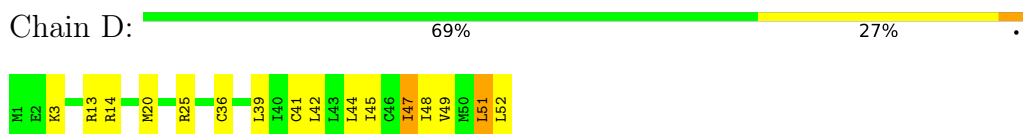
- Molecule 1: Cardiac phospholamban



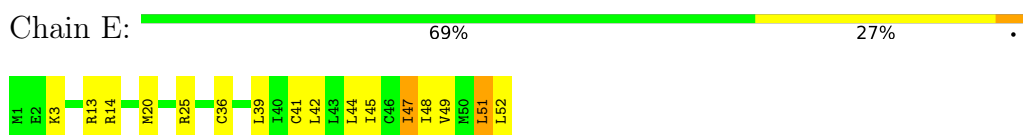
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

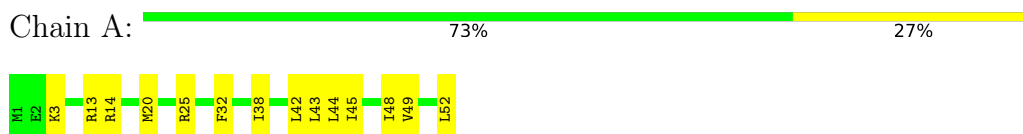


- Molecule 1: Cardiac phospholamban



4.2.166 Score per residue for model 166

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.167 Score per residue for model 167

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



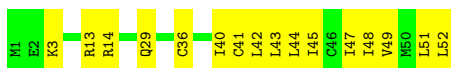


- Molecule 1: Cardiac phospholamban



4.2.168 Score per residue for model 168

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

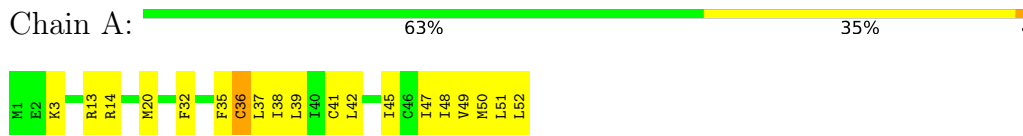


- Molecule 1: Cardiac phospholamban

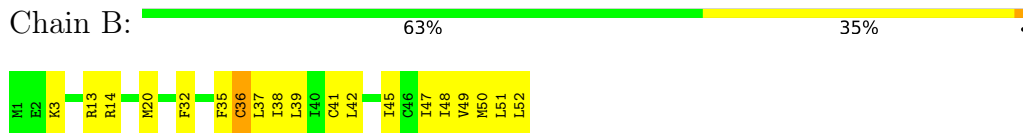


4.2.169 Score per residue for model 169

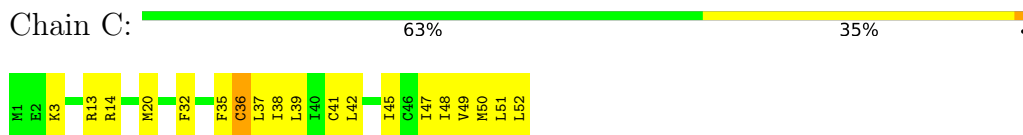
- Molecule 1: Cardiac phospholamban



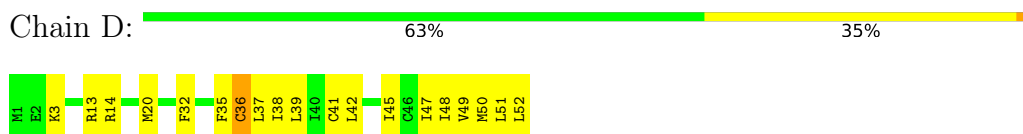
- Molecule 1: Cardiac phospholamban



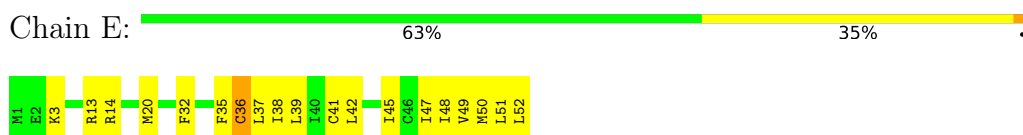
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

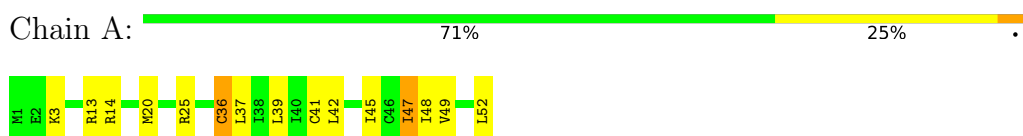


- Molecule 1: Cardiac phospholamban



4.2.170 Score per residue for model 170

- Molecule 1: Cardiac phospholamban

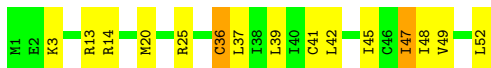


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

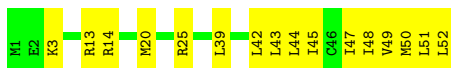


- Molecule 1: Cardiac phospholamban

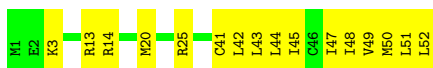


4.2.171 Score per residue for model 171

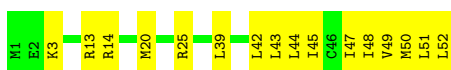
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

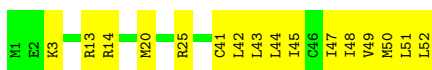


- Molecule 1: Cardiac phospholamban

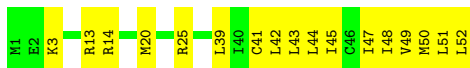


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban

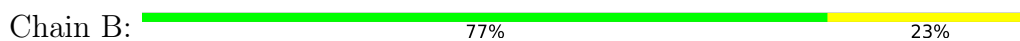


4.2.172 Score per residue for model 172

- Molecule 1: Cardiac phospholamban



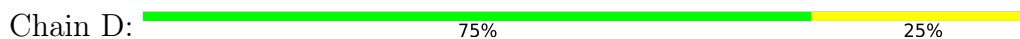
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

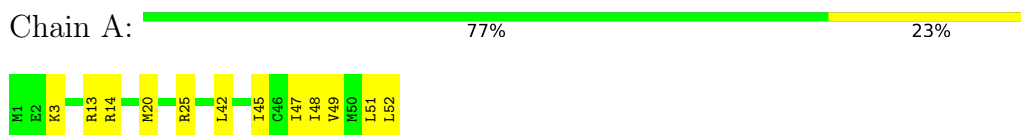


- Molecule 1: Cardiac phospholamban

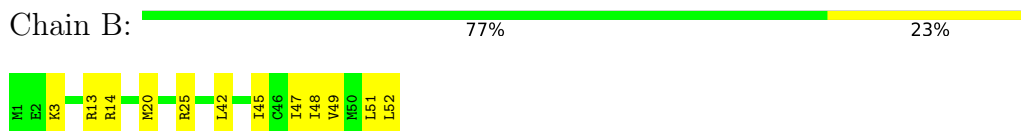


4.2.173 Score per residue for model 173

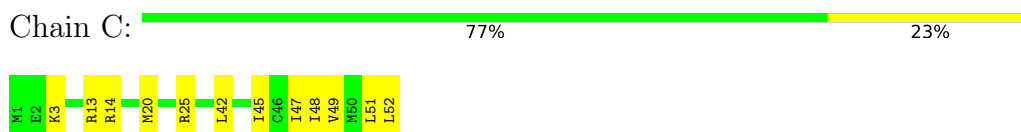
- Molecule 1: Cardiac phospholamban



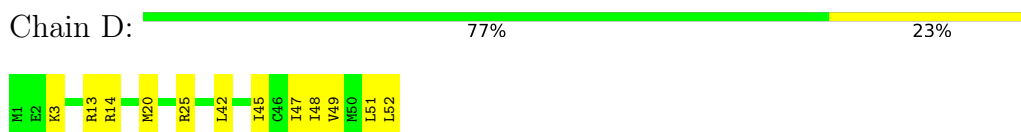
- Molecule 1: Cardiac phospholamban



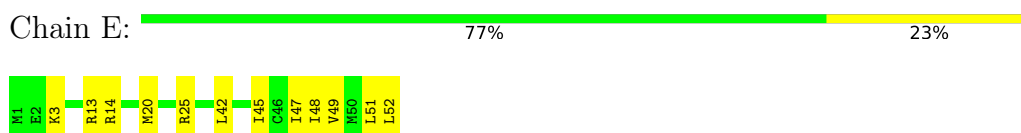
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

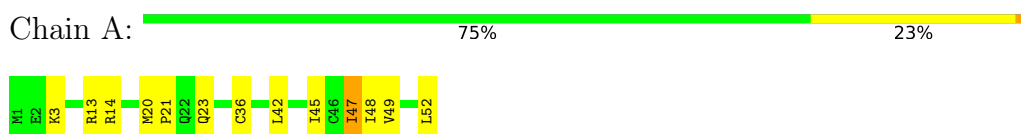


- Molecule 1: Cardiac phospholamban

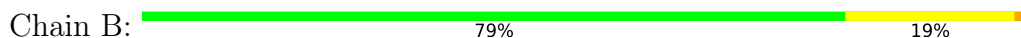


4.2.174 Score per residue for model 174

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

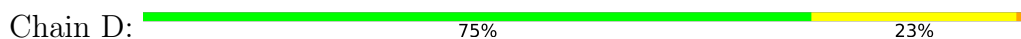




- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.175 Score per residue for model 175

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

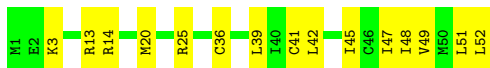


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



4.2.176 Score per residue for model 176

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



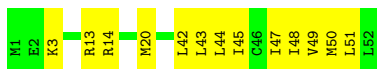
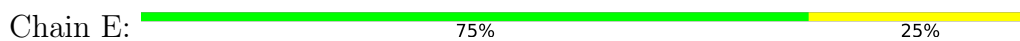
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

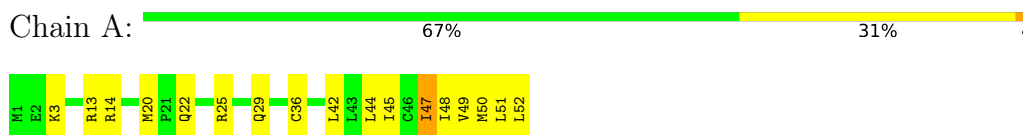


- Molecule 1: Cardiac phospholamban

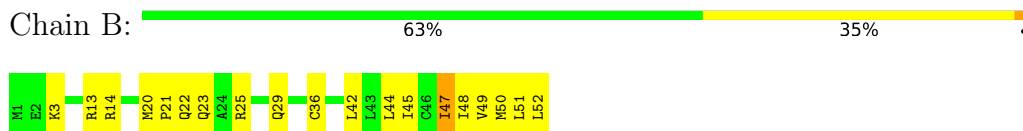


4.2.177 Score per residue for model 177

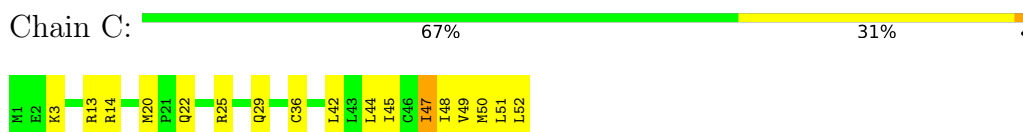
- Molecule 1: Cardiac phospholamban



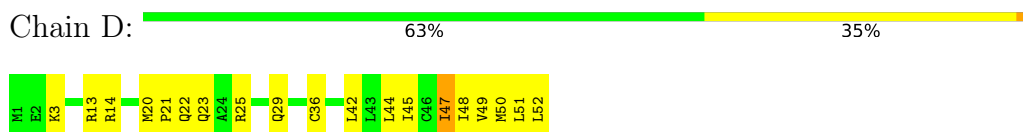
- Molecule 1: Cardiac phospholamban



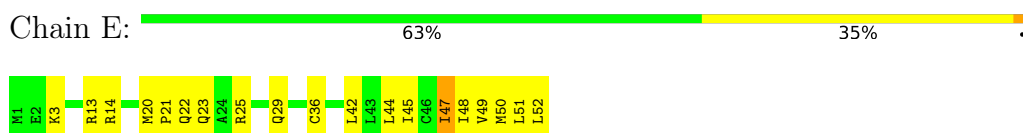
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

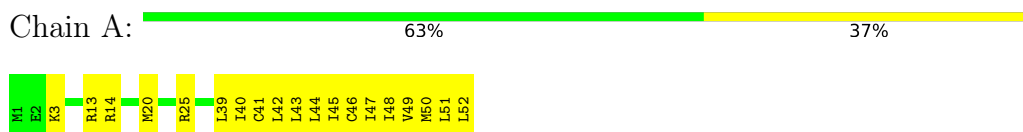


- Molecule 1: Cardiac phospholamban



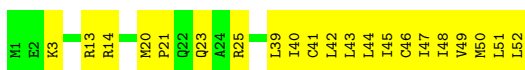
4.2.178 Score per residue for model 178

- Molecule 1: Cardiac phospholamban

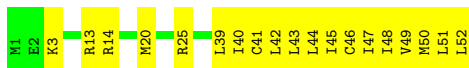


- Molecule 1: Cardiac phospholamban

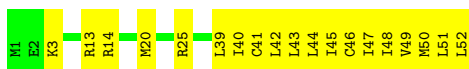




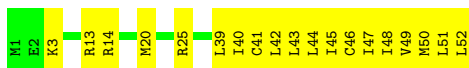
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

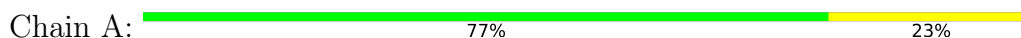


- Molecule 1: Cardiac phospholamban

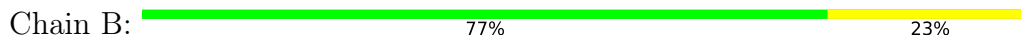


4.2.179 Score per residue for model 179

- Molecule 1: Cardiac phospholamban



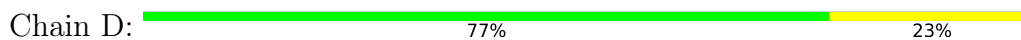
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

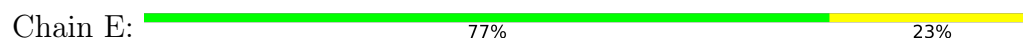


- Molecule 1: Cardiac phospholamban





- Molecule 1: Cardiac phospholamban



4.2.180 Score per residue for model 180

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

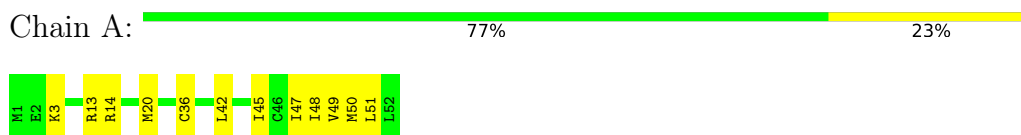


- Molecule 1: Cardiac phospholamban

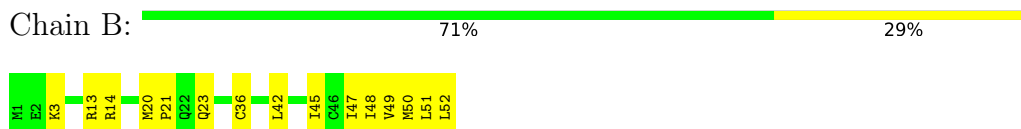


4.2.181 Score per residue for model 181

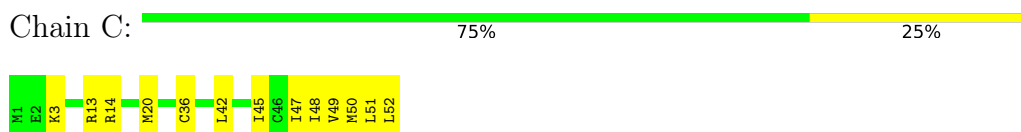
- Molecule 1: Cardiac phospholamban



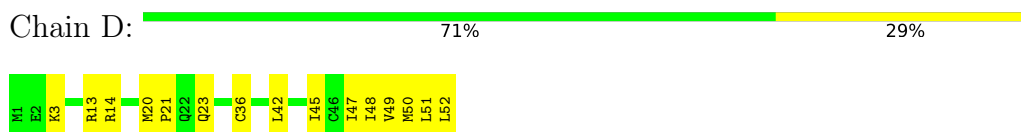
- Molecule 1: Cardiac phospholamban



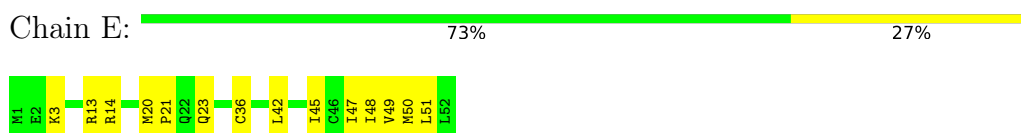
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

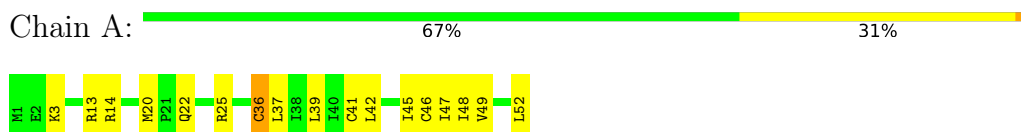


- Molecule 1: Cardiac phospholamban



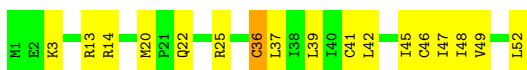
4.2.182 Score per residue for model 182

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

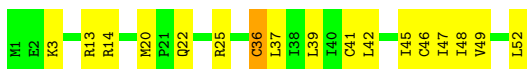




- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



4.2.183 Score per residue for model 183

- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban

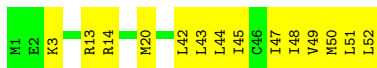


- Molecule 1: Cardiac phospholamban



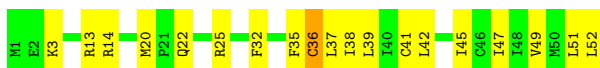


- Molecule 1: Cardiac phospholamban

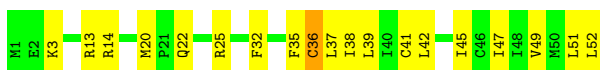


4.2.184 Score per residue for model 184

- Molecule 1: Cardiac phospholamban



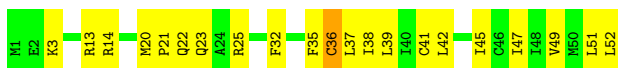
- Molecule 1: Cardiac phospholamban



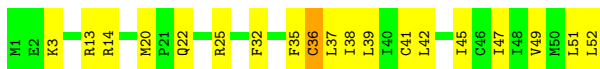
- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



- Molecule 1: Cardiac phospholamban



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Complete SCS search, Energy-minimization.*

Of the 184 calculated structures, 184 were deposited, based on the following criterion: *All calculated structures were submitted. Our method guarantees that the ensemble represents all structures that satisfy the data and have good vdW packing within a user-defined similarity level (chosen as 1 Å)..*

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

Software name	Classification	Version
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	424	475	475	26±15
1	B	424	475	475	26±15
1	C	424	475	475	26±15
1	D	424	475	475	26±15
1	E	423	475	475	26±15
All	All	389896	436810	436810	14112

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LEU:HD23	1:E:48:ILE:HD12	1.12	1.17	66	33
1:A:48:ILE:HD12	1:B:43:LEU:HD23	1.12	1.17	66	33
1:D:48:ILE:HD12	1:E:43:LEU:HD23	1.11	1.17	66	33
1:A:48:ILE:CD1	1:B:43:LEU:HD23	1.10	1.76	56	38
1:D:48:ILE:CD1	1:E:43:LEU:HD23	1.09	1.76	56	38
1:A:43:LEU:HD23	1:E:48:ILE:CD1	1.09	1.76	56	38
1:C:48:ILE:HD12	1:D:43:LEU:HD23	1.09	1.14	112	33
1:B:48:ILE:CD1	1:C:43:LEU:HD23	1.09	1.76	56	38
1:C:48:ILE:CD1	1:D:43:LEU:HD23	1.08	1.76	56	38
1:C:48:ILE:HD12	1:D:43:LEU:CD2	1.07	1.79	56	38

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:48:ILE:HD12	1:E:43:LEU:CD2	1.07	1.79	56	39
1:B:48:ILE:HD12	1:C:43:LEU:HD23	1.07	1.17	66	33
1:B:48:ILE:HD12	1:C:43:LEU:CD2	1.06	1.79	56	40
1:A:43:LEU:CD2	1:E:48:ILE:HD12	1.06	1.79	56	40
1:A:48:ILE:HD12	1:B:43:LEU:CD2	1.06	1.79	56	39
1:A:44:LEU:HB2	1:B:43:LEU:HD13	1.00	1.34	36	37
1:A:43:LEU:HD13	1:E:44:LEU:HB2	0.99	1.34	36	37
1:C:44:LEU:HB2	1:D:43:LEU:HD13	0.98	1.33	36	37
1:A:43:LEU:HD13	1:E:44:LEU:CB	0.98	1.89	73	17
1:A:44:LEU:CB	1:B:43:LEU:HD13	0.98	1.88	73	17
1:B:44:LEU:CB	1:C:43:LEU:HD13	0.98	1.88	73	17
1:C:44:LEU:CB	1:D:43:LEU:HD13	0.98	1.88	73	17
1:D:44:LEU:CB	1:E:43:LEU:HD13	0.97	1.88	73	18
1:B:44:LEU:HB2	1:C:43:LEU:HD13	0.95	1.34	36	37
1:D:44:LEU:HB2	1:E:43:LEU:HD13	0.95	1.34	36	37
1:B:37:LEU:HD13	1:C:36:CYS:CB	0.89	1.97	19	9
1:C:37:LEU:HD13	1:D:36:CYS:CB	0.89	1.97	19	9
1:D:37:LEU:HD13	1:E:36:CYS:CB	0.89	1.97	19	9
1:A:37:LEU:HD13	1:B:36:CYS:CB	0.89	1.97	19	9
1:A:36:CYS:CB	1:E:37:LEU:HD13	0.88	1.97	19	9
1:A:47:ILE:HG22	1:E:51:LEU:HD12	0.88	1.44	129	5
1:A:32:PHE:CE1	1:E:37:LEU:HD12	0.88	2.04	147	13
1:D:48:ILE:CD1	1:E:43:LEU:HD22	0.88	1.99	6	9
1:C:37:LEU:HD12	1:D:32:PHE:CE1	0.87	2.04	147	13
1:A:43:LEU:HD22	1:E:48:ILE:HD12	0.87	1.47	71	30
1:B:48:ILE:CD1	1:C:43:LEU:HD22	0.87	1.99	6	9
1:A:48:ILE:CD1	1:B:43:LEU:HD22	0.87	1.99	6	8
1:A:37:LEU:HD12	1:B:32:PHE:CE1	0.87	2.04	147	12
1:B:48:ILE:HD12	1:C:43:LEU:HD22	0.86	1.47	71	29
1:D:37:LEU:HD12	1:E:32:PHE:CE1	0.86	2.04	147	13
1:A:51:LEU:HD12	1:B:50:MET:HB2	0.86	1.45	84	1
1:C:48:ILE:HD12	1:D:43:LEU:HD22	0.86	1.47	71	30
1:C:48:ILE:CD1	1:D:43:LEU:HD22	0.86	1.99	6	9
1:B:37:LEU:HD12	1:C:32:PHE:CE1	0.86	2.05	147	13
1:A:48:ILE:HG12	1:B:47:ILE:HG23	0.86	1.48	45	13
1:A:43:LEU:HD22	1:E:48:ILE:CD1	0.85	1.99	6	9
1:D:48:ILE:HD12	1:E:43:LEU:HD22	0.85	1.47	71	30
1:A:37:LEU:HD13	1:B:33:ILE:HA	0.85	1.49	38	8
1:D:48:ILE:HG12	1:E:47:ILE:HG23	0.84	1.48	45	13
1:A:47:ILE:HG23	1:E:48:ILE:CG1	0.84	2.03	45	4
1:D:37:LEU:HD13	1:E:33:ILE:HA	0.84	1.49	38	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:48:ILE:CG1	1:D:47:ILE:HG23	0.84	2.03	45	3
1:A:33:ILE:HA	1:E:37:LEU:HD13	0.84	1.49	38	8
1:D:45:ILE:HD11	1:E:39:LEU:HD21	0.84	1.49	59	14
1:C:37:LEU:HD13	1:D:33:ILE:HA	0.84	1.49	38	8
1:A:48:ILE:HD12	1:B:43:LEU:HD22	0.84	1.47	71	29
1:C:48:ILE:HG12	1:D:47:ILE:HG23	0.84	1.48	45	14
1:A:48:ILE:CG1	1:B:47:ILE:HG23	0.84	2.03	45	4
1:B:51:LEU:HD12	1:C:50:MET:HB2	0.84	1.50	147	1
1:A:42:LEU:HA	1:A:45:ILE:HD12	0.83	1.50	68	183
1:A:45:ILE:HD11	1:B:39:LEU:HD21	0.83	1.49	59	14
1:D:42:LEU:HA	1:D:45:ILE:HD12	0.83	1.50	68	183
1:B:42:LEU:HA	1:B:45:ILE:HD12	0.83	1.50	68	184
1:C:42:LEU:HA	1:C:45:ILE:HD12	0.83	1.50	68	184
1:B:48:ILE:HG12	1:C:47:ILE:HG23	0.83	1.48	45	13
1:A:38:ILE:HD11	1:B:32:PHE:CZ	0.83	2.09	13	7
1:C:38:ILE:HD11	1:D:32:PHE:CZ	0.83	2.09	13	7
1:C:38:ILE:HG12	1:D:32:PHE:CZ	0.83	2.09	28	42
1:A:38:ILE:HG12	1:B:32:PHE:CZ	0.83	2.09	28	41
1:D:38:ILE:HG12	1:E:32:PHE:CZ	0.83	2.09	28	41
1:D:38:ILE:HD11	1:E:32:PHE:CZ	0.83	2.09	13	7
1:B:48:ILE:CG1	1:C:47:ILE:HG23	0.83	2.03	45	3
1:B:45:ILE:HD11	1:C:39:LEU:HD21	0.82	1.49	59	14
1:D:48:ILE:CG1	1:E:47:ILE:HG23	0.82	2.03	45	3
1:C:45:ILE:HD11	1:D:39:LEU:HD21	0.82	1.49	59	14
1:B:51:LEU:HD22	1:C:51:LEU:CD2	0.82	2.04	84	12
1:B:37:LEU:HD13	1:C:33:ILE:HA	0.82	1.49	38	8
1:C:51:LEU:CD1	1:D:47:ILE:HG22	0.82	2.04	129	6
1:A:40:ILE:HD11	1:E:41:CYS:SG	0.82	2.15	5	21
1:A:32:PHE:CZ	1:E:38:ILE:HD11	0.82	2.09	13	7
1:C:37:LEU:HD22	1:D:36:CYS:SG	0.82	2.15	69	37
1:A:38:ILE:CG1	1:B:32:PHE:CZ	0.82	2.63	22	39
1:A:47:ILE:HG23	1:E:48:ILE:HG12	0.82	1.48	45	14
1:B:38:ILE:CG1	1:C:32:PHE:CZ	0.82	2.63	22	41
1:A:37:LEU:HD22	1:B:36:CYS:SG	0.81	2.15	69	36
1:A:39:LEU:HD21	1:E:45:ILE:HD11	0.81	1.50	37	14
1:D:48:ILE:HD11	1:E:47:ILE:HG12	0.81	1.52	15	39
1:B:45:ILE:HG12	1:C:43:LEU:HD21	0.81	1.52	44	17
1:B:38:ILE:HD11	1:C:32:PHE:CZ	0.81	2.09	13	7
1:D:38:ILE:CG1	1:E:32:PHE:CZ	0.81	2.63	22	41
1:B:37:LEU:HD22	1:C:36:CYS:SG	0.81	2.15	69	36
1:C:41:CYS:SG	1:D:40:ILE:HD11	0.81	2.15	5	21

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:41:CYS:SG	1:E:40:ILE:HD11	0.81	2.15	5	21
1:A:32:PHE:CZ	1:E:38:ILE:HG12	0.81	2.09	28	42
1:A:45:ILE:HG12	1:B:43:LEU:HD21	0.81	1.53	32	16
1:A:41:CYS:SG	1:B:40:ILE:HD11	0.81	2.15	5	21
1:B:38:ILE:HG12	1:C:32:PHE:CZ	0.81	2.09	28	41
1:A:43:LEU:HD21	1:E:45:ILE:HG12	0.81	1.52	44	17
1:C:45:ILE:HG12	1:D:43:LEU:HD21	0.81	1.53	32	16
1:A:36:CYS:SG	1:E:37:LEU:HD22	0.81	2.15	69	36
1:E:42:LEU:HA	1:E:45:ILE:HD12	0.81	1.50	68	184
1:A:32:PHE:CZ	1:E:38:ILE:CG1	0.81	2.63	22	40
1:C:38:ILE:CG1	1:D:32:PHE:CZ	0.81	2.63	22	41
1:D:37:LEU:HD22	1:E:36:CYS:SG	0.81	2.15	69	36
1:B:41:CYS:SG	1:C:40:ILE:HD11	0.81	2.15	5	22
1:D:45:ILE:HG12	1:E:43:LEU:HD21	0.81	1.52	44	16
1:B:48:ILE:HD11	1:C:47:ILE:HG12	0.80	1.52	15	38
1:A:38:ILE:HG23	1:B:32:PHE:CZ	0.80	2.11	27	8
1:C:38:ILE:HG23	1:D:32:PHE:CZ	0.80	2.11	27	8
1:A:32:PHE:CE1	1:E:38:ILE:HG13	0.80	2.12	28	18
1:A:38:ILE:HG13	1:B:32:PHE:CE1	0.80	2.12	28	17
1:B:38:ILE:HG13	1:C:32:PHE:CE1	0.80	2.12	28	16
1:C:38:ILE:HG13	1:D:32:PHE:CE1	0.80	2.12	28	16
1:A:32:PHE:CZ	1:E:38:ILE:HG23	0.80	2.11	27	8
1:D:38:ILE:HG23	1:E:32:PHE:CZ	0.80	2.11	27	8
1:D:38:ILE:HG13	1:E:32:PHE:CE1	0.80	2.12	28	16
1:B:51:LEU:HD22	1:C:51:LEU:HD22	0.80	1.53	84	1
1:B:38:ILE:HG23	1:C:32:PHE:CZ	0.79	2.11	27	8
1:A:48:ILE:HD11	1:B:47:ILE:HG12	0.79	1.52	15	39
1:B:37:LEU:HD13	1:C:36:CYS:HB3	0.79	1.53	19	5
1:D:51:LEU:HD12	1:E:50:MET:HB2	0.79	1.54	129	2
1:D:37:LEU:HB3	1:E:36:CYS:SG	0.79	2.17	51	45
1:A:47:ILE:HG12	1:E:48:ILE:HD11	0.78	1.52	15	38
1:A:37:LEU:HD13	1:B:36:CYS:HB3	0.78	1.53	19	5
1:A:36:CYS:HB3	1:E:37:LEU:HD13	0.78	1.53	19	5
1:B:44:LEU:HB3	1:C:43:LEU:HD22	0.78	1.54	65	16
1:C:48:ILE:HD11	1:D:47:ILE:HG12	0.78	1.52	15	39
1:D:37:LEU:HD13	1:E:36:CYS:HB3	0.78	1.53	19	5
1:C:38:ILE:CG1	1:D:32:PHE:CE1	0.78	2.67	7	28
1:C:37:LEU:HD13	1:D:36:CYS:HB3	0.78	1.53	19	5
1:A:44:LEU:CD1	1:B:40:ILE:HG23	0.78	2.09	59	47
1:D:38:ILE:CG1	1:E:32:PHE:CE1	0.78	2.67	7	29
1:D:44:LEU:HB3	1:E:43:LEU:HD22	0.78	1.54	65	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:51:LEU:HD13	1:C:47:ILE:HA	0.78	1.56	26	8
1:A:32:PHE:CE1	1:E:38:ILE:CG1	0.78	2.67	7	29
1:C:44:LEU:HB3	1:D:43:LEU:HD22	0.78	1.54	65	15
1:C:37:LEU:HB3	1:D:36:CYS:SG	0.78	2.18	51	45
1:A:40:ILE:HG23	1:E:44:LEU:CD1	0.78	2.09	59	47
1:D:41:CYS:SG	1:E:39:LEU:HD22	0.77	2.20	35	21
1:A:38:ILE:CG1	1:B:32:PHE:CE1	0.77	2.67	7	28
1:D:38:ILE:HA	1:E:36:CYS:SG	0.77	2.19	59	6
1:D:44:LEU:CD1	1:E:40:ILE:HG23	0.77	2.10	37	47
1:B:38:ILE:HA	1:C:36:CYS:SG	0.77	2.20	37	6
1:A:43:LEU:HD22	1:E:44:LEU:HB3	0.77	1.54	65	16
1:B:44:LEU:CD1	1:C:40:ILE:HG23	0.77	2.09	59	47
1:A:41:CYS:SG	1:B:39:LEU:CD2	0.77	2.74	1	41
1:B:41:CYS:SG	1:C:39:LEU:HD22	0.77	2.20	35	21
1:A:36:CYS:SG	1:E:38:ILE:HA	0.77	2.20	37	6
1:B:38:ILE:CG1	1:C:32:PHE:CE1	0.77	2.67	7	28
1:D:38:ILE:HG13	1:E:32:PHE:CZ	0.77	2.15	10	24
1:D:41:CYS:SG	1:E:39:LEU:CD2	0.76	2.73	1	43
1:A:38:ILE:HG13	1:B:32:PHE:CZ	0.76	2.15	10	24
1:C:41:CYS:SG	1:D:39:LEU:CD2	0.76	2.73	1	43
1:A:38:ILE:HA	1:B:36:CYS:SG	0.76	2.20	59	6
1:C:38:ILE:HA	1:D:36:CYS:SG	0.76	2.20	37	6
1:A:44:LEU:HB3	1:B:43:LEU:HD22	0.76	1.54	65	15
1:B:41:CYS:SG	1:C:39:LEU:CD2	0.76	2.73	1	43
1:C:44:LEU:CD1	1:D:40:ILE:HG23	0.76	2.09	59	47
1:A:41:CYS:SG	1:B:39:LEU:HD22	0.76	2.20	35	21
1:B:38:ILE:HG13	1:C:32:PHE:CZ	0.76	2.15	10	24
1:D:51:LEU:HD13	1:E:47:ILE:HA	0.76	1.56	26	7
1:A:39:LEU:CD2	1:E:41:CYS:SG	0.76	2.74	1	42
1:A:39:LEU:HD22	1:E:41:CYS:SG	0.76	2.20	35	21
1:B:37:LEU:HB3	1:C:36:CYS:SG	0.76	2.21	10	46
1:D:38:ILE:HA	1:D:41:CYS:SG	0.76	2.21	47	22
1:E:38:ILE:HA	1:E:41:CYS:SG	0.76	2.21	47	22
1:A:38:ILE:HA	1:A:41:CYS:SG	0.76	2.21	47	22
1:C:51:LEU:HD13	1:D:47:ILE:HA	0.76	1.56	26	7
1:A:36:CYS:SG	1:E:37:LEU:HB3	0.76	2.21	105	44
1:A:51:LEU:HD13	1:B:47:ILE:HA	0.76	1.56	26	8
1:B:44:LEU:HD11	1:C:40:ILE:HG23	0.75	1.58	36	26
1:A:37:LEU:HB3	1:B:36:CYS:SG	0.75	2.22	105	46
1:B:38:ILE:HA	1:B:41:CYS:SG	0.75	2.21	9	22
1:C:41:CYS:SG	1:D:39:LEU:HD22	0.75	2.20	35	21

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:38:ILE:HA	1:C:41:CYS:SG	0.75	2.21	47	22
1:C:48:ILE:CD1	1:D:43:LEU:CD2	0.75	2.65	52	15
1:C:38:ILE:HG13	1:D:32:PHE:CZ	0.75	2.15	10	24
1:A:32:PHE:CZ	1:E:38:ILE:HG13	0.75	2.17	22	25
1:A:47:ILE:HA	1:E:51:LEU:HD13	0.75	1.56	26	7
1:A:48:ILE:CD1	1:B:43:LEU:CD2	0.74	2.65	52	16
1:B:48:ILE:CD1	1:C:43:LEU:CD2	0.74	2.65	52	16
1:D:44:LEU:HD11	1:E:40:ILE:HG23	0.74	1.58	36	26
1:A:40:ILE:HG23	1:E:44:LEU:HD11	0.74	1.58	36	26
1:A:43:LEU:CD2	1:E:48:ILE:CD1	0.74	2.65	52	15
1:A:51:LEU:HD22	1:B:51:LEU:CD2	0.74	2.13	12	11
1:D:51:LEU:HD22	1:E:51:LEU:CD2	0.74	2.13	12	12
1:C:44:LEU:HD11	1:D:40:ILE:HG23	0.74	1.58	36	26
1:A:44:LEU:HD11	1:B:40:ILE:HG23	0.74	1.58	36	27
1:C:51:LEU:HD22	1:D:51:LEU:CD2	0.73	2.13	12	12
1:D:48:ILE:CD1	1:E:43:LEU:CD2	0.73	2.66	30	15
1:E:36:CYS:SG	1:E:37:LEU:HD23	0.73	2.24	1	5
1:C:36:CYS:SG	1:C:37:LEU:HD23	0.73	2.24	1	5
1:D:48:ILE:CG1	1:E:47:ILE:CG1	0.73	2.67	3	16
1:B:36:CYS:SG	1:B:37:LEU:HD23	0.73	2.24	1	5
1:D:38:ILE:HG12	1:E:32:PHE:CE1	0.73	2.19	41	35
1:D:36:CYS:SG	1:D:37:LEU:HD23	0.72	2.24	1	5
1:A:47:ILE:CG1	1:E:48:ILE:CG1	0.72	2.67	3	17
1:C:51:LEU:HD11	1:D:47:ILE:HG23	0.72	1.61	175	23
1:A:38:ILE:HG12	1:B:32:PHE:CE1	0.72	2.19	41	36
1:B:38:ILE:HG12	1:C:32:PHE:CE1	0.72	2.19	101	36
1:A:51:LEU:CD2	1:E:51:LEU:HD22	0.72	2.13	12	14
1:C:38:ILE:HG12	1:D:32:PHE:CE1	0.72	2.19	41	36
1:A:36:CYS:SG	1:A:37:LEU:HD23	0.72	2.24	1	5
1:B:48:ILE:CG1	1:C:47:ILE:CG1	0.72	2.67	3	16
1:A:32:PHE:CE1	1:E:38:ILE:HG12	0.72	2.19	101	36
1:A:47:ILE:HG23	1:E:51:LEU:CD1	0.72	2.15	3	24
1:D:51:LEU:HD11	1:E:47:ILE:HG23	0.72	1.61	175	23
1:A:43:LEU:HB3	1:E:44:LEU:HB3	0.72	1.62	36	21
1:A:47:ILE:HG23	1:E:51:LEU:HD11	0.72	1.61	175	22
1:A:48:ILE:CG1	1:B:47:ILE:CG1	0.72	2.67	3	16
1:A:51:LEU:CD1	1:B:47:ILE:HG23	0.72	2.15	3	24
1:C:44:LEU:HB3	1:D:43:LEU:HB3	0.71	1.62	36	20
1:C:37:LEU:HD13	1:D:36:CYS:SG	0.71	2.26	11	19
1:C:48:ILE:CG1	1:D:47:ILE:CG1	0.71	2.67	3	16
1:B:51:LEU:CD1	1:C:47:ILE:HG23	0.71	2.15	3	27

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:37:LEU:HD13	1:E:36:CYS:SG	0.71	2.26	11	19
1:B:51:LEU:HD11	1:C:47:ILE:HG23	0.71	1.61	175	22
1:A:37:LEU:HD13	1:B:36:CYS:SG	0.71	2.26	11	19
1:C:37:LEU:HB3	1:D:36:CYS:HB2	0.71	1.62	1	13
1:B:51:LEU:HD13	1:C:51:LEU:HG	0.70	1.63	147	8
1:D:51:LEU:CD1	1:E:47:ILE:HG23	0.70	2.15	3	23
1:B:37:LEU:HB3	1:C:36:CYS:HB2	0.70	1.63	1	12
1:B:37:LEU:HD13	1:C:36:CYS:SG	0.70	2.26	11	19
1:A:51:LEU:HD11	1:B:47:ILE:HG23	0.70	1.61	175	23
1:D:48:ILE:HD11	1:E:43:LEU:O	0.70	1.86	20	22
1:C:51:LEU:CD1	1:D:47:ILE:HG23	0.70	2.15	3	24
1:B:51:LEU:HD13	1:C:51:LEU:HD21	0.70	1.63	84	3
1:A:36:CYS:HB2	1:E:37:LEU:HB3	0.70	1.63	1	13
1:D:51:LEU:HB3	1:E:50:MET:CB	0.70	2.17	48	24
1:D:34:ASN:HA	1:D:37:LEU:HD12	0.70	1.64	38	16
1:B:37:LEU:HB3	1:C:36:CYS:CB	0.70	2.17	1	21
1:D:37:LEU:HB3	1:E:36:CYS:HB2	0.70	1.63	1	12
1:A:48:ILE:HD11	1:B:43:LEU:O	0.70	1.86	20	21
1:B:48:ILE:HD11	1:C:43:LEU:O	0.70	1.86	20	22
1:B:34:ASN:HA	1:B:37:LEU:HD12	0.70	1.64	38	14
1:A:36:CYS:SG	1:E:37:LEU:HD13	0.70	2.26	11	18
1:A:43:LEU:O	1:E:48:ILE:HD11	0.70	1.86	20	22
1:A:48:ILE:HD11	1:B:43:LEU:HD23	0.70	1.64	140	7
1:A:36:CYS:CB	1:E:37:LEU:HB3	0.70	2.17	1	21
1:A:37:LEU:HB3	1:B:36:CYS:HB2	0.70	1.62	1	12
1:C:37:LEU:HB3	1:D:36:CYS:CB	0.70	2.17	1	21
1:A:51:LEU:HB3	1:B:50:MET:CB	0.70	2.17	48	24
1:C:48:ILE:HD11	1:D:43:LEU:O	0.70	1.86	20	21
1:A:44:LEU:HB3	1:B:43:LEU:HB3	0.70	1.62	36	20
1:B:44:LEU:HB3	1:C:43:LEU:HB3	0.70	1.62	36	21
1:B:51:LEU:CD1	1:C:47:ILE:HG22	0.70	2.17	31	5
1:A:34:ASN:HA	1:A:37:LEU:HD12	0.69	1.64	38	16
1:D:44:LEU:HB3	1:E:43:LEU:HB3	0.69	1.62	36	20
1:D:51:LEU:CD1	1:E:47:ILE:HG22	0.69	2.17	31	5
1:D:37:LEU:HB3	1:E:36:CYS:CB	0.69	2.17	1	21
1:C:48:ILE:HD11	1:D:47:ILE:CD1	0.69	2.17	17	10
1:A:43:LEU:HD23	1:E:48:ILE:HD11	0.69	1.64	140	9
1:C:51:LEU:HB3	1:D:50:MET:CB	0.69	2.17	48	24
1:B:48:ILE:HD11	1:C:47:ILE:CD1	0.69	2.17	17	11
1:D:48:ILE:HD11	1:E:47:ILE:CD1	0.69	2.17	17	12
1:A:37:LEU:HB3	1:B:36:CYS:CB	0.69	2.17	1	21

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:37:LEU:HD12	1:E:32:PHE:HE1	0.69	1.48	147	4
1:A:51:LEU:CD1	1:B:47:ILE:HG22	0.69	2.17	31	6
1:D:48:ILE:CG1	1:E:47:ILE:HG12	0.69	2.18	31	37
1:A:47:ILE:CD1	1:E:48:ILE:HD11	0.69	2.17	17	11
1:A:48:ILE:HG23	1:B:50:MET:HG3	0.69	1.64	147	2
1:D:36:CYS:SG	1:D:40:ILE:HD12	0.69	2.28	54	21
1:E:34:ASN:HA	1:E:37:LEU:HD12	0.69	1.64	38	17
1:A:48:ILE:HD11	1:B:47:ILE:CD1	0.69	2.17	17	12
1:C:48:ILE:HD11	1:D:43:LEU:HD23	0.69	1.64	140	8
1:C:48:ILE:CG1	1:D:47:ILE:HG12	0.69	2.18	31	37
1:A:47:ILE:HD11	1:E:48:ILE:HD11	0.69	1.65	75	7
1:A:50:MET:CB	1:E:51:LEU:HB3	0.69	2.17	48	24
1:B:51:LEU:HB3	1:C:50:MET:CB	0.69	2.17	48	24
1:A:36:CYS:SG	1:A:40:ILE:HD12	0.69	2.28	54	21
1:B:36:CYS:SG	1:B:40:ILE:HD12	0.68	2.28	54	22
1:A:32:PHE:HE1	1:E:37:LEU:HD12	0.68	1.48	147	4
1:E:36:CYS:SG	1:E:40:ILE:HD12	0.68	2.28	54	21
1:A:40:ILE:HG13	1:E:41:CYS:SG	0.68	2.29	40	21
1:A:41:CYS:SG	1:B:40:ILE:HG13	0.68	2.29	40	22
1:C:41:CYS:SG	1:D:40:ILE:HG13	0.68	2.29	40	21
1:B:48:ILE:HD11	1:C:43:LEU:HD23	0.68	1.64	140	9
1:B:45:ILE:CG1	1:C:43:LEU:HD21	0.68	2.19	106	14
1:D:45:ILE:CG1	1:E:43:LEU:HD21	0.68	2.18	106	13
1:A:47:ILE:HG12	1:E:48:ILE:CG1	0.68	2.18	31	36
1:B:48:ILE:CG1	1:C:47:ILE:HG12	0.68	2.18	31	34
1:A:47:ILE:HG22	1:E:51:LEU:CD1	0.68	2.17	31	6
1:C:48:ILE:CG1	1:D:47:ILE:HA	0.68	2.19	147	2
1:C:51:LEU:HD11	1:D:47:ILE:CG2	0.68	2.17	84	1
1:A:48:ILE:CG1	1:B:47:ILE:HG12	0.68	2.18	31	36
1:B:41:CYS:SG	1:C:40:ILE:HG13	0.68	2.28	40	22
1:C:45:ILE:CG1	1:D:43:LEU:HD21	0.68	2.18	106	14
1:B:44:LEU:CB	1:C:43:LEU:HD22	0.68	2.18	35	9
1:D:48:ILE:HD11	1:E:47:ILE:HD11	0.68	1.65	75	7
1:D:37:LEU:HD23	1:E:36:CYS:SG	0.68	2.29	125	10
1:A:43:LEU:HD21	1:E:45:ILE:CG1	0.68	2.19	106	14
1:A:46:CYS:CB	1:E:48:ILE:HD13	0.68	2.19	32	13
1:C:34:ASN:HA	1:C:37:LEU:HD12	0.68	1.64	38	15
1:D:44:LEU:CB	1:E:43:LEU:HD22	0.68	2.18	35	10
1:B:48:ILE:CG1	1:C:47:ILE:HA	0.68	2.19	147	2
1:A:45:ILE:CG1	1:B:43:LEU:HD21	0.68	2.18	106	14
1:C:48:ILE:HD13	1:D:46:CYS:CB	0.68	2.19	32	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:37:LEU:HD12	1:D:32:PHE:HE1	0.68	1.48	147	4
1:A:48:ILE:CG1	1:B:47:ILE:HA	0.68	2.18	147	2
1:A:32:PHE:CD1	1:E:37:LEU:HD12	0.68	2.24	19	9
1:C:36:CYS:SG	1:C:40:ILE:HD12	0.68	2.28	54	22
1:A:47:ILE:HA	1:E:48:ILE:CG1	0.68	2.19	147	2
1:C:44:LEU:CB	1:D:43:LEU:HD22	0.68	2.18	35	13
1:A:37:LEU:HD23	1:B:36:CYS:SG	0.68	2.28	125	10
1:C:37:LEU:HD12	1:D:32:PHE:CD1	0.67	2.24	19	9
1:A:48:ILE:HD11	1:B:47:ILE:HD11	0.67	1.65	75	7
1:A:43:LEU:HD22	1:E:44:LEU:CB	0.67	2.19	35	11
1:C:48:ILE:HD11	1:D:47:ILE:HD11	0.67	1.66	57	7
1:D:48:ILE:CG1	1:E:47:ILE:HD13	0.67	2.19	64	7
1:A:48:ILE:HD11	1:B:47:ILE:CG1	0.67	2.20	45	15
1:A:48:ILE:CG1	1:B:47:ILE:HD13	0.67	2.19	64	7
1:D:48:ILE:HD11	1:E:43:LEU:HD23	0.67	1.64	140	8
1:A:47:ILE:CG1	1:E:48:ILE:HD11	0.67	2.20	45	15
1:D:48:ILE:HD11	1:E:47:ILE:CG1	0.67	2.20	45	14
1:B:48:ILE:HD11	1:C:47:ILE:CG1	0.67	2.20	45	14
1:A:37:LEU:HD12	1:B:32:PHE:CD1	0.67	2.24	19	9
1:C:51:LEU:HD13	1:D:47:ILE:HG23	0.67	1.67	5	2
1:D:41:CYS:SG	1:E:40:ILE:HG13	0.67	2.29	40	21
1:A:39:LEU:HD23	1:E:41:CYS:SG	0.67	2.30	11	43
1:A:48:ILE:HD13	1:B:46:CYS:CB	0.67	2.19	32	12
1:A:47:ILE:HD13	1:E:48:ILE:CG1	0.67	2.19	64	6
1:B:48:ILE:HD11	1:C:47:ILE:HD11	0.67	1.65	75	7
1:B:48:ILE:HD13	1:C:46:CYS:CB	0.67	2.19	32	12
1:A:44:LEU:CB	1:B:43:LEU:HD22	0.67	2.19	35	12
1:B:37:LEU:HD12	1:C:32:PHE:CD1	0.67	2.24	19	9
1:C:48:ILE:HG13	1:D:47:ILE:CG1	0.67	2.20	3	10
1:B:48:ILE:CG1	1:C:47:ILE:HD13	0.67	2.19	64	7
1:B:48:ILE:HG13	1:C:47:ILE:CG1	0.67	2.20	3	10
1:B:36:CYS:SG	1:B:40:ILE:CD1	0.67	2.83	54	25
1:D:48:ILE:CG1	1:E:47:ILE:HA	0.67	2.20	147	2
1:A:48:ILE:HG13	1:B:47:ILE:CG1	0.66	2.20	3	10
1:A:36:CYS:SG	1:A:40:ILE:CD1	0.66	2.83	54	25
1:D:37:LEU:HD12	1:E:33:ILE:HG23	0.66	1.67	59	2
1:C:48:ILE:CG1	1:D:47:ILE:HD13	0.66	2.19	64	6
1:A:44:LEU:C	1:B:43:LEU:HD22	0.66	2.11	36	9
1:A:51:LEU:HG	1:E:51:LEU:HD13	0.66	1.67	129	9
1:D:48:ILE:HD13	1:E:46:CYS:CB	0.66	2.19	32	12
1:C:44:LEU:C	1:D:43:LEU:HD22	0.66	2.11	36	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:51:LEU:CD2	1:C:51:LEU:HD21	0.66	2.21	12	8
1:D:41:CYS:SG	1:E:39:LEU:HD23	0.66	2.30	11	42
1:B:37:LEU:HD12	1:C:32:PHE:HE1	0.66	1.48	147	4
1:A:51:LEU:HD21	1:E:51:LEU:CD2	0.66	2.21	12	8
1:D:51:LEU:CD2	1:E:51:LEU:HD21	0.66	2.21	12	8
1:B:38:ILE:CD1	1:C:32:PHE:CZ	0.66	2.79	33	6
1:A:43:LEU:HD22	1:E:44:LEU:C	0.66	2.11	36	9
1:D:37:LEU:HD12	1:E:32:PHE:CD1	0.66	2.24	19	9
1:C:48:ILE:HD11	1:D:47:ILE:CG1	0.66	2.20	45	15
1:A:41:CYS:SG	1:B:39:LEU:HD23	0.66	2.30	11	43
1:C:41:CYS:SG	1:D:39:LEU:HD23	0.66	2.30	11	43
1:D:48:ILE:HG13	1:E:47:ILE:CG1	0.66	2.20	3	10
1:E:36:CYS:SG	1:E:40:ILE:CD1	0.66	2.83	54	24
1:B:41:CYS:SG	1:C:39:LEU:HD23	0.66	2.30	11	43
1:C:36:CYS:SG	1:C:40:ILE:CD1	0.66	2.83	54	25
1:A:32:PHE:CZ	1:E:38:ILE:CD1	0.66	2.79	33	6
1:D:44:LEU:C	1:E:43:LEU:HD22	0.66	2.11	36	9
1:D:36:CYS:SG	1:D:40:ILE:CD1	0.66	2.83	54	25
1:D:38:ILE:CD1	1:E:32:PHE:CZ	0.66	2.79	33	5
1:B:44:LEU:HD22	1:C:44:LEU:CD2	0.66	2.21	32	7
1:D:44:LEU:HD22	1:E:44:LEU:CD2	0.66	2.21	32	7
1:C:51:LEU:CD2	1:D:51:LEU:HD21	0.66	2.20	12	8
1:A:44:LEU:HD22	1:B:44:LEU:CD2	0.66	2.21	32	7
1:A:44:LEU:CD2	1:E:44:LEU:HD22	0.66	2.21	32	7
1:A:51:LEU:HD12	1:B:47:ILE:HG22	0.66	1.68	60	5
1:A:51:LEU:HD13	1:B:47:ILE:HG23	0.65	1.67	5	2
1:A:37:LEU:HD12	1:B:33:ILE:HG23	0.65	1.67	59	2
1:C:38:ILE:CD1	1:D:32:PHE:CZ	0.65	2.79	33	5
1:B:51:LEU:HD13	1:C:51:LEU:CD2	0.65	2.21	84	4
1:B:38:ILE:HG23	1:C:32:PHE:HZ	0.65	1.51	102	6
1:A:47:ILE:CG1	1:E:48:ILE:HG13	0.65	2.20	3	10
1:A:51:LEU:CD2	1:B:51:LEU:HD21	0.65	2.20	12	8
1:A:38:ILE:CD1	1:B:32:PHE:CZ	0.65	2.79	33	6
1:A:37:LEU:HD12	1:B:32:PHE:HE1	0.65	1.48	147	4
1:B:44:LEU:C	1:C:43:LEU:HD22	0.65	2.11	36	10
1:B:44:LEU:HA	1:B:47:ILE:HG13	0.65	1.68	45	27
1:B:51:LEU:HD12	1:C:47:ILE:HG22	0.65	1.68	60	5
1:D:51:LEU:HD12	1:E:47:ILE:HG22	0.65	1.68	60	4
1:D:51:LEU:HD13	1:E:47:ILE:HG23	0.65	1.67	5	2
1:C:37:LEU:HD12	1:D:33:ILE:HG23	0.65	1.67	59	2
1:D:44:LEU:HA	1:D:47:ILE:HG13	0.65	1.68	45	28

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:51:LEU:HD13	1:C:47:ILE:HG23	0.65	1.67	5	2
1:C:44:LEU:HD22	1:D:44:LEU:CD2	0.65	2.21	32	7
1:C:51:LEU:HD12	1:D:47:ILE:HG22	0.65	1.68	60	4
1:A:32:PHE:HZ	1:E:38:ILE:HG23	0.65	1.51	102	6
1:A:47:ILE:HG23	1:E:51:LEU:HD13	0.65	1.67	5	2
1:A:38:ILE:HG23	1:B:32:PHE:HZ	0.65	1.51	102	6
1:B:51:LEU:HD12	1:C:50:MET:CB	0.64	2.20	147	1
1:D:49:VAL:HA	1:D:52:LEU:HD12	0.64	1.70	129	171
1:A:51:LEU:HD22	1:B:51:LEU:HD21	0.64	1.69	12	9
1:B:48:ILE:CD1	1:C:47:ILE:HG12	0.64	2.22	64	30
1:D:48:ILE:CD1	1:E:47:ILE:HG12	0.64	2.22	64	30
1:B:51:LEU:HD12	1:C:51:LEU:HD21	0.64	1.70	45	1
1:B:37:LEU:HD12	1:C:33:ILE:HG23	0.64	1.67	59	2
1:C:44:LEU:HA	1:C:47:ILE:HG13	0.64	1.68	45	28
1:D:37:LEU:HD13	1:E:33:ILE:HG23	0.64	1.70	41	3
1:A:33:ILE:HG23	1:E:37:LEU:HD12	0.64	1.67	59	2
1:D:38:ILE:HG23	1:E:32:PHE:HZ	0.64	1.51	102	6
1:B:51:LEU:HD22	1:C:51:LEU:HD21	0.64	1.69	12	8
1:C:51:LEU:HD12	1:D:47:ILE:HG23	0.64	1.70	25	5
1:C:51:LEU:HD22	1:D:51:LEU:HD21	0.64	1.69	12	9
1:A:48:ILE:CD1	1:B:47:ILE:HG12	0.64	2.23	29	29
1:C:48:ILE:CD1	1:D:47:ILE:HG12	0.64	2.23	29	31
1:A:37:LEU:HD13	1:B:33:ILE:HG23	0.64	1.70	41	3
1:C:38:ILE:HG23	1:D:32:PHE:HZ	0.64	1.50	102	6
1:A:47:ILE:HG12	1:E:48:ILE:CD1	0.64	2.23	29	29
1:D:41:CYS:HB3	1:E:39:LEU:CD2	0.64	2.23	106	20
1:A:50:MET:HG3	1:E:48:ILE:HG23	0.64	1.70	147	2
1:C:48:ILE:HG23	1:D:50:MET:HG3	0.64	1.70	147	2
1:E:44:LEU:HA	1:E:47:ILE:HG13	0.63	1.68	45	27
1:A:39:LEU:CD2	1:E:41:CYS:HB3	0.63	2.23	106	21
1:D:51:LEU:HD12	1:E:51:LEU:HD21	0.63	1.69	45	1
1:B:41:CYS:HB3	1:C:39:LEU:CD2	0.63	2.23	106	21
1:C:51:LEU:HD13	1:D:51:LEU:HG	0.63	1.70	84	7
1:A:33:ILE:HG23	1:E:37:LEU:HD13	0.63	1.69	41	4
1:A:47:ILE:HG23	1:E:51:LEU:HD12	0.63	1.69	25	5
1:A:51:LEU:HD21	1:E:51:LEU:HD22	0.63	1.69	12	8
1:D:51:LEU:HD12	1:E:47:ILE:HG23	0.63	1.70	25	5
1:C:51:LEU:HD12	1:D:51:LEU:HD21	0.63	1.70	45	1
1:C:44:LEU:HD12	1:D:43:LEU:HD13	0.63	1.71	65	5
1:A:51:LEU:HD12	1:B:51:LEU:HD21	0.63	1.70	45	1
1:D:51:LEU:HD11	1:E:47:ILE:CG2	0.63	2.24	147	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LEU:HD12	1:B:47:ILE:HG23	0.62	1.70	25	5
1:D:51:LEU:HD22	1:E:51:LEU:HD21	0.62	1.69	12	8
1:C:41:CYS:SG	1:D:36:CYS:HA	0.62	2.34	23	4
1:E:49:VAL:HA	1:E:52:LEU:HD12	0.62	1.71	36	171
1:A:51:LEU:HD21	1:E:51:LEU:HD12	0.62	1.69	45	1
1:A:37:LEU:CD1	1:B:33:ILE:HA	0.62	2.25	24	10
1:A:41:CYS:HB3	1:B:39:LEU:CD2	0.62	2.24	106	19
1:A:36:CYS:HA	1:E:41:CYS:SG	0.62	2.35	23	4
1:D:41:CYS:SG	1:E:36:CYS:HA	0.62	2.34	23	4
1:B:37:LEU:HD13	1:C:33:ILE:HG23	0.62	1.70	41	3
1:C:49:VAL:HA	1:C:52:LEU:HD12	0.62	1.70	145	164
1:D:51:LEU:CB	1:E:50:MET:CB	0.62	2.77	119	9
1:A:41:CYS:SG	1:B:36:CYS:HA	0.62	2.34	23	4
1:A:43:LEU:HD13	1:E:44:LEU:HD12	0.62	1.71	65	5
1:A:33:ILE:HA	1:E:37:LEU:CD1	0.62	2.25	24	10
1:A:36:CYS:SG	1:E:37:LEU:HD23	0.62	2.35	72	9
1:A:50:MET:CB	1:E:51:LEU:CB	0.62	2.77	119	9
1:A:44:LEU:HA	1:A:47:ILE:HG13	0.62	1.68	45	28
1:C:37:LEU:HD13	1:D:33:ILE:HG23	0.62	1.70	41	4
1:C:41:CYS:HB3	1:D:39:LEU:CD2	0.62	2.24	106	19
1:B:51:LEU:CB	1:C:50:MET:CB	0.62	2.77	119	9
1:C:37:LEU:HD23	1:D:36:CYS:SG	0.62	2.35	72	9
1:A:51:LEU:CB	1:B:50:MET:CB	0.62	2.77	119	9
1:A:44:LEU:HD12	1:B:43:LEU:HD13	0.62	1.71	65	5
1:A:49:VAL:HA	1:A:52:LEU:HD12	0.62	1.71	36	164
1:B:37:LEU:CD1	1:C:33:ILE:HA	0.62	2.25	24	10
1:A:40:ILE:HG12	1:E:40:ILE:HG22	0.62	1.71	59	7
1:C:44:LEU:HD13	1:D:43:LEU:CB	0.62	2.25	35	7
1:D:37:LEU:CD1	1:E:33:ILE:HA	0.62	2.25	24	10
1:C:51:LEU:HD13	1:D:51:LEU:CD2	0.62	2.25	147	6
1:D:48:ILE:HG23	1:E:50:MET:HG3	0.62	1.69	147	2
1:A:43:LEU:CB	1:E:44:LEU:HD13	0.61	2.25	35	7
1:D:44:LEU:HD13	1:E:43:LEU:CB	0.61	2.25	35	7
1:B:51:LEU:HD12	1:C:47:ILE:HG23	0.61	1.70	25	5
1:A:48:ILE:HD11	1:B:43:LEU:HA	0.61	1.72	36	10
1:D:48:ILE:HD11	1:E:43:LEU:HA	0.61	1.72	36	11
1:A:41:CYS:HB3	1:B:39:LEU:HD21	0.61	1.72	1	5
1:A:44:LEU:HD13	1:B:43:LEU:CB	0.61	2.25	65	7
1:C:40:ILE:HG22	1:D:40:ILE:HG12	0.61	1.71	59	6
1:C:38:ILE:HD13	1:D:32:PHE:CZ	0.61	2.30	51	5
1:B:44:LEU:HD13	1:C:43:LEU:CB	0.61	2.26	65	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:49:VAL:HA	1:B:52:LEU:HD12	0.61	1.70	145	165
1:C:37:LEU:CD1	1:D:33:ILE:HA	0.61	2.25	24	10
1:A:51:LEU:HD23	1:E:51:LEU:HD13	0.61	1.71	84	1
1:A:36:CYS:HB3	1:E:37:LEU:HB3	0.61	1.73	33	3
1:D:37:LEU:HD12	1:E:33:ILE:HA	0.61	1.73	22	1
1:B:41:CYS:SG	1:C:36:CYS:HA	0.61	2.34	23	4
1:D:44:LEU:HD12	1:E:43:LEU:HD13	0.61	1.71	65	5
1:B:44:LEU:HD12	1:C:40:ILE:HG23	0.61	1.73	59	10
1:C:51:LEU:HB3	1:D:50:MET:HB3	0.61	1.72	48	19
1:A:38:ILE:HD13	1:B:32:PHE:CZ	0.61	2.30	51	5
1:B:44:LEU:HB3	1:C:43:LEU:HD13	0.61	1.73	74	3
1:B:37:LEU:HD23	1:C:36:CYS:SG	0.61	2.35	72	10
1:C:37:LEU:HD12	1:D:33:ILE:HA	0.61	1.72	22	1
1:B:40:ILE:HG22	1:C:40:ILE:HG12	0.61	1.71	59	7
1:D:40:ILE:HG22	1:E:40:ILE:HG12	0.61	1.71	59	7
1:C:44:LEU:HD12	1:D:40:ILE:HG23	0.61	1.72	37	9
1:C:51:LEU:CB	1:D:50:MET:CB	0.61	2.77	119	9
1:B:41:CYS:HB3	1:C:39:LEU:HD21	0.61	1.73	1	5
1:D:44:LEU:HD12	1:E:40:ILE:HG23	0.61	1.72	37	9
1:B:44:LEU:HD12	1:C:43:LEU:HD13	0.61	1.71	65	5
1:A:40:ILE:HG22	1:B:40:ILE:HG12	0.60	1.71	59	7
1:A:44:LEU:HB3	1:B:43:LEU:HD13	0.60	1.73	74	3
1:A:51:LEU:CD1	1:B:50:MET:HB2	0.60	2.25	84	1
1:C:41:CYS:HB3	1:D:39:LEU:HD21	0.60	1.72	1	5
1:C:37:LEU:CD1	1:D:36:CYS:CB	0.60	2.78	19	3
1:A:43:LEU:HA	1:E:48:ILE:HD11	0.60	1.72	36	10
1:C:51:LEU:HD13	1:D:47:ILE:HG22	0.60	1.73	129	1
1:A:39:LEU:CD2	1:E:41:CYS:CB	0.60	2.80	103	15
1:C:48:ILE:HD11	1:D:43:LEU:HA	0.60	1.72	36	10
1:B:51:LEU:HB3	1:C:50:MET:HB3	0.60	1.73	48	17
1:B:41:CYS:CB	1:C:39:LEU:CD2	0.60	2.80	103	15
1:A:44:LEU:HD12	1:B:40:ILE:HG23	0.60	1.73	59	8
1:D:51:LEU:HB3	1:E:50:MET:HB3	0.60	1.72	48	17
1:D:37:LEU:O	1:D:41:CYS:SG	0.60	2.58	49	25
1:A:40:ILE:HG23	1:E:44:LEU:HD12	0.60	1.72	37	9
1:B:37:LEU:CD1	1:C:36:CYS:CB	0.60	2.78	19	2
1:C:41:CYS:CB	1:D:39:LEU:CD2	0.60	2.80	103	15
1:D:41:CYS:HB3	1:E:39:LEU:HD21	0.60	1.73	1	5
1:D:41:CYS:CB	1:E:39:LEU:CD2	0.60	2.80	35	15
1:A:48:ILE:HD11	1:B:43:LEU:C	0.60	2.17	25	9
1:D:44:LEU:HB3	1:E:43:LEU:HD13	0.60	1.73	74	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LEU:C	1:E:48:ILE:HD11	0.60	2.17	20	10
1:B:48:ILE:HD11	1:C:43:LEU:C	0.60	2.17	20	9
1:D:48:ILE:HD11	1:E:43:LEU:C	0.60	2.18	20	8
1:A:36:CYS:CB	1:E:37:LEU:CD1	0.60	2.78	19	2
1:A:37:LEU:HD12	1:B:33:ILE:HA	0.60	1.72	22	1
1:B:37:LEU:C	1:C:36:CYS:HG	0.60	2.00	72	1
1:D:48:ILE:HD11	1:E:43:LEU:CA	0.60	2.27	20	6
1:A:47:ILE:HD13	1:E:48:ILE:HG13	0.60	1.74	64	3
1:A:48:ILE:HG13	1:B:47:ILE:HD13	0.60	1.74	64	3
1:A:50:MET:HB3	1:E:51:LEU:HB3	0.60	1.72	48	18
1:C:48:ILE:HD11	1:D:43:LEU:C	0.59	2.17	25	8
1:D:37:LEU:HB3	1:E:36:CYS:HB3	0.59	1.73	33	3
1:A:51:LEU:CD2	1:E:51:LEU:HD13	0.59	2.27	12	4
1:A:39:LEU:HD21	1:E:41:CYS:HB3	0.59	1.72	1	6
1:D:48:ILE:HG13	1:E:47:ILE:HD13	0.59	1.74	64	3
1:D:37:LEU:CD1	1:E:36:CYS:CB	0.59	2.78	19	3
1:B:48:ILE:HD11	1:C:43:LEU:CA	0.59	2.27	20	6
1:D:51:LEU:HD13	1:E:51:LEU:CD2	0.59	2.27	12	3
1:A:48:ILE:HD11	1:B:43:LEU:CA	0.59	2.27	20	4
1:A:51:LEU:HB3	1:B:50:MET:HB3	0.59	1.74	133	18
1:D:38:ILE:HD13	1:E:32:PHE:CZ	0.59	2.32	51	5
1:A:48:ILE:CG1	1:B:47:ILE:HG13	0.59	2.28	3	5
1:B:48:ILE:HG13	1:C:47:ILE:HG12	0.59	1.75	3	12
1:A:37:LEU:HB3	1:B:36:CYS:HB3	0.59	1.73	33	3
1:C:48:ILE:HD11	1:D:43:LEU:CA	0.59	2.27	20	6
1:B:37:LEU:O	1:B:41:CYS:SG	0.59	2.58	49	24
1:A:43:LEU:CA	1:E:48:ILE:HD11	0.59	2.27	20	6
1:B:38:ILE:HD13	1:C:32:PHE:CZ	0.59	2.33	51	5
1:E:37:LEU:O	1:E:41:CYS:SG	0.59	2.58	49	24
1:C:48:ILE:CG1	1:D:47:ILE:HG13	0.59	2.28	3	4
1:D:48:ILE:CG1	1:E:47:ILE:HG13	0.59	2.28	3	5
1:C:37:LEU:HB3	1:D:36:CYS:HB3	0.59	1.73	33	3
1:D:51:LEU:HD13	1:E:51:LEU:HG	0.59	1.74	147	9
1:B:37:LEU:HB3	1:C:36:CYS:HB3	0.59	1.73	33	3
1:B:48:ILE:HD11	1:C:43:LEU:HA	0.59	1.72	36	11
1:A:33:ILE:HA	1:E:37:LEU:HD12	0.59	1.72	22	1
1:B:37:LEU:HD12	1:C:33:ILE:HA	0.59	1.72	22	1
1:A:41:CYS:CB	1:B:39:LEU:CD2	0.59	2.80	35	15
1:A:51:LEU:HD13	1:B:51:LEU:CD2	0.59	2.27	12	4
1:C:44:LEU:HD13	1:D:43:LEU:HB3	0.59	1.75	34	6
1:A:47:ILE:HG13	1:E:48:ILE:CG1	0.59	2.28	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:48:ILE:HD13	1:C:46:CYS:HB2	0.59	1.75	32	4
1:A:32:PHE:CZ	1:E:38:ILE:HD13	0.59	2.33	51	5
1:A:37:LEU:CD1	1:B:36:CYS:CB	0.58	2.78	19	3
1:D:48:ILE:HG12	1:E:47:ILE:CG1	0.58	2.28	3	10
1:D:44:LEU:HD13	1:E:43:LEU:HB3	0.58	1.75	35	6
1:A:48:ILE:HA	1:A:51:LEU:HD12	0.58	1.74	104	27
1:A:37:LEU:O	1:A:41:CYS:SG	0.58	2.57	1	21
1:B:38:ILE:HD11	1:C:32:PHE:CE1	0.58	2.34	40	5
1:C:37:LEU:C	1:D:36:CYS:HG	0.58	2.02	72	1
1:B:44:LEU:HD13	1:C:43:LEU:HB3	0.58	1.75	35	6
1:A:39:LEU:CD2	1:E:45:ILE:HD11	0.58	2.28	76	6
1:A:45:ILE:HD11	1:B:39:LEU:CD2	0.58	2.28	76	7
1:D:45:ILE:HD11	1:E:39:LEU:CD2	0.58	2.28	76	6
1:B:45:ILE:HD11	1:C:39:LEU:CD2	0.58	2.28	76	7
1:A:38:ILE:HD11	1:B:32:PHE:CE1	0.58	2.34	40	5
1:A:48:ILE:HD13	1:B:46:CYS:HB2	0.58	1.75	32	4
1:C:51:LEU:HD13	1:D:51:LEU:HD23	0.58	1.75	129	1
1:A:43:LEU:HB3	1:E:44:LEU:HD13	0.58	1.75	35	6
1:E:48:ILE:HA	1:E:51:LEU:HD12	0.58	1.74	104	24
1:C:40:ILE:HA	1:C:43:LEU:HD12	0.58	1.76	52	15
1:C:44:LEU:CD1	1:D:43:LEU:HD13	0.58	2.29	65	8
1:A:41:CYS:SG	1:B:40:ILE:CD1	0.58	2.92	37	2
1:C:48:ILE:HG12	1:D:47:ILE:CG1	0.58	2.28	3	10
1:D:38:ILE:HD11	1:E:32:PHE:CE1	0.58	2.34	40	5
1:C:48:ILE:HG13	1:D:47:ILE:HD13	0.58	1.74	64	4
1:C:37:LEU:O	1:C:41:CYS:SG	0.57	2.58	49	24
1:A:48:ILE:HG13	1:B:47:ILE:HG12	0.57	1.75	3	12
1:D:41:CYS:SG	1:E:40:ILE:CD1	0.57	2.92	37	2
1:A:51:LEU:HD13	1:B:47:ILE:O	0.57	1.99	84	1
1:B:48:ILE:CG1	1:C:47:ILE:HG13	0.57	2.27	3	5
1:A:46:CYS:HB2	1:E:48:ILE:HD13	0.57	1.75	32	4
1:C:48:ILE:HA	1:C:51:LEU:HD12	0.57	1.76	169	29
1:D:48:ILE:HA	1:D:51:LEU:HD12	0.57	1.76	169	26
1:A:51:LEU:HD13	1:B:51:LEU:HD23	0.57	1.76	147	1
1:A:44:LEU:HD13	1:B:43:LEU:HB3	0.57	1.75	35	6
1:B:48:ILE:HA	1:B:51:LEU:HD12	0.57	1.76	169	29
1:C:48:ILE:HG12	1:D:47:ILE:HG12	0.57	1.77	5	25
1:A:48:ILE:HG12	1:B:47:ILE:CG1	0.57	2.28	3	10
1:B:48:ILE:HG12	1:C:47:ILE:CG1	0.57	2.28	3	10
1:C:48:ILE:HD13	1:D:46:CYS:HB2	0.57	1.75	32	5
1:B:44:LEU:CD1	1:C:43:LEU:HD13	0.57	2.29	65	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:44:LEU:CD1	1:E:43:LEU:HD13	0.57	2.29	65	8
1:A:40:ILE:CD1	1:E:41:CYS:SG	0.57	2.92	37	2
1:B:41:CYS:SG	1:C:40:ILE:CD1	0.57	2.92	37	2
1:A:48:ILE:HG12	1:B:47:ILE:HG12	0.57	1.77	5	26
1:A:47:ILE:HG12	1:E:48:ILE:HG13	0.57	1.75	3	13
1:A:32:PHE:CE1	1:E:38:ILE:HD11	0.57	2.34	40	5
1:C:38:ILE:HD11	1:D:32:PHE:CE1	0.57	2.34	40	5
1:C:41:CYS:SG	1:D:40:ILE:CD1	0.57	2.92	37	2
1:A:47:ILE:CG1	1:E:48:ILE:HG12	0.57	2.28	3	10
1:B:40:ILE:HA	1:B:43:LEU:HD12	0.57	1.76	52	14
1:C:45:ILE:HD11	1:D:39:LEU:CD2	0.57	2.28	76	7
1:D:48:ILE:HD13	1:E:46:CYS:HB2	0.57	1.75	32	4
1:B:48:ILE:HG13	1:C:47:ILE:HD13	0.57	1.74	64	4
1:E:40:ILE:HA	1:E:43:LEU:HD12	0.57	1.76	52	14
1:D:44:LEU:HD22	1:E:44:LEU:HD23	0.57	1.77	32	2
1:A:40:ILE:HA	1:A:43:LEU:HD12	0.56	1.76	52	16
1:A:43:LEU:HD13	1:E:44:LEU:CD1	0.56	2.29	65	9
1:A:47:ILE:HG12	1:E:48:ILE:HG12	0.56	1.77	5	25
1:D:48:ILE:HG13	1:E:47:ILE:HG12	0.56	1.75	3	13
1:A:34:ASN:HA	1:B:32:PHE:CE1	0.56	2.35	19	1
1:A:43:LEU:HD13	1:E:44:LEU:HB3	0.56	1.76	73	3
1:A:44:LEU:CD2	1:B:44:LEU:HD21	0.56	2.30	32	4
1:D:34:ASN:HA	1:E:32:PHE:CE1	0.56	2.35	19	1
1:A:44:LEU:CD1	1:B:43:LEU:HD13	0.56	2.29	65	8
1:C:48:ILE:HG13	1:D:47:ILE:HG12	0.56	1.75	3	13
1:A:44:LEU:HD21	1:E:44:LEU:CD2	0.56	2.30	32	4
1:A:37:LEU:CB	1:B:36:CYS:SG	0.56	2.94	28	14
1:B:37:LEU:CB	1:C:36:CYS:SG	0.56	2.94	28	16
1:A:44:LEU:HD22	1:B:44:LEU:HD23	0.56	1.77	32	2
1:C:44:LEU:HB3	1:D:43:LEU:HD13	0.56	1.76	73	3
1:E:36:CYS:SG	1:E:37:LEU:N	0.56	2.78	51	23
1:D:37:LEU:CB	1:E:36:CYS:SG	0.56	2.94	28	16
1:C:44:LEU:CD2	1:D:44:LEU:HD21	0.56	2.31	32	4
1:A:51:LEU:HD23	1:E:51:LEU:HD22	0.56	1.77	84	2
1:A:36:CYS:SG	1:E:37:LEU:CB	0.56	2.94	28	14
1:A:32:PHE:CE1	1:E:34:ASN:HA	0.56	2.36	19	1
1:C:34:ASN:HA	1:D:32:PHE:CE1	0.56	2.36	19	1
1:C:51:LEU:HD22	1:D:51:LEU:HD22	0.56	1.76	147	1
1:A:51:LEU:HD13	1:B:51:LEU:HG	0.56	1.77	31	8
1:B:44:LEU:CD2	1:C:44:LEU:HD21	0.56	2.30	32	4
1:D:51:LEU:CD1	1:E:50:MET:HB2	0.56	2.29	129	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:CYS:SG	1:A:37:LEU:N	0.56	2.79	18	24
1:B:36:CYS:SG	1:B:37:LEU:N	0.56	2.79	18	24
1:D:48:ILE:HG12	1:E:47:ILE:HG12	0.56	1.77	5	27
1:D:41:CYS:HB3	1:E:39:LEU:HD23	0.56	1.78	13	2
1:B:48:ILE:HG12	1:C:47:ILE:HG12	0.56	1.77	5	26
1:D:40:ILE:HA	1:D:43:LEU:HD12	0.56	1.76	52	15
1:A:38:ILE:CG1	1:B:32:PHE:HZ	0.56	2.14	11	20
1:C:37:LEU:CB	1:D:36:CYS:SG	0.55	2.94	28	15
1:A:32:PHE:HZ	1:E:38:ILE:CG1	0.55	2.14	11	20
1:C:38:ILE:CG1	1:D:32:PHE:HZ	0.55	2.14	11	21
1:C:51:LEU:HB3	1:D:50:MET:HG3	0.55	1.79	26	1
1:D:38:ILE:CG1	1:E:32:PHE:HZ	0.55	2.14	11	23
1:D:33:ILE:HA	1:D:36:CYS:SG	0.55	2.42	13	1
1:D:44:LEU:CD2	1:E:44:LEU:HD21	0.55	2.30	32	4
1:B:48:ILE:HG12	1:C:47:ILE:HA	0.55	1.77	147	7
1:C:36:CYS:SG	1:C:37:LEU:N	0.55	2.79	18	23
1:C:44:LEU:CD2	1:D:44:LEU:CD2	0.55	2.85	32	5
1:A:33:ILE:HA	1:A:36:CYS:SG	0.55	2.42	13	2
1:B:44:LEU:HD22	1:C:44:LEU:HD23	0.55	1.77	32	2
1:C:41:CYS:HB3	1:D:39:LEU:HD23	0.55	1.78	13	2
1:E:33:ILE:HA	1:E:36:CYS:SG	0.55	2.42	13	1
1:A:50:MET:HG3	1:E:51:LEU:HB3	0.55	1.79	26	1
1:B:34:ASN:HA	1:C:32:PHE:CE1	0.55	2.35	19	1
1:A:51:LEU:HB3	1:B:50:MET:HG3	0.55	1.79	26	1
1:B:44:LEU:CB	1:C:43:LEU:CD1	0.55	2.78	73	1
1:D:36:CYS:SG	1:D:37:LEU:N	0.55	2.79	18	25
1:A:44:LEU:CD2	1:E:44:LEU:CD2	0.55	2.85	32	5
1:D:44:LEU:CD2	1:E:44:LEU:CD2	0.55	2.85	32	5
1:A:48:ILE:HG12	1:B:47:ILE:HA	0.55	1.79	84	5
1:A:33:ILE:HG23	1:E:37:LEU:CD1	0.54	2.32	27	5
1:A:37:LEU:CD1	1:B:33:ILE:HG23	0.54	2.32	27	7
1:A:44:LEU:CD2	1:B:44:LEU:CD2	0.54	2.85	32	5
1:A:41:CYS:HB3	1:B:39:LEU:HD23	0.54	1.79	13	2
1:B:51:LEU:CD2	1:C:51:LEU:HG	0.54	2.31	129	1
1:B:37:LEU:CD1	1:C:33:ILE:HG23	0.54	2.32	27	5
1:A:37:LEU:CD2	1:B:36:CYS:SG	0.54	2.95	147	10
1:A:38:ILE:HG23	1:B:32:PHE:CE1	0.54	2.38	37	5
1:C:37:LEU:CD1	1:D:33:ILE:HG23	0.54	2.32	27	6
1:A:44:LEU:HD23	1:E:44:LEU:HD22	0.54	1.77	32	2
1:C:33:ILE:HA	1:C:36:CYS:SG	0.54	2.42	13	2
1:D:37:LEU:CD1	1:E:33:ILE:HG23	0.54	2.32	27	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:38:ILE:CG1	1:C:32:PHE:HZ	0.54	2.16	24	21
1:B:41:CYS:HB3	1:C:39:LEU:HD23	0.54	1.79	13	2
1:D:44:LEU:HD13	1:E:44:LEU:HG	0.54	1.79	13	4
1:D:38:ILE:HG23	1:E:32:PHE:CE1	0.54	2.38	37	5
1:B:44:LEU:CD2	1:C:44:LEU:CD2	0.54	2.85	32	5
1:C:48:ILE:HD11	1:D:47:ILE:N	0.54	2.18	147	1
1:A:44:LEU:CD2	1:E:44:LEU:HD21	0.54	2.33	44	3
1:B:33:ILE:HA	1:B:36:CYS:SG	0.54	2.42	13	1
1:B:44:LEU:HD13	1:C:44:LEU:HG	0.54	1.79	13	4
1:A:43:LEU:HB3	1:E:44:LEU:CB	0.54	2.33	103	5
1:A:32:PHE:CE1	1:E:37:LEU:HB2	0.54	2.38	34	2
1:C:44:LEU:HD22	1:D:44:LEU:HD23	0.54	1.77	32	2
1:C:44:LEU:CB	1:D:43:LEU:HB3	0.54	2.33	103	4
1:B:37:LEU:CD2	1:C:36:CYS:SG	0.54	2.95	147	10
1:B:51:LEU:HB3	1:C:50:MET:HG3	0.54	1.79	26	1
1:A:48:ILE:HD11	1:B:47:ILE:N	0.54	2.18	147	1
1:A:45:ILE:HG13	1:B:43:LEU:HD21	0.54	1.79	103	3
1:C:51:LEU:CD1	1:D:51:LEU:HD23	0.54	2.33	129	1
1:B:37:LEU:HB2	1:C:32:PHE:CE1	0.53	2.38	34	2
1:C:38:ILE:HG23	1:D:32:PHE:CE1	0.53	2.38	37	5
1:A:39:LEU:HD23	1:E:41:CYS:HB3	0.53	1.78	13	2
1:C:44:LEU:HD13	1:D:44:LEU:HG	0.53	1.80	68	4
1:A:43:LEU:CD1	1:E:44:LEU:CB	0.53	2.78	73	2
1:A:37:LEU:HB2	1:B:32:PHE:CE1	0.53	2.38	34	2
1:A:44:LEU:HD21	1:B:44:LEU:CD2	0.53	2.33	44	3
1:A:44:LEU:HG	1:E:44:LEU:HD13	0.53	1.80	68	4
1:B:45:ILE:HA	1:C:43:LEU:HD22	0.53	1.81	20	3
1:A:44:LEU:HD13	1:B:44:LEU:HG	0.53	1.80	13	4
1:B:44:LEU:CB	1:C:43:LEU:HB3	0.53	2.33	103	7
1:D:48:ILE:HD11	1:E:47:ILE:N	0.53	2.18	147	1
1:D:37:LEU:HB2	1:E:32:PHE:CE1	0.53	2.38	34	2
1:B:41:CYS:HB3	1:C:40:ILE:HG13	0.53	1.81	9	8
1:B:44:LEU:HD21	1:C:44:LEU:CD2	0.53	2.33	44	3
1:B:45:ILE:HG13	1:C:43:LEU:HD21	0.53	1.79	103	3
1:C:45:ILE:HG13	1:D:43:LEU:HD21	0.53	1.79	103	3
1:C:37:LEU:HB2	1:D:32:PHE:CE1	0.53	2.38	34	2
1:D:45:ILE:HA	1:E:43:LEU:HD22	0.53	1.81	20	3
1:D:44:LEU:CB	1:E:43:LEU:HB3	0.53	2.33	103	5
1:D:51:LEU:HD13	1:E:47:ILE:O	0.53	2.03	129	1
1:D:51:LEU:HD11	1:E:47:ILE:HA	0.53	1.79	129	1
1:C:44:LEU:HD21	1:D:44:LEU:CD2	0.53	2.33	44	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LEU:HD21	1:E:45:ILE:HG13	0.53	1.79	103	3
1:A:32:PHE:CE1	1:E:38:ILE:HG23	0.53	2.38	37	6
1:C:41:CYS:HB3	1:D:40:ILE:HG13	0.53	1.81	9	8
1:D:51:LEU:HB3	1:E:50:MET:HG3	0.53	1.79	26	1
1:D:51:LEU:HB3	1:E:50:MET:CG	0.53	2.34	26	3
1:A:47:ILE:N	1:E:48:ILE:HD11	0.53	2.19	147	1
1:A:45:ILE:HA	1:B:43:LEU:HD22	0.53	1.81	8	3
1:A:32:PHE:HZ	1:E:38:ILE:HG13	0.53	1.63	33	3
1:D:44:LEU:HD21	1:E:44:LEU:CD2	0.53	2.33	44	3
1:A:45:ILE:HA	1:B:43:LEU:CD2	0.53	2.34	145	7
1:A:40:ILE:HG13	1:E:41:CYS:HB3	0.52	1.81	9	8
1:A:47:ILE:HD11	1:E:48:ILE:CG1	0.52	2.34	54	2
1:A:36:CYS:SG	1:E:37:LEU:CD2	0.52	2.96	147	10
1:B:44:LEU:HD13	1:C:44:LEU:CD2	0.52	2.35	32	2
1:A:50:MET:CG	1:E:51:LEU:HB3	0.52	2.34	26	3
1:C:51:LEU:HB3	1:D:50:MET:CG	0.52	2.34	26	3
1:B:38:ILE:HG23	1:C:32:PHE:CE1	0.52	2.39	59	5
1:A:41:CYS:HB3	1:B:40:ILE:HG13	0.52	1.81	9	8
1:C:48:ILE:CG1	1:D:47:ILE:HD11	0.52	2.34	54	2
1:C:45:ILE:HA	1:D:43:LEU:CD2	0.52	2.34	145	7
1:A:47:ILE:HA	1:E:48:ILE:HG12	0.52	1.80	84	5
1:B:48:ILE:HD11	1:C:47:ILE:N	0.52	2.20	147	1
1:D:44:LEU:HD13	1:E:44:LEU:CD2	0.52	2.35	32	2
1:B:45:ILE:HA	1:C:43:LEU:CD2	0.52	2.34	20	7
1:A:37:LEU:HD22	1:B:36:CYS:HB3	0.52	1.81	39	2
1:A:30:ASN:HA	1:A:33:ILE:HD12	0.52	1.81	6	1
1:D:37:LEU:CD2	1:E:36:CYS:SG	0.52	2.95	147	11
1:A:43:LEU:CD2	1:E:45:ILE:HA	0.52	2.35	20	7
1:A:36:CYS:HG	1:E:37:LEU:C	0.52	2.07	72	1
1:A:36:CYS:HB3	1:E:37:LEU:HD22	0.52	1.81	39	2
1:C:48:ILE:HG12	1:D:47:ILE:HA	0.52	1.80	84	4
1:A:51:LEU:CB	1:B:50:MET:HB2	0.52	2.35	58	4
1:D:45:ILE:HA	1:E:43:LEU:CD2	0.52	2.35	20	6
1:A:44:LEU:CB	1:B:43:LEU:HB3	0.52	2.33	103	5
1:E:38:ILE:O	1:E:41:CYS:SG	0.52	2.68	98	3
1:D:45:ILE:HG13	1:E:43:LEU:HD21	0.52	1.79	103	3
1:B:45:ILE:O	1:B:49:VAL:HG23	0.52	2.05	76	175
1:C:45:ILE:HA	1:D:43:LEU:HD22	0.52	1.81	20	3
1:B:30:ASN:HA	1:B:33:ILE:HD12	0.52	1.81	6	1
1:A:43:LEU:HD22	1:E:45:ILE:HA	0.52	1.81	8	3
1:B:48:ILE:CG1	1:C:47:ILE:HD11	0.52	2.34	54	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:51:LEU:CB	1:E:50:MET:HB2	0.52	2.35	58	4
1:A:51:LEU:HB3	1:B:50:MET:CG	0.52	2.34	26	3
1:D:51:LEU:CD1	1:E:47:ILE:HA	0.52	2.34	26	2
1:B:48:ILE:HG12	1:C:47:ILE:CG2	0.52	2.32	45	2
1:B:38:ILE:CD1	1:C:32:PHE:CE1	0.52	2.93	7	7
1:D:38:ILE:CG1	1:E:32:PHE:HE1	0.52	2.17	7	8
1:D:48:ILE:CG1	1:E:47:ILE:HD11	0.52	2.34	54	2
1:A:44:LEU:CD2	1:E:44:LEU:HD13	0.52	2.35	32	2
1:B:37:LEU:HD22	1:C:36:CYS:HB3	0.52	1.81	39	2
1:C:37:LEU:HD22	1:D:36:CYS:HB3	0.52	1.81	39	2
1:D:41:CYS:SG	1:E:36:CYS:SG	0.52	3.08	58	9
1:E:45:ILE:O	1:E:49:VAL:HG23	0.51	2.05	76	175
1:A:41:CYS:CB	1:B:40:ILE:HD11	0.51	2.35	54	6
1:B:41:CYS:CB	1:C:40:ILE:HD11	0.51	2.35	54	7
1:C:38:ILE:CD1	1:D:32:PHE:CE1	0.51	2.93	7	7
1:A:38:ILE:O	1:A:41:CYS:SG	0.51	2.68	98	3
1:A:48:ILE:CG1	1:B:47:ILE:HD11	0.51	2.34	54	2
1:A:36:CYS:SG	1:A:40:ILE:HD11	0.51	2.46	135	11
1:B:36:CYS:SG	1:B:40:ILE:HD11	0.51	2.46	135	10
1:A:44:LEU:HD13	1:B:44:LEU:CD2	0.51	2.35	32	2
1:A:51:LEU:HD13	1:B:50:MET:HB2	0.51	1.83	14	1
1:D:41:CYS:CB	1:E:40:ILE:HD11	0.51	2.35	54	7
1:C:38:ILE:O	1:C:41:CYS:SG	0.51	2.68	98	3
1:A:38:ILE:HG13	1:B:32:PHE:HZ	0.51	1.63	33	3
1:C:38:ILE:HG13	1:D:32:PHE:HZ	0.51	1.63	33	4
1:C:44:LEU:HD13	1:D:44:LEU:CD2	0.51	2.35	32	2
1:A:50:MET:HB2	1:E:51:LEU:HD13	0.51	1.83	14	1
1:B:51:LEU:HB3	1:C:50:MET:CG	0.51	2.34	26	3
1:C:41:CYS:SG	1:D:36:CYS:SG	0.51	3.08	58	13
1:B:41:CYS:HB2	1:C:40:ILE:HD11	0.51	1.82	88	1
1:A:45:ILE:O	1:A:49:VAL:HG23	0.51	2.05	76	177
1:D:45:ILE:O	1:D:49:VAL:HG23	0.51	2.05	76	176
1:A:40:ILE:HD11	1:E:41:CYS:CB	0.51	2.35	54	7
1:A:38:ILE:CG1	1:B:32:PHE:HE1	0.51	2.17	7	8
1:C:51:LEU:HD13	1:D:50:MET:HB2	0.51	1.83	14	1
1:A:40:ILE:HD11	1:E:41:CYS:HB2	0.51	1.83	88	1
1:C:41:CYS:CB	1:D:40:ILE:HD11	0.51	2.35	54	7
1:D:36:CYS:SG	1:D:40:ILE:HD11	0.51	2.46	135	11
1:B:51:LEU:CD1	1:C:47:ILE:HA	0.51	2.34	26	3
1:C:44:LEU:HB2	1:D:43:LEU:CD1	0.51	2.26	73	4
1:C:44:LEU:CB	1:D:43:LEU:CD1	0.51	2.78	73	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:45:ILE:O	1:C:49:VAL:HG23	0.51	2.06	52	175
1:B:38:ILE:O	1:B:41:CYS:SG	0.51	2.68	98	3
1:D:38:ILE:O	1:D:41:CYS:SG	0.51	2.68	98	3
1:D:41:CYS:HB3	1:E:40:ILE:HG13	0.51	1.81	9	8
1:C:36:CYS:SG	1:C:40:ILE:HD11	0.51	2.46	135	11
1:A:48:ILE:HG12	1:B:47:ILE:CA	0.51	2.36	32	3
1:D:48:ILE:HG12	1:E:47:ILE:CA	0.51	2.36	32	2
1:D:48:ILE:HG12	1:E:47:ILE:CG2	0.51	2.35	64	3
1:A:41:CYS:HB2	1:B:40:ILE:HD11	0.51	1.82	88	1
1:D:41:CYS:HB2	1:E:40:ILE:HD11	0.51	1.82	88	1
1:D:38:ILE:CD1	1:E:32:PHE:CE1	0.51	2.93	7	6
1:B:41:CYS:CB	1:C:39:LEU:HD23	0.51	2.36	106	4
1:A:48:ILE:HA	1:A:51:LEU:CD1	0.51	2.36	84	1
1:B:33:ILE:O	1:B:37:LEU:HG	0.51	2.06	19	7
1:E:30:ASN:HA	1:E:33:ILE:HD12	0.51	1.83	6	1
1:C:51:LEU:CB	1:D:50:MET:HB2	0.51	2.35	58	4
1:C:41:CYS:CB	1:D:39:LEU:HD23	0.51	2.36	106	4
1:A:43:LEU:HA	1:E:48:ILE:CD1	0.51	2.36	56	2
1:A:33:ILE:O	1:A:37:LEU:HG	0.51	2.06	19	8
1:D:30:ASN:HA	1:D:33:ILE:HD12	0.51	1.81	6	1
1:A:32:PHE:CE1	1:E:38:ILE:CD1	0.51	2.93	7	7
1:A:39:LEU:HD23	1:E:41:CYS:CB	0.51	2.36	106	4
1:A:44:LEU:HB2	1:B:43:LEU:CD1	0.51	2.27	26	4
1:D:37:LEU:HD22	1:E:36:CYS:HB3	0.51	1.81	39	2
1:E:36:CYS:SG	1:E:40:ILE:HD11	0.51	2.46	38	10
1:B:51:LEU:CB	1:C:50:MET:HB2	0.51	2.35	58	4
1:A:36:CYS:SG	1:E:41:CYS:SG	0.51	3.08	58	11
1:A:41:CYS:CB	1:B:39:LEU:HD23	0.51	2.36	106	4
1:D:51:LEU:HD13	1:E:50:MET:HB2	0.51	1.83	14	1
1:B:48:ILE:CD1	1:C:43:LEU:HA	0.51	2.36	56	3
1:C:48:ILE:CD1	1:D:43:LEU:HA	0.51	2.36	56	3
1:D:48:ILE:CD1	1:E:43:LEU:HA	0.51	2.36	56	2
1:A:50:MET:HB2	1:E:51:LEU:CB	0.50	2.36	12	4
1:B:48:ILE:HD13	1:C:46:CYS:HB3	0.50	1.84	32	4
1:B:51:LEU:CB	1:C:50:MET:HB3	0.50	2.36	119	3
1:A:48:ILE:CG1	1:B:47:ILE:CD1	0.50	2.89	46	4
1:A:47:ILE:CA	1:E:48:ILE:HG12	0.50	2.36	32	3
1:B:47:ILE:HB	1:C:47:ILE:HD13	0.50	1.83	32	1
1:A:37:LEU:C	1:B:36:CYS:HG	0.50	2.10	72	1
1:A:47:ILE:CD1	1:E:48:ILE:CG1	0.50	2.90	46	5
1:C:48:ILE:HG12	1:D:47:ILE:CG2	0.50	2.35	64	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:CYS:HB3	1:E:48:ILE:HD13	0.50	1.84	32	4
1:A:45:ILE:HG12	1:B:43:LEU:CD2	0.50	2.33	32	3
1:D:48:ILE:CG1	1:E:47:ILE:CD1	0.50	2.90	46	5
1:A:47:ILE:HD13	1:E:47:ILE:HB	0.50	1.83	32	1
1:D:38:ILE:HG12	1:E:32:PHE:CE2	0.50	2.42	38	1
1:A:41:CYS:SG	1:B:36:CYS:SG	0.50	3.08	58	11
1:A:47:ILE:CG2	1:E:48:ILE:HG12	0.50	2.35	64	3
1:B:38:ILE:HD13	1:C:32:PHE:CE1	0.50	2.42	72	3
1:C:32:PHE:C	1:C:32:PHE:CD1	0.50	2.85	41	16
1:C:51:LEU:CD1	1:D:51:LEU:HD21	0.50	2.37	12	1
1:B:51:LEU:HD13	1:C:50:MET:HB2	0.50	1.82	14	1
1:C:48:ILE:CG1	1:D:47:ILE:CD1	0.50	2.90	46	5
1:A:43:LEU:CD1	1:E:44:LEU:HB2	0.50	2.27	26	3
1:C:47:ILE:HB	1:D:47:ILE:HD13	0.50	1.83	32	1
1:A:32:PHE:CE1	1:E:38:ILE:HD13	0.50	2.42	59	3
1:C:33:ILE:O	1:C:37:LEU:HG	0.50	2.06	19	6
1:B:38:ILE:CG1	1:C:32:PHE:HE1	0.50	2.20	68	7
1:C:37:LEU:CD2	1:D:36:CYS:SG	0.50	2.96	147	10
1:C:48:ILE:HG12	1:D:47:ILE:CA	0.50	2.36	32	4
1:D:48:ILE:HG12	1:E:47:ILE:HA	0.50	1.84	147	6
1:C:38:ILE:HD13	1:D:32:PHE:CE1	0.50	2.42	59	3
1:A:44:LEU:CB	1:B:43:LEU:CD1	0.50	2.78	73	2
1:D:48:ILE:HG13	1:E:47:ILE:HA	0.50	1.83	147	1
1:A:38:ILE:CD1	1:B:32:PHE:CE1	0.50	2.93	7	5
1:C:38:ILE:CG1	1:D:32:PHE:HE1	0.50	2.20	68	8
1:A:48:ILE:CD1	1:B:43:LEU:HA	0.50	2.37	20	2
1:D:38:ILE:HD13	1:E:32:PHE:CE1	0.50	2.42	72	3
1:D:51:LEU:HD12	1:E:50:MET:CB	0.50	2.33	129	1
1:D:33:ILE:O	1:D:37:LEU:HG	0.50	2.06	19	7
1:A:32:PHE:C	1:A:32:PHE:CD1	0.50	2.85	41	15
1:D:38:ILE:HG13	1:E:32:PHE:HZ	0.50	1.63	33	5
1:D:47:ILE:HB	1:E:47:ILE:HD13	0.50	1.83	32	1
1:C:38:ILE:HG12	1:D:32:PHE:CE2	0.50	2.41	38	1
1:A:38:ILE:HD13	1:B:32:PHE:CE1	0.50	2.42	59	3
1:B:51:LEU:HB3	1:C:50:MET:HB2	0.50	1.84	67	8
1:E:32:PHE:C	1:E:32:PHE:CD1	0.50	2.85	41	17
1:A:43:LEU:HD22	1:E:45:ILE:N	0.50	2.22	58	7
1:A:45:ILE:N	1:B:43:LEU:HD22	0.50	2.22	58	7
1:A:51:LEU:CB	1:B:50:MET:HB3	0.50	2.36	119	3
1:D:45:ILE:N	1:E:43:LEU:HD22	0.50	2.22	58	7
1:B:38:ILE:HG12	1:C:32:PHE:CE2	0.50	2.41	38	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:41:CYS:SG	1:C:36:CYS:SG	0.50	3.08	58	13
1:A:51:LEU:HD23	1:E:51:LEU:CD1	0.50	2.37	84	1
1:C:51:LEU:HD13	1:D:51:LEU:HD21	0.50	1.81	147	2
1:A:32:PHE:HE1	1:E:38:ILE:CG1	0.50	2.17	7	9
1:A:41:CYS:HB3	1:B:40:ILE:CD1	0.50	2.37	98	3
1:A:51:LEU:CD1	1:B:51:LEU:HD21	0.50	2.37	12	1
1:A:50:MET:HB3	1:E:51:LEU:HD22	0.50	1.84	114	2
1:B:48:ILE:HG12	1:C:47:ILE:CA	0.50	2.36	32	3
1:A:32:PHE:CE2	1:E:38:ILE:HG12	0.50	2.42	38	1
1:D:48:ILE:HG12	1:E:47:ILE:HG13	0.49	1.84	3	2
1:B:32:PHE:CD1	1:B:32:PHE:C	0.49	2.86	28	22
1:A:47:ILE:HB	1:B:47:ILE:HD13	0.49	1.83	32	1
1:B:51:LEU:HD22	1:C:50:MET:HB3	0.49	1.84	114	1
1:E:33:ILE:O	1:E:37:LEU:HG	0.49	2.06	19	6
1:D:45:ILE:HG12	1:E:43:LEU:CD2	0.49	2.33	32	3
1:A:47:ILE:HA	1:E:51:LEU:CD1	0.49	2.34	26	3
1:B:48:ILE:CD1	1:C:46:CYS:HB2	0.49	2.37	48	7
1:A:38:ILE:HG12	1:B:32:PHE:CE2	0.49	2.41	38	1
1:A:48:ILE:HG13	1:B:47:ILE:HA	0.49	1.83	147	1
1:B:45:ILE:N	1:C:43:LEU:HD22	0.49	2.22	58	7
1:C:48:ILE:HD13	1:D:46:CYS:HB3	0.49	1.84	32	4
1:C:41:CYS:HB3	1:D:40:ILE:CD1	0.49	2.37	98	3
1:D:48:ILE:CD1	1:E:47:ILE:HD11	0.49	2.38	9	2
1:A:51:LEU:HD21	1:E:51:LEU:CD1	0.49	2.37	12	1
1:C:51:LEU:CB	1:D:50:MET:HB3	0.49	2.36	119	3
1:D:41:CYS:CB	1:E:39:LEU:HD23	0.49	2.36	106	4
1:A:51:LEU:HD22	1:B:51:LEU:HG	0.49	1.85	129	1
1:A:50:MET:HB2	1:E:51:LEU:HB3	0.49	1.84	67	9
1:A:40:ILE:CD1	1:E:41:CYS:HB3	0.49	2.38	98	3
1:B:51:LEU:CD1	1:C:51:LEU:HD21	0.49	2.37	12	2
1:D:48:ILE:HD13	1:E:46:CYS:HB3	0.49	1.84	32	4
1:B:48:ILE:CG1	1:C:47:ILE:CD1	0.49	2.90	46	4
1:D:44:LEU:HD12	1:E:40:ILE:HG12	0.49	1.84	56	2
1:A:51:LEU:HD12	1:B:50:MET:CB	0.49	2.27	84	1
1:D:51:LEU:HD13	1:E:51:LEU:HD21	0.49	1.84	94	3
1:D:51:LEU:CD1	1:E:51:LEU:HD21	0.49	2.37	12	1
1:A:43:LEU:CD2	1:E:45:ILE:HG12	0.49	2.33	32	2
1:B:38:ILE:HA	1:C:32:PHE:CZ	0.49	2.43	27	1
1:A:44:LEU:CD1	1:B:43:LEU:HB3	0.49	2.38	1	3
1:D:32:PHE:C	1:D:32:PHE:CD1	0.49	2.86	7	17
1:A:47:ILE:HD11	1:E:48:ILE:CD1	0.49	2.38	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LEU:HD21	1:E:44:LEU:HD22	0.49	1.85	14	3
1:A:32:PHE:CZ	1:E:38:ILE:HA	0.49	2.43	27	1
1:C:41:CYS:HB2	1:D:40:ILE:HD11	0.49	1.82	88	1
1:D:51:LEU:HD22	1:E:50:MET:HB3	0.49	1.84	114	1
1:D:44:LEU:CD1	1:E:43:LEU:HB3	0.49	2.38	1	3
1:A:46:CYS:HB3	1:E:48:ILE:CG2	0.49	2.38	58	3
1:C:45:ILE:HG12	1:D:43:LEU:CD2	0.49	2.33	32	3
1:D:44:LEU:HB3	1:E:47:ILE:HD11	0.49	1.85	19	1
1:C:51:LEU:CD1	1:D:47:ILE:HA	0.49	2.34	26	2
1:A:46:CYS:HB2	1:E:48:ILE:CD1	0.49	2.37	48	6
1:A:48:ILE:CD1	1:B:46:CYS:HB2	0.49	2.37	48	8
1:C:48:ILE:CD1	1:D:46:CYS:HB2	0.49	2.37	48	7
1:C:37:LEU:O	1:D:36:CYS:SG	0.49	2.71	59	2
1:C:30:ASN:HA	1:C:33:ILE:HD12	0.49	1.83	6	1
1:A:48:ILE:HG13	1:B:47:ILE:CD1	0.49	2.38	14	1
1:A:36:CYS:SG	1:E:37:LEU:O	0.49	2.71	101	2
1:A:37:LEU:O	1:B:36:CYS:SG	0.49	2.71	101	2
1:D:37:LEU:O	1:E:36:CYS:SG	0.49	2.71	59	2
1:A:51:LEU:HD13	1:B:51:LEU:HD21	0.49	1.84	94	2
1:A:43:LEU:CD2	1:E:44:LEU:HB3	0.49	2.38	73	2
1:B:41:CYS:HB3	1:C:40:ILE:CD1	0.48	2.38	98	3
1:D:41:CYS:HB3	1:E:40:ILE:CD1	0.48	2.38	98	3
1:A:48:ILE:CG2	1:B:46:CYS:HB3	0.48	2.38	58	3
1:D:48:ILE:CG2	1:E:46:CYS:HB3	0.48	2.38	58	4
1:A:47:ILE:CD1	1:E:48:ILE:HG13	0.48	2.38	14	1
1:D:44:LEU:HB3	1:E:43:LEU:CD2	0.48	2.38	73	2
1:A:38:ILE:HA	1:B:32:PHE:CZ	0.48	2.43	27	1
1:A:47:ILE:HA	1:E:48:ILE:HG13	0.48	1.84	147	1
1:A:47:ILE:HG13	1:E:48:ILE:HG12	0.48	1.84	3	2
1:C:51:LEU:HB3	1:D:50:MET:HB2	0.48	1.84	67	8
1:A:48:ILE:CD1	1:B:47:ILE:HD11	0.48	2.38	9	2
1:A:47:ILE:HD11	1:E:44:LEU:HB3	0.48	1.85	19	1
1:A:44:LEU:HB3	1:B:47:ILE:HD11	0.48	1.85	19	1
1:C:38:ILE:HA	1:D:32:PHE:CZ	0.48	2.43	27	1
1:B:44:LEU:HB2	1:C:43:LEU:CD1	0.48	2.26	73	4
1:A:40:ILE:HG12	1:E:44:LEU:HD12	0.48	1.84	56	2
1:A:44:LEU:HB3	1:B:43:LEU:CD2	0.48	2.38	73	2
1:D:51:LEU:HB3	1:E:50:MET:HB2	0.48	1.85	48	7
1:A:51:LEU:HD13	1:B:51:LEU:CG	0.48	2.39	12	2
1:C:45:ILE:N	1:D:43:LEU:HD22	0.48	2.22	58	7
1:B:48:ILE:HG13	1:C:47:ILE:CD1	0.48	2.38	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:37:LEU:CB	1:D:36:CYS:HB2	0.48	2.37	1	1
1:A:48:ILE:HD13	1:B:46:CYS:HB3	0.48	1.86	106	4
1:A:50:MET:HB3	1:E:51:LEU:CB	0.48	2.36	119	3
1:C:51:LEU:HB2	1:D:50:MET:CB	0.48	2.38	84	4
1:D:51:LEU:HD13	1:E:51:LEU:CG	0.48	2.39	12	3
1:D:44:LEU:HD22	1:E:44:LEU:HD21	0.48	1.85	14	3
1:A:44:LEU:HD12	1:B:40:ILE:HG12	0.48	1.84	56	2
1:A:37:LEU:CB	1:B:36:CYS:HB2	0.48	2.36	1	1
1:B:37:LEU:CB	1:C:36:CYS:HB2	0.48	2.37	1	1
1:A:51:LEU:HB3	1:B:50:MET:HB2	0.48	1.84	67	7
1:B:48:ILE:HG12	1:C:47:ILE:N	0.48	2.24	12	3
1:B:51:LEU:HD13	1:C:51:LEU:CG	0.48	2.39	12	3
1:C:44:LEU:HD22	1:D:44:LEU:HD21	0.48	1.85	14	2
1:D:33:ILE:O	1:D:36:CYS:SG	0.48	2.69	95	2
1:D:44:LEU:HB2	1:E:43:LEU:CD1	0.48	2.24	36	4
1:D:38:ILE:HA	1:E:32:PHE:CZ	0.48	2.43	27	1
1:A:51:LEU:HD22	1:B:50:MET:HB3	0.48	1.84	114	1
1:A:36:CYS:HB2	1:E:37:LEU:CB	0.48	2.37	1	1
1:B:44:LEU:CD1	1:C:43:LEU:HB3	0.48	2.38	1	3
1:D:51:LEU:CB	1:E:50:MET:HB3	0.48	2.36	119	3
1:C:44:LEU:HB3	1:D:47:ILE:HD11	0.48	1.84	19	1
1:A:51:LEU:CG	1:E:51:LEU:HD13	0.48	2.39	12	4
1:C:51:LEU:HD13	1:D:51:LEU:CG	0.48	2.39	12	3
1:D:48:ILE:HG12	1:E:47:ILE:N	0.48	2.24	12	3
1:B:44:LEU:HB3	1:C:47:ILE:HD11	0.48	1.84	19	1
1:B:44:LEU:HD12	1:C:40:ILE:HG12	0.48	1.85	56	2
1:B:37:LEU:O	1:C:36:CYS:SG	0.48	2.71	101	2
1:C:44:LEU:HB2	1:D:43:LEU:HD22	0.48	1.86	35	3
1:B:33:ILE:O	1:B:36:CYS:SG	0.48	2.70	95	3
1:D:48:ILE:HG12	1:E:47:ILE:CD1	0.48	2.39	5	2
1:A:51:LEU:HD21	1:E:51:LEU:HD13	0.48	1.84	94	2
1:C:48:ILE:CG2	1:D:46:CYS:HB3	0.48	2.38	58	3
1:B:45:ILE:HG12	1:C:43:LEU:CD2	0.48	2.33	32	2
1:C:51:LEU:HD22	1:D:50:MET:HB3	0.48	1.84	114	2
1:D:48:ILE:HG13	1:E:47:ILE:CD1	0.48	2.38	14	1
1:C:51:LEU:HB2	1:D:50:MET:HB3	0.48	1.86	84	1
1:A:43:LEU:HB3	1:E:44:LEU:CD1	0.47	2.38	1	3
1:C:44:LEU:CD1	1:D:43:LEU:HB3	0.47	2.38	1	3
1:C:48:ILE:HG12	1:D:47:ILE:CD1	0.47	2.39	5	2
1:A:47:ILE:N	1:E:48:ILE:HG12	0.47	2.24	12	3
1:D:48:ILE:CD1	1:E:46:CYS:HB2	0.47	2.37	48	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:48:ILE:HG12	1:C:47:ILE:HG13	0.47	1.84	3	2
1:B:38:ILE:HG13	1:C:32:PHE:HZ	0.47	1.62	33	4
1:A:48:ILE:HA	1:A:51:LEU:HD11	0.47	1.85	84	1
1:C:48:ILE:CD1	1:D:46:CYS:CB	0.47	2.92	103	1
1:A:41:CYS:HA	1:B:43:LEU:HD13	0.47	1.86	147	1
1:A:48:ILE:HG12	1:B:47:ILE:HG13	0.47	1.84	3	2
1:A:44:LEU:HD22	1:B:44:LEU:HD21	0.47	1.85	14	3
1:A:51:LEU:HD12	1:B:47:ILE:CG2	0.47	2.39	129	5
1:B:37:LEU:CA	1:C:36:CYS:SG	0.47	3.03	28	3
1:B:37:LEU:CB	1:C:32:PHE:HE1	0.47	2.23	65	3
1:B:48:ILE:CD1	1:C:46:CYS:CB	0.47	2.93	103	1
1:C:41:CYS:HA	1:D:43:LEU:HD13	0.47	1.86	147	1
1:B:48:ILE:CG2	1:C:46:CYS:HB3	0.47	2.38	58	3
1:B:44:LEU:HD22	1:C:44:LEU:HD21	0.47	1.85	14	2
1:A:41:CYS:SG	1:B:40:ILE:CG1	0.47	3.03	17	4
1:D:41:CYS:SG	1:E:40:ILE:CG1	0.47	3.03	64	5
1:C:37:LEU:CA	1:D:36:CYS:SG	0.47	3.03	28	3
1:A:37:LEU:HB2	1:B:32:PHE:HE1	0.47	1.70	34	4
1:D:41:CYS:SG	1:E:36:CYS:HB2	0.47	2.50	56	2
1:D:41:CYS:SG	1:E:39:LEU:HD21	0.47	2.49	147	1
1:A:47:ILE:CD1	1:E:48:ILE:HG12	0.47	2.39	5	2
1:C:48:ILE:HG13	1:D:47:ILE:CD1	0.47	2.38	14	1
1:A:36:CYS:SG	1:E:37:LEU:CA	0.47	3.03	28	3
1:D:37:LEU:CA	1:E:36:CYS:SG	0.47	3.03	28	3
1:C:41:CYS:SG	1:D:39:LEU:HD21	0.47	2.49	147	1
1:B:48:ILE:HG12	1:C:47:ILE:CD1	0.47	2.39	5	1
1:A:43:LEU:CD2	1:E:45:ILE:CG1	0.47	2.93	32	3
1:E:33:ILE:O	1:E:36:CYS:SG	0.47	2.70	95	4
1:C:37:LEU:CD1	1:D:36:CYS:HB3	0.47	2.40	22	3
1:D:37:LEU:CD1	1:E:36:CYS:HB3	0.47	2.40	22	2
1:B:44:LEU:HB3	1:C:43:LEU:CD2	0.47	2.38	73	3
1:A:37:LEU:CA	1:B:36:CYS:SG	0.47	3.02	28	3
1:A:50:MET:SD	1:E:52:LEU:HD23	0.47	2.50	31	2
1:B:37:LEU:HB2	1:C:32:PHE:HE1	0.47	1.70	34	5
1:A:32:PHE:HE1	1:E:37:LEU:CB	0.47	2.23	65	3
1:A:37:LEU:CB	1:B:32:PHE:HE1	0.47	2.23	65	3
1:A:41:CYS:SG	1:B:36:CYS:HB2	0.47	2.50	56	2
1:C:44:LEU:HB3	1:D:43:LEU:CD2	0.47	2.38	73	2
1:B:51:LEU:CD2	1:C:51:LEU:CD2	0.47	2.87	84	1
1:A:39:LEU:HD21	1:E:41:CYS:SG	0.47	2.49	147	1
1:D:41:CYS:HA	1:E:43:LEU:HD13	0.47	1.86	147	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:48:ILE:HG12	1:D:47:ILE:HG13	0.47	1.84	3	2
1:A:48:ILE:HG12	1:B:47:ILE:CD1	0.47	2.39	5	1
1:B:52:LEU:HD23	1:C:50:MET:SD	0.47	2.50	31	2
1:C:41:CYS:SG	1:D:40:ILE:CG1	0.47	3.03	64	3
1:A:41:CYS:SG	1:B:36:CYS:CA	0.47	3.03	23	1
1:B:51:LEU:HD12	1:C:47:ILE:CG2	0.47	2.40	130	3
1:C:51:LEU:HD11	1:D:47:ILE:HG22	0.47	1.85	84	4
1:C:52:LEU:HD23	1:D:50:MET:SD	0.47	2.50	31	1
1:C:41:CYS:SG	1:D:36:CYS:HB2	0.47	2.50	56	2
1:C:44:LEU:HD12	1:D:40:ILE:HG12	0.47	1.85	56	2
1:D:44:LEU:CB	1:E:43:LEU:CD1	0.47	2.78	73	2
1:A:41:CYS:SG	1:B:39:LEU:HD21	0.47	2.49	147	1
1:B:41:CYS:SG	1:C:39:LEU:HD21	0.47	2.49	147	1
1:A:45:ILE:CG1	1:B:43:LEU:CD2	0.47	2.93	32	3
1:B:45:ILE:CG1	1:C:43:LEU:CD2	0.47	2.93	32	3
1:C:45:ILE:CG1	1:D:43:LEU:CD2	0.47	2.93	32	3
1:C:48:ILE:HG12	1:D:47:ILE:N	0.47	2.24	12	3
1:A:36:CYS:HB3	1:E:37:LEU:CD1	0.47	2.40	22	2
1:B:41:CYS:SG	1:C:36:CYS:CA	0.47	3.03	23	1
1:A:46:CYS:CB	1:E:48:ILE:CD1	0.47	2.93	103	1
1:A:48:ILE:CD1	1:B:46:CYS:CB	0.47	2.93	103	1
1:A:48:ILE:HG12	1:B:47:ILE:N	0.47	2.24	12	3
1:C:33:ILE:O	1:C:36:CYS:SG	0.47	2.70	95	3
1:A:40:ILE:CG1	1:E:41:CYS:SG	0.47	3.03	17	4
1:B:37:LEU:CD1	1:C:36:CYS:HB3	0.47	2.40	22	2
1:D:51:LEU:HD12	1:E:47:ILE:CG2	0.47	2.40	130	4
1:D:37:LEU:CB	1:E:32:PHE:HE1	0.47	2.23	65	3
1:D:48:ILE:HD11	1:E:46:CYS:HB2	0.47	1.87	84	1
1:B:44:LEU:CD1	1:C:43:LEU:CB	0.47	2.93	35	3
1:B:41:CYS:SG	1:C:40:ILE:CG1	0.47	3.03	64	3
1:A:51:LEU:CD1	1:B:47:ILE:O	0.47	2.63	84	1
1:B:41:CYS:HA	1:C:43:LEU:HD13	0.47	1.87	147	1
1:D:45:ILE:CG1	1:E:43:LEU:CD2	0.46	2.93	32	3
1:A:37:LEU:CD1	1:B:36:CYS:HB3	0.46	2.40	22	2
1:A:51:LEU:CD1	1:B:51:LEU:HG	0.46	2.40	60	3
1:A:52:LEU:HD23	1:B:50:MET:SD	0.46	2.50	31	2
1:A:51:LEU:HD12	1:B:47:ILE:HA	0.46	1.87	145	2
1:A:44:LEU:CD1	1:B:43:LEU:CB	0.46	2.93	35	2
1:C:44:LEU:CD1	1:D:43:LEU:CB	0.46	2.93	35	2
1:B:51:LEU:CD1	1:C:51:LEU:HG	0.46	2.40	60	3
1:C:51:LEU:CD1	1:D:51:LEU:HG	0.46	2.40	60	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:37:LEU:CB	1:D:32:PHE:HE1	0.46	2.23	65	3
1:A:47:ILE:HG23	1:E:48:ILE:HG13	0.46	1.85	45	1
1:A:41:CYS:HB2	1:B:39:LEU:CD2	0.46	2.41	147	1
1:B:47:ILE:HG21	1:C:47:ILE:HD13	0.46	1.87	58	4
1:D:41:CYS:SG	1:E:36:CYS:CA	0.46	3.03	23	1
1:C:51:LEU:HD12	1:D:47:ILE:CG2	0.46	2.40	130	4
1:A:47:ILE:CG2	1:E:51:LEU:HD12	0.46	2.40	130	4
1:A:41:CYS:HA	1:B:40:ILE:HG13	0.46	1.88	37	2
1:A:48:ILE:HG12	1:B:47:ILE:CG2	0.46	2.35	64	3
1:B:41:CYS:SG	1:C:36:CYS:HB2	0.46	2.50	56	2
1:D:37:LEU:CB	1:E:36:CYS:HB2	0.46	2.37	1	1
1:A:51:LEU:CD1	1:B:47:ILE:HA	0.46	2.34	26	2
1:A:38:ILE:CA	1:B:36:CYS:SG	0.46	3.02	59	1
1:D:37:LEU:C	1:E:36:CYS:HG	0.46	2.13	72	1
1:C:41:CYS:HB2	1:D:39:LEU:CD2	0.46	2.41	147	1
1:A:44:LEU:HB2	1:B:43:LEU:HD22	0.46	1.86	35	3
1:D:38:ILE:CA	1:D:41:CYS:SG	0.46	3.03	92	5
1:D:37:LEU:HD11	1:E:33:ILE:HG23	0.46	1.87	10	1
1:D:48:ILE:CD1	1:E:46:CYS:CB	0.46	2.93	103	1
1:C:48:ILE:HG13	1:D:47:ILE:HA	0.46	1.84	147	1
1:C:48:ILE:CD1	1:D:47:ILE:HD11	0.46	2.38	9	1
1:D:51:LEU:CD1	1:E:51:LEU:HG	0.46	2.40	60	2
1:A:40:ILE:HG13	1:E:41:CYS:HA	0.46	1.88	37	2
1:C:41:CYS:HA	1:D:40:ILE:HG13	0.46	1.88	37	2
1:A:43:LEU:HD22	1:E:45:ILE:CA	0.46	2.40	44	1
1:A:36:CYS:HB2	1:E:41:CYS:SG	0.46	2.50	56	2
1:A:38:ILE:CA	1:A:41:CYS:SG	0.46	3.02	9	9
1:B:48:ILE:CD1	1:C:47:ILE:HD11	0.46	2.38	9	1
1:A:40:ILE:CG1	1:E:41:CYS:HA	0.46	2.41	21	4
1:A:41:CYS:HA	1:B:40:ILE:CG1	0.46	2.41	21	4
1:C:41:CYS:SG	1:D:36:CYS:CA	0.46	3.03	23	1
1:B:44:LEU:CD1	1:C:40:ILE:HA	0.46	2.41	73	1
1:A:43:LEU:CB	1:E:44:LEU:CD1	0.46	2.93	35	2
1:C:41:CYS:HA	1:D:40:ILE:CG1	0.46	2.41	21	4
1:A:36:CYS:CA	1:E:41:CYS:SG	0.46	3.03	23	1
1:A:51:LEU:HG	1:E:51:LEU:CD1	0.46	2.40	60	2
1:C:45:ILE:CA	1:D:43:LEU:HD22	0.46	2.40	44	1
1:B:41:CYS:HB2	1:C:39:LEU:CD2	0.46	2.41	147	1
1:C:37:LEU:HD11	1:D:33:ILE:HG23	0.46	1.87	10	2
1:D:52:LEU:HD23	1:E:50:MET:SD	0.46	2.50	31	3
1:A:43:LEU:HD13	1:E:41:CYS:HA	0.46	1.86	147	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:44:LEU:CD1	1:E:43:LEU:CB	0.46	2.93	35	2
1:A:33:ILE:HG23	1:E:37:LEU:HD11	0.46	1.87	10	1
1:D:45:ILE:CA	1:E:43:LEU:HD22	0.46	2.41	44	1
1:B:48:ILE:HG13	1:C:47:ILE:HG23	0.46	1.85	45	1
1:D:44:LEU:CD1	1:E:40:ILE:HA	0.46	2.41	73	1
1:D:47:ILE:HG22	1:D:51:LEU:HD11	0.45	1.87	26	1
1:B:51:LEU:HD11	1:C:47:ILE:HG22	0.45	1.87	31	3
1:B:44:LEU:HD21	1:C:44:LEU:HD21	0.45	1.88	44	1
1:B:48:ILE:HD11	1:C:46:CYS:HB2	0.45	1.88	84	1
1:A:47:ILE:HA	1:E:51:LEU:HD12	0.45	1.87	145	2
1:C:51:LEU:HD12	1:D:47:ILE:HA	0.45	1.87	145	2
1:D:41:CYS:HB2	1:E:39:LEU:CD2	0.45	2.41	147	1
1:B:38:ILE:CA	1:B:41:CYS:SG	0.45	3.03	92	4
1:A:47:ILE:HG22	1:E:51:LEU:HD11	0.45	1.87	31	3
1:A:45:ILE:CA	1:B:43:LEU:HD22	0.45	2.40	44	1
1:A:47:ILE:HD13	1:E:48:ILE:HG12	0.45	1.88	46	1
1:C:44:LEU:CD1	1:D:40:ILE:HA	0.45	2.41	73	1
1:A:44:LEU:HD21	1:E:44:LEU:HD21	0.45	1.88	44	1
1:D:51:LEU:HD12	1:E:47:ILE:HA	0.45	1.87	145	2
1:B:51:LEU:HD22	1:C:51:LEU:HG	0.45	1.88	129	1
1:A:47:ILE:HG21	1:B:47:ILE:HD13	0.45	1.87	58	4
1:B:45:ILE:CA	1:C:43:LEU:HD22	0.45	2.40	44	1
1:C:44:LEU:HD21	1:D:44:LEU:HD21	0.45	1.88	44	1
1:B:41:CYS:HA	1:C:40:ILE:CG1	0.45	2.41	21	4
1:B:41:CYS:HB3	1:C:39:LEU:HD22	0.45	1.88	27	1
1:D:41:CYS:HB3	1:E:39:LEU:HD22	0.45	1.88	27	1
1:C:48:ILE:HG12	1:D:47:ILE:HD13	0.45	1.89	46	1
1:A:44:LEU:CD1	1:B:40:ILE:HA	0.45	2.41	73	1
1:B:48:ILE:HG23	1:C:50:MET:HG3	0.45	1.87	84	1
1:A:39:LEU:CD2	1:E:41:CYS:HB2	0.45	2.41	147	1
1:A:37:LEU:HD11	1:B:33:ILE:HG23	0.45	1.87	10	2
1:C:22:GLN:HA	1:C:25:ARG:HD3	0.45	1.89	145	27
1:D:44:LEU:HD21	1:E:44:LEU:HD21	0.45	1.88	44	1
1:A:40:ILE:HA	1:E:44:LEU:CD1	0.45	2.41	73	1
1:A:48:ILE:HD11	1:B:46:CYS:HB2	0.45	1.88	84	1
1:B:47:ILE:HG22	1:B:51:LEU:HD11	0.45	1.87	26	2
1:B:22:GLN:HA	1:B:25:ARG:HD3	0.45	1.89	124	24
1:A:32:PHE:HE1	1:E:37:LEU:HB2	0.45	1.70	34	4
1:A:43:LEU:HD22	1:E:44:LEU:HB2	0.45	1.88	1	3
1:A:47:ILE:HD13	1:E:47:ILE:HG21	0.45	1.89	48	4
1:C:47:ILE:HG21	1:D:47:ILE:HD13	0.45	1.88	58	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:47:ILE:HG21	1:E:47:ILE:HD13	0.45	1.88	58	4
1:E:22:GLN:HA	1:E:25:ARG:HD3	0.45	1.89	168	24
1:A:44:LEU:HD21	1:B:44:LEU:HD21	0.45	1.88	44	1
1:D:48:ILE:HG12	1:E:47:ILE:HD13	0.45	1.89	46	1
1:A:46:CYS:HB2	1:E:48:ILE:HD11	0.45	1.87	84	1
1:A:50:MET:CB	1:E:51:LEU:HB2	0.45	2.41	12	3
1:A:32:PHE:CD1	1:A:32:PHE:C	0.45	2.89	22	6
1:C:37:LEU:HB2	1:D:32:PHE:HE1	0.45	1.69	34	5
1:B:51:LEU:HB2	1:C:50:MET:CB	0.45	2.41	12	1
1:C:37:LEU:CD1	1:D:36:CYS:SG	0.45	3.05	147	2
1:E:32:PHE:CD1	1:E:32:PHE:C	0.45	2.89	22	7
1:A:48:ILE:HG12	1:B:47:ILE:HD13	0.45	1.89	46	1
1:D:44:LEU:HB2	1:E:43:LEU:HD22	0.44	1.89	1	3
1:E:38:ILE:CA	1:E:41:CYS:SG	0.44	3.02	9	4
1:A:47:ILE:HG22	1:A:51:LEU:HD11	0.44	1.87	26	1
1:C:44:LEU:HD12	1:D:40:ILE:HA	0.44	1.89	36	1
1:D:14:ARG:NH2	1:D:15:ALA:HB2	0.44	2.27	75	3
1:C:38:ILE:CA	1:C:41:CYS:SG	0.44	3.02	9	7
1:D:51:LEU:HB2	1:E:50:MET:CB	0.44	2.41	12	2
1:D:41:CYS:HA	1:E:40:ILE:CG1	0.44	2.41	21	4
1:E:47:ILE:HG22	1:E:51:LEU:HD11	0.44	1.87	26	1
1:A:39:LEU:HD22	1:E:41:CYS:HB3	0.44	1.88	27	1
1:A:41:CYS:HB3	1:B:39:LEU:HD22	0.44	1.88	27	1
1:C:41:CYS:CB	1:D:39:LEU:HD22	0.44	2.42	27	1
1:D:41:CYS:CB	1:E:39:LEU:HD22	0.44	2.42	27	1
1:A:22:GLN:HA	1:A:25:ARG:HD3	0.44	1.89	159	29
1:D:37:LEU:HB2	1:E:32:PHE:HE1	0.44	1.70	34	5
1:B:48:ILE:HG13	1:C:47:ILE:HA	0.44	1.88	147	2
1:B:37:LEU:CD1	1:C:32:PHE:CE1	0.44	2.92	147	1
1:A:37:LEU:CD1	1:B:36:CYS:SG	0.44	3.05	147	2
1:A:14:ARG:NH2	1:A:15:ALA:HB2	0.44	2.27	180	4
1:A:44:LEU:HD12	1:B:40:ILE:HA	0.44	1.89	36	1
1:B:51:LEU:HD12	1:C:47:ILE:HA	0.44	1.87	145	2
1:C:41:CYS:HA	1:D:43:LEU:CD1	0.44	2.43	147	1
1:B:44:LEU:HB2	1:C:43:LEU:HD22	0.44	1.86	35	3
1:B:37:LEU:HD11	1:C:33:ILE:HG23	0.44	1.87	10	1
1:C:47:ILE:HG22	1:C:51:LEU:HD11	0.44	1.87	26	1
1:A:45:ILE:HA	1:B:43:LEU:HD21	0.44	1.90	56	1
1:D:22:GLN:HA	1:D:25:ARG:HD3	0.44	1.90	52	26
1:A:51:LEU:HB2	1:B:50:MET:CB	0.44	2.41	12	1
1:A:38:ILE:HA	1:B:32:PHE:CE1	0.44	2.48	27	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LEU:HD21	1:E:45:ILE:HA	0.44	1.89	56	1
1:B:41:CYS:HA	1:C:43:LEU:CD1	0.44	2.43	147	1
1:B:45:ILE:CD1	1:C:39:LEU:HD21	0.44	2.43	66	1
1:B:38:ILE:CA	1:C:36:CYS:SG	0.44	3.02	59	2
1:D:41:CYS:HB3	1:E:40:ILE:CG1	0.44	2.43	9	2
1:C:32:PHE:CD1	1:C:32:PHE:C	0.44	2.91	39	9
1:B:41:CYS:HA	1:C:40:ILE:HG13	0.44	1.88	37	2
1:D:41:CYS:HA	1:E:40:ILE:HG13	0.44	1.88	37	2
1:D:38:ILE:HG23	1:E:32:PHE:HE1	0.44	1.73	98	1
1:D:48:ILE:HA	1:D:51:LEU:HD11	0.44	1.90	129	1
1:D:37:LEU:CD1	1:E:32:PHE:CE1	0.44	2.92	147	1
1:A:36:CYS:SG	1:E:38:ILE:CA	0.44	3.02	59	2
1:A:41:CYS:CB	1:B:39:LEU:HD22	0.44	2.42	27	1
1:D:38:ILE:HA	1:E:32:PHE:CE1	0.44	2.48	27	1
1:A:39:LEU:HD21	1:E:45:ILE:CD1	0.44	2.43	66	1
1:E:14:ARG:NH2	1:E:15:ALA:HB2	0.44	2.27	180	2
1:A:38:ILE:HG23	1:B:32:PHE:HE1	0.44	1.73	98	1
1:D:41:CYS:HA	1:E:43:LEU:CD1	0.44	2.43	147	1
1:A:41:CYS:HB3	1:B:40:ILE:CG1	0.44	2.43	9	1
1:C:14:ARG:NH2	1:C:15:ALA:HB2	0.44	2.27	180	3
1:B:48:ILE:HG12	1:C:47:ILE:HD13	0.44	1.88	46	1
1:A:43:LEU:CD1	1:E:41:CYS:HA	0.44	2.43	147	1
1:A:51:LEU:HD11	1:B:47:ILE:HG22	0.43	1.87	31	3
1:C:45:ILE:HA	1:D:43:LEU:HD21	0.43	1.89	56	1
1:D:45:ILE:CD1	1:E:39:LEU:HD21	0.43	2.43	66	1
1:A:32:PHE:HE1	1:E:38:ILE:HG23	0.43	1.73	98	1
1:B:41:CYS:HB3	1:C:40:ILE:CG1	0.43	2.43	9	2
1:E:27:LYS:HB3	1:E:31:LEU:HD12	0.43	1.91	10	1
1:A:39:LEU:HD22	1:E:41:CYS:CB	0.43	2.42	27	1
1:A:44:LEU:CD2	1:E:44:LEU:CD1	0.43	2.96	32	1
1:A:44:LEU:CD1	1:B:44:LEU:CD2	0.43	2.96	32	1
1:B:51:LEU:CB	1:C:50:MET:HG3	0.43	2.43	36	2
1:A:51:LEU:HD23	1:E:51:LEU:CD2	0.43	2.41	84	1
1:B:14:ARG:NH2	1:B:15:ALA:HB2	0.43	2.27	180	2
1:C:48:ILE:HG12	1:D:47:ILE:CB	0.43	2.43	129	1
1:C:41:CYS:HB3	1:D:40:ILE:CG1	0.43	2.43	9	3
1:B:41:CYS:CB	1:C:39:LEU:HD22	0.43	2.42	27	1
1:C:38:ILE:HA	1:D:32:PHE:CE1	0.43	2.48	27	1
1:C:44:LEU:CD1	1:D:44:LEU:CD2	0.43	2.96	32	1
1:D:44:LEU:CD1	1:E:44:LEU:CD2	0.43	2.96	32	1
1:D:44:LEU:HD12	1:E:40:ILE:HA	0.43	1.89	36	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:48:ILE:HD11	1:D:46:CYS:HB2	0.43	1.89	84	1
1:A:40:ILE:CG1	1:E:41:CYS:HB3	0.43	2.43	9	1
1:B:37:LEU:CD1	1:C:36:CYS:SG	0.43	3.05	147	2
1:A:32:PHE:CE1	1:E:38:ILE:HA	0.43	2.48	27	1
1:B:45:ILE:HA	1:C:43:LEU:HD21	0.43	1.89	56	1
1:D:45:ILE:HA	1:E:43:LEU:HD21	0.43	1.90	56	1
1:D:41:CYS:HG	1:E:36:CYS:HG	0.43	1.57	104	2
1:C:41:CYS:HB3	1:D:39:LEU:HD22	0.43	1.88	27	1
1:B:44:LEU:CD1	1:C:44:LEU:CD2	0.43	2.96	32	1
1:B:44:LEU:HD12	1:C:40:ILE:HA	0.43	1.89	36	1
1:A:41:CYS:HA	1:B:43:LEU:CD1	0.43	2.43	147	1
1:B:38:ILE:HA	1:C:32:PHE:CE1	0.43	2.48	27	1
1:C:37:LEU:CD1	1:D:33:ILE:HG12	0.43	2.44	38	1
1:C:37:LEU:HD13	1:D:33:ILE:HG12	0.43	1.91	77	1
1:D:32:PHE:CE1	1:D:36:CYS:SG	0.43	3.11	155	1
1:B:34:ASN:ND2	1:C:32:PHE:HB3	0.43	2.29	33	2
1:D:51:LEU:HD11	1:E:47:ILE:HG22	0.43	1.87	31	3
1:D:37:LEU:CD1	1:E:33:ILE:HG12	0.43	2.44	38	1
1:A:48:ILE:HG23	1:B:46:CYS:HB3	0.43	1.91	48	1
1:C:51:LEU:HD12	1:D:50:MET:HB2	0.43	1.89	84	1
1:A:47:ILE:CG2	1:E:51:LEU:CD1	0.43	2.94	3	2
1:A:51:LEU:CD1	1:B:47:ILE:CG2	0.43	2.94	3	1
1:A:33:ILE:HG12	1:E:37:LEU:CD1	0.43	2.44	38	1
1:A:37:LEU:CD1	1:B:33:ILE:HG12	0.43	2.44	38	1
1:B:51:LEU:CD1	1:C:47:ILE:CG2	0.43	2.96	25	2
1:A:48:ILE:HG21	1:B:46:CYS:HB3	0.43	1.91	12	1
1:A:40:ILE:HA	1:E:44:LEU:HD12	0.43	1.89	36	1
1:D:48:ILE:HG23	1:E:50:MET:CG	0.43	2.44	84	1
1:B:38:ILE:HG23	1:C:32:PHE:HE1	0.43	1.73	98	1
1:A:47:ILE:CB	1:E:48:ILE:HG12	0.43	2.44	129	1
1:B:35:PHE:CZ	1:B:39:LEU:HD13	0.43	2.49	69	3
1:A:51:LEU:CD2	1:B:51:LEU:HG	0.43	2.44	129	1
1:C:27:LYS:HB3	1:C:31:LEU:HD12	0.42	1.91	10	1
1:C:48:ILE:HG21	1:D:46:CYS:HB3	0.42	1.91	12	1
1:A:46:CYS:HB3	1:E:48:ILE:HG23	0.42	1.91	48	1
1:C:48:ILE:HG23	1:D:46:CYS:HB3	0.42	1.91	48	1
1:A:35:PHE:CZ	1:A:39:LEU:HD13	0.42	2.49	79	3
1:C:38:ILE:HG23	1:D:32:PHE:HE1	0.42	1.73	98	1
1:C:32:PHE:CE1	1:C:36:CYS:SG	0.42	3.11	155	1
1:A:28:LEU:O	1:A:32:PHE:CB	0.42	2.68	34	2
1:B:28:LEU:O	1:B:32:PHE:CB	0.42	2.68	34	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:37:LEU:CD1	1:E:36:CYS:SG	0.42	3.05	147	2
1:C:34:ASN:ND2	1:D:32:PHE:HB3	0.42	2.29	33	2
1:A:43:LEU:HB3	1:E:48:ILE:CD1	0.42	2.44	5	1
1:A:36:CYS:SG	1:E:37:LEU:CD1	0.42	3.05	147	2
1:A:32:PHE:HB3	1:E:34:ASN:ND2	0.42	2.29	33	2
1:D:51:LEU:CB	1:E:50:MET:HG3	0.42	2.44	36	2
1:C:41:CYS:CB	1:D:39:LEU:HD21	0.42	2.45	1	1
1:D:51:LEU:CD1	1:E:47:ILE:CG2	0.42	2.94	3	1
1:B:48:ILE:CD1	1:C:43:LEU:HB3	0.42	2.44	5	1
1:D:27:LYS:HB3	1:D:31:LEU:HD12	0.42	1.91	10	1
1:A:33:ILE:O	1:A:36:CYS:SG	0.42	2.76	15	4
1:A:34:ASN:ND2	1:B:32:PHE:HB3	0.42	2.29	33	1
1:A:37:LEU:HD13	1:B:33:ILE:HG12	0.42	1.91	77	1
1:D:48:ILE:HG21	1:E:46:CYS:HB3	0.42	1.91	12	1
1:D:34:ASN:ND2	1:E:32:PHE:HB3	0.42	2.29	33	2
1:C:51:LEU:CD1	1:D:47:ILE:CG2	0.42	2.94	3	1
1:D:35:PHE:CZ	1:D:39:LEU:HD13	0.42	2.49	69	4
1:D:32:PHE:CD1	1:D:32:PHE:C	0.42	2.93	27	7
1:A:51:LEU:HD22	1:B:51:LEU:HD23	0.42	1.92	131	1
1:C:28:LEU:O	1:C:32:PHE:CB	0.42	2.68	34	2
1:E:28:LEU:O	1:E:32:PHE:CB	0.42	2.68	34	2
1:A:48:ILE:CD1	1:B:43:LEU:HB3	0.42	2.44	5	1
1:C:35:PHE:CZ	1:C:39:LEU:HD13	0.42	2.49	79	4
1:D:28:LEU:O	1:D:32:PHE:CB	0.42	2.68	34	1
1:E:44:LEU:CA	1:E:47:ILE:HG13	0.42	2.44	45	1
1:A:45:ILE:CD1	1:B:39:LEU:HD21	0.42	2.43	66	1
1:C:48:ILE:CD1	1:D:43:LEU:HB3	0.42	2.44	5	1
1:D:48:ILE:CD1	1:E:43:LEU:HB3	0.42	2.44	5	1
1:B:48:ILE:HG21	1:C:46:CYS:HB3	0.42	1.91	12	1
1:B:37:LEU:HD13	1:C:33:ILE:HG12	0.42	1.91	77	1
1:A:46:CYS:HB3	1:E:48:ILE:HG21	0.42	1.91	12	1
1:A:51:LEU:CB	1:B:50:MET:HG3	0.42	2.45	36	2
1:A:37:LEU:CD1	1:B:32:PHE:CE1	0.42	2.92	147	1
1:D:21:PRO:O	1:D:23:GLN:N	0.41	2.53	135	69
1:E:21:PRO:O	1:E:23:GLN:N	0.41	2.53	135	56
1:B:27:LYS:HB3	1:B:31:LEU:HD12	0.41	1.91	10	1
1:B:44:LEU:CD2	1:C:44:LEU:HD23	0.41	2.45	12	1
1:A:47:ILE:CA	1:E:48:ILE:CG1	0.41	2.97	84	1
1:B:21:PRO:O	1:B:23:GLN:N	0.41	2.54	114	56
1:B:37:LEU:CD1	1:C:33:ILE:HG12	0.41	2.44	38	1
1:A:21:PRO:O	1:A:23:GLN:N	0.41	2.54	89	53

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LEU:CD2	1:B:44:LEU:HD23	0.41	2.46	12	1
1:C:51:LEU:CB	1:D:50:MET:HG3	0.41	2.45	36	2
1:C:38:ILE:CA	1:D:36:CYS:SG	0.41	3.02	59	1
1:C:21:PRO:O	1:C:23:GLN:N	0.41	2.53	151	60
1:A:50:MET:HG3	1:E:51:LEU:CB	0.41	2.46	176	2
1:D:48:ILE:HG23	1:E:46:CYS:HB3	0.41	1.91	48	1
1:D:51:LEU:HD22	1:E:51:LEU:HD23	0.41	1.92	131	1
1:E:35:PHE:CZ	1:E:39:LEU:HD13	0.41	2.49	69	3
1:B:48:ILE:HG23	1:C:46:CYS:HB3	0.41	1.91	48	1
1:A:51:LEU:HG	1:E:51:LEU:HD11	0.41	1.93	165	1
1:A:27:LYS:HB3	1:A:31:LEU:HD12	0.41	1.91	10	1
1:C:51:LEU:HD11	1:D:51:LEU:HG	0.41	1.93	165	1
1:A:44:LEU:HD23	1:E:44:LEU:CD2	0.41	2.45	12	1
1:D:38:ILE:CA	1:E:36:CYS:SG	0.41	3.02	59	1
1:C:44:LEU:CD2	1:D:44:LEU:HD23	0.41	2.45	12	1
1:A:44:LEU:HD13	1:B:44:LEU:CG	0.41	2.46	13	1
1:A:44:LEU:CG	1:E:44:LEU:HD13	0.41	2.46	13	1
1:C:51:LEU:HD22	1:D:51:LEU:HD23	0.41	1.92	131	1
1:A:48:ILE:CD1	1:B:47:ILE:CG1	0.41	2.99	55	1
1:D:37:LEU:HD13	1:E:33:ILE:HG12	0.41	1.91	77	1
1:D:44:LEU:CD2	1:E:44:LEU:HD23	0.40	2.46	12	1
1:C:48:ILE:HG13	1:D:47:ILE:HG23	0.40	1.85	45	1
1:A:33:ILE:HG12	1:E:37:LEU:HD13	0.40	1.91	77	1
1:B:51:LEU:HB2	1:C:50:MET:HB2	0.40	1.93	12	1
1:B:48:ILE:HG12	1:C:47:ILE:CB	0.40	2.46	129	1
1:B:51:LEU:HD22	1:C:51:LEU:HD23	0.40	1.92	131	1
1:A:50:MET:HB2	1:E:51:LEU:HB2	0.40	1.93	12	1
1:A:36:CYS:O	1:E:41:CYS:SG	0.40	2.80	59	1
1:B:41:CYS:SG	1:C:36:CYS:O	0.40	2.80	59	1
1:C:41:CYS:SG	1:D:36:CYS:O	0.40	2.80	59	1
1:B:44:LEU:HD13	1:C:44:LEU:CG	0.40	2.46	13	1
1:C:44:LEU:HD13	1:D:44:LEU:CG	0.40	2.46	13	1
1:D:48:ILE:HG13	1:E:47:ILE:HG23	0.40	1.85	45	1
1:B:34:ASN:O	1:B:38:ILE:HG13	0.40	2.17	59	1
1:C:34:ASN:O	1:C:38:ILE:HG13	0.40	2.17	59	1
1:D:34:ASN:O	1:D:38:ILE:HG13	0.40	2.17	59	1
1:D:48:ILE:CG1	1:E:47:ILE:CA	0.40	2.98	84	1
1:D:48:ILE:O	1:D:51:LEU:HG	0.40	2.17	129	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	50/52 (96%)	45±1 (89±1%)	5±1 (11±1%)	0±0 (0±0%)	100	100
1	B	50/52 (96%)	45±1 (89±1%)	5±1 (11±1%)	0±0 (0±0%)	100	100
1	C	50/52 (96%)	45±1 (89±1%)	5±1 (11±1%)	0±0 (0±0%)	100	100
1	D	50/52 (96%)	45±1 (89±1%)	5±1 (11±1%)	0±0 (0±0%)	100	100
1	E	50/52 (96%)	45±1 (89±1%)	5±1 (11±1%)	0±0 (0±0%)	100	100
All	All	46000/47840 (96%)	41111 (89%)	4889 (11%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	49/49 (100%)	43±1 (87±3%)	6±1 (13±3%)	7	48
1	B	49/49 (100%)	43±1 (87±3%)	6±1 (13±3%)	7	48
1	C	49/49 (100%)	43±1 (87±3%)	6±1 (13±3%)	7	48
1	D	49/49 (100%)	43±1 (87±3%)	6±1 (13±3%)	7	48
1	E	49/49 (100%)	43±1 (87±3%)	6±1 (13±3%)	7	48
All	All	45080/45080 (100%)	39207 (87%)	5873 (13%)	7	48

All 100 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	13	ARG	184
1	B	13	ARG	184

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Mol	Chain	Res	Type	Models (Total)
1	C	13	ARG	184
1	D	13	ARG	184
1	E	13	ARG	184
1	C	20	MET	178
1	A	3	LYS	177
1	B	3	LYS	177
1	B	20	MET	177
1	C	3	LYS	177
1	D	3	LYS	177
1	D	20	MET	177
1	E	3	LYS	177
1	E	20	MET	176
1	A	20	MET	175
1	A	14	ARG	154
1	B	14	ARG	154
1	C	14	ARG	154
1	D	14	ARG	154
1	E	14	ARG	154
1	A	36	CYS	146
1	B	36	CYS	146
1	C	36	CYS	146
1	D	36	CYS	146
1	E	36	CYS	146
1	B	25	ARG	99
1	C	25	ARG	98
1	A	25	ARG	96
1	D	25	ARG	96
1	E	25	ARG	96
1	A	29	GLN	62
1	D	29	GLN	62
1	B	29	GLN	61
1	C	29	GLN	61
1	E	29	GLN	60
1	A	47	ILE	41
1	B	47	ILE	41
1	C	47	ILE	41
1	D	47	ILE	41
1	E	47	ILE	41
1	E	41	CYS	36
1	A	41	CYS	35
1	B	41	CYS	35
1	C	41	CYS	35

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Mol	Chain	Res	Type	Models (Total)
1	D	41	CYS	35
1	A	34	ASN	23
1	B	34	ASN	23
1	C	34	ASN	23
1	D	34	ASN	23
1	E	34	ASN	23
1	A	35	PHE	22
1	D	35	PHE	22
1	B	35	PHE	21
1	C	35	PHE	21
1	E	35	PHE	21
1	A	37	LEU	19
1	B	37	LEU	19
1	D	37	LEU	19
1	C	37	LEU	18
1	E	37	LEU	17
1	A	38	ILE	12
1	B	38	ILE	12
1	C	38	ILE	12
1	D	38	ILE	12
1	E	38	ILE	12
1	A	46	CYS	8
1	B	46	CYS	8
1	C	46	CYS	8
1	D	46	CYS	8
1	E	46	CYS	8
1	A	51	LEU	6
1	B	51	LEU	6
1	C	51	LEU	6
1	D	51	LEU	6
1	A	50	MET	6
1	B	50	MET	6
1	C	50	MET	6
1	D	50	MET	6
1	E	50	MET	6
1	E	51	LEU	5
1	A	23	GLN	3
1	A	27	LYS	3
1	B	23	GLN	3
1	B	27	LYS	3
1	C	23	GLN	3
1	C	27	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	D	23	GLN	3
1	D	27	LYS	3
1	E	23	GLN	3
1	E	27	LYS	3
1	A	39	LEU	1
1	B	39	LEU	1
1	C	39	LEU	1
1	D	39	LEU	1
1	E	39	LEU	1
1	A	48	ILE	1
1	B	48	ILE	1
1	C	48	ILE	1
1	D	48	ILE	1
1	E	48	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

No chemical shift data were provided