



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:25 AM UTC

PDB ID : 2TMP / pdb\_00002tmp  
Title : N-TERMINAL DOMAIN OF TISSUE INHIBITOR OF  
METALLOPROTEINASE-2 (N-TIMP-2), NMR, 49 STRUCTURES  
Authors : Muskett, F.W.; Frenkiel, T.A.; Feeney, J.; Freedman, R.B.; Carr, M.D.;  
Williamson, R.A.  
Deposited on : 1998-05-26

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

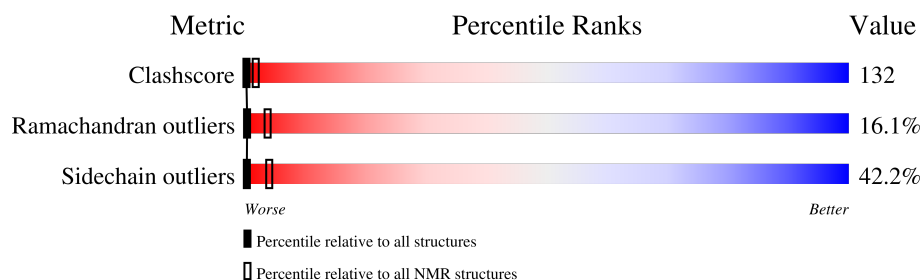
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	127	

## 2 Ensemble composition and analysis

This entry contains 49 models. Model 20 is the overall representative, medoid model (most similar to other models). The authors have identified model 3 as representative.

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:3-A:119 (117)	0.34	20

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 10 clusters and 5 single-model clusters were found.

Cluster number	Models
1	3, 4, 5, 6, 23, 25, 26, 37, 38, 40, 42
2	7, 14, 15, 29, 35, 36, 48
3	2, 9, 11, 19, 20, 27
4	8, 13, 21, 32, 44
5	1, 12, 31, 34
6	16, 30, 46
7	24, 47
8	18, 41
9	10, 17
10	22, 33
Single-model clusters	28; 39; 43; 45; 49

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1958 atoms, of which 974 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TISSUE INHIBITOR OF METALLOPROTEINASES-2.

Mol	Chain	Residues	Atoms						Trace
1	A	127	Total	C	H	N	O	S	0
			1958	620	974	166	189	9	

There is a discrepancy between the modelled and reference sequences:

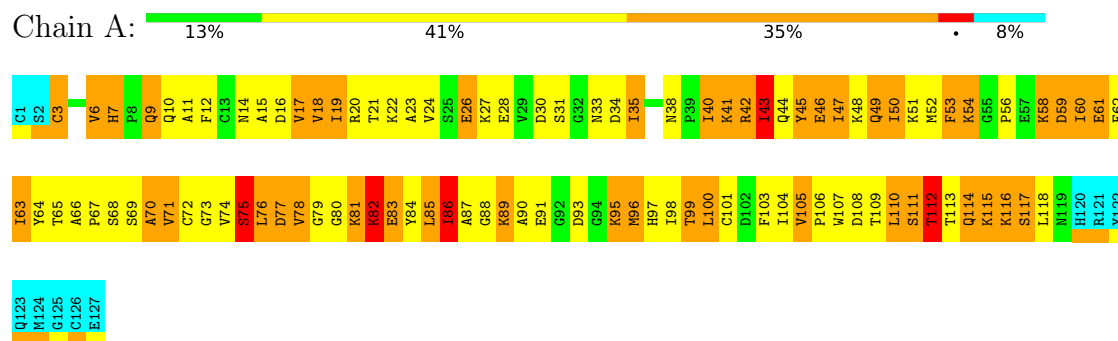
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	THR	ALA	conflict	UNP P16035

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2

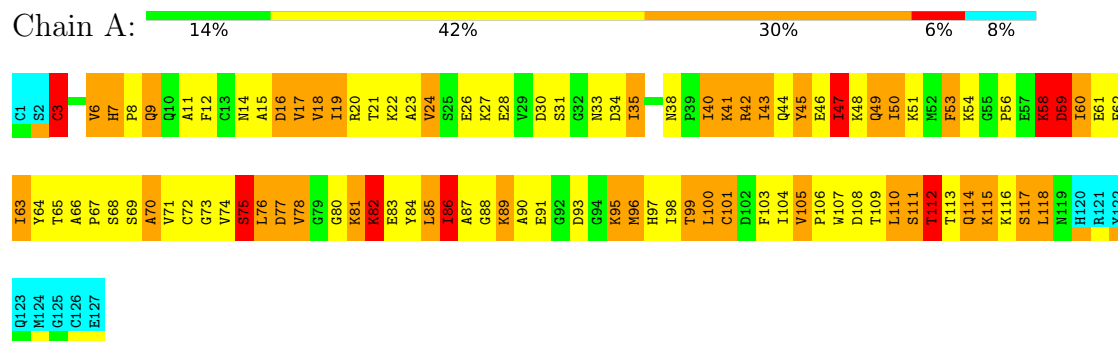


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

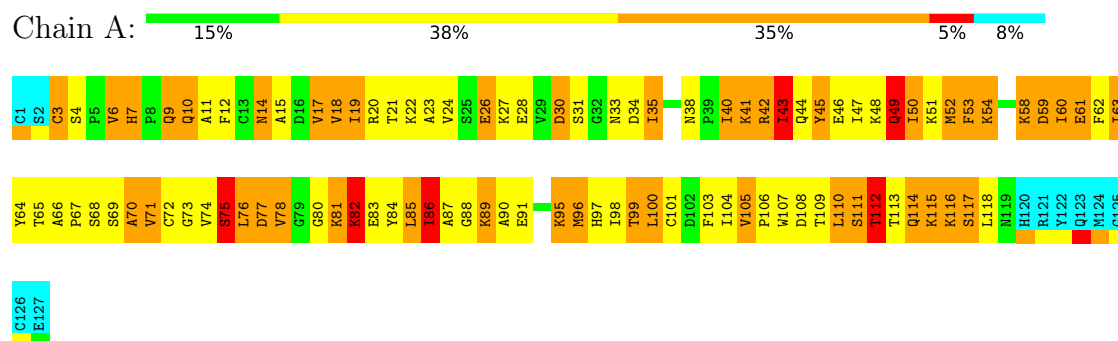
#### 4.2.1 Score per residue for model 1

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



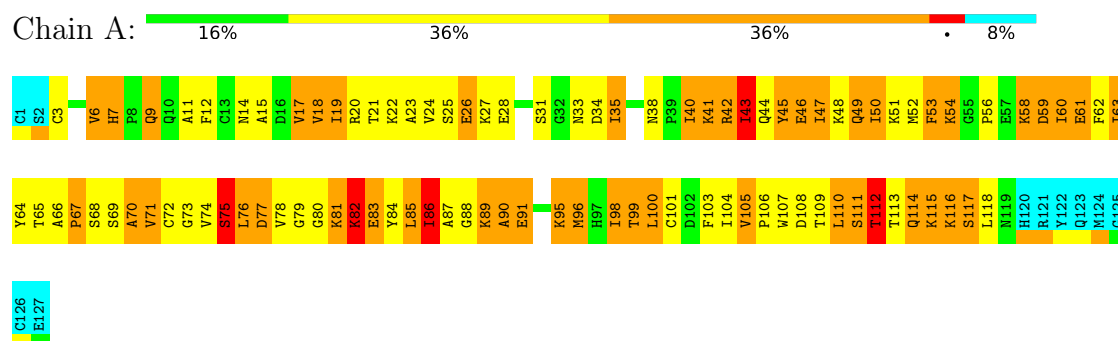
### 4.2.2 Score per residue for model 2

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



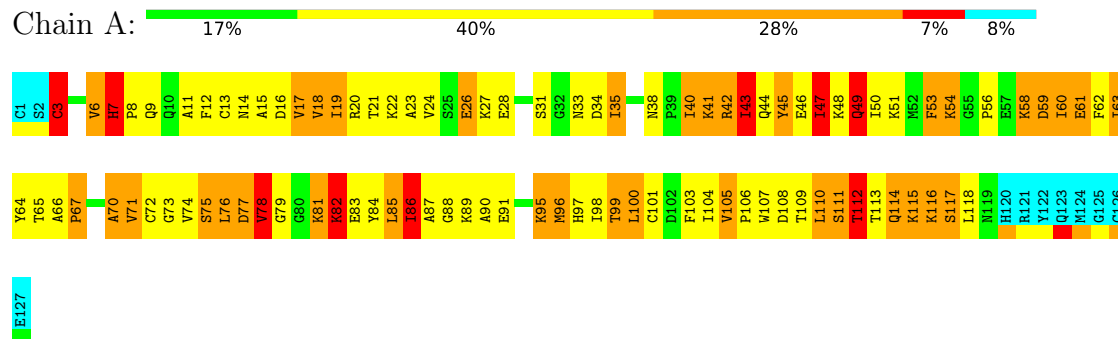
### 4.2.3 Score per residue for model 3

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



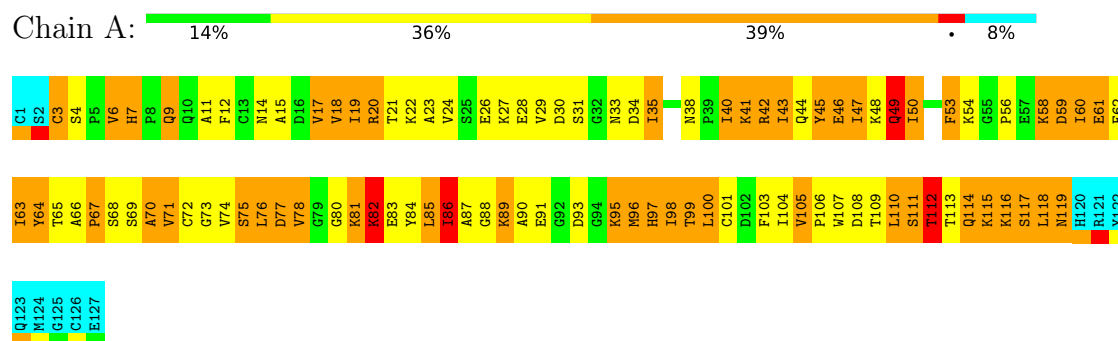
### 4.2.4 Score per residue for model 4

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



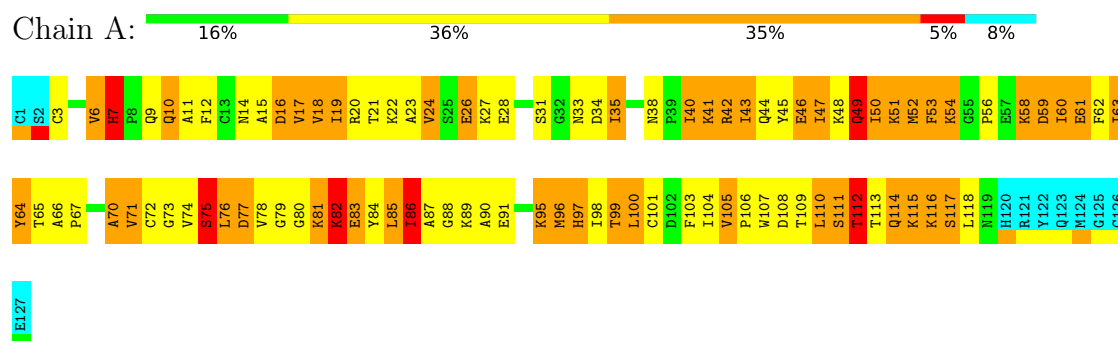
### 4.2.5 Score per residue for model 5

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



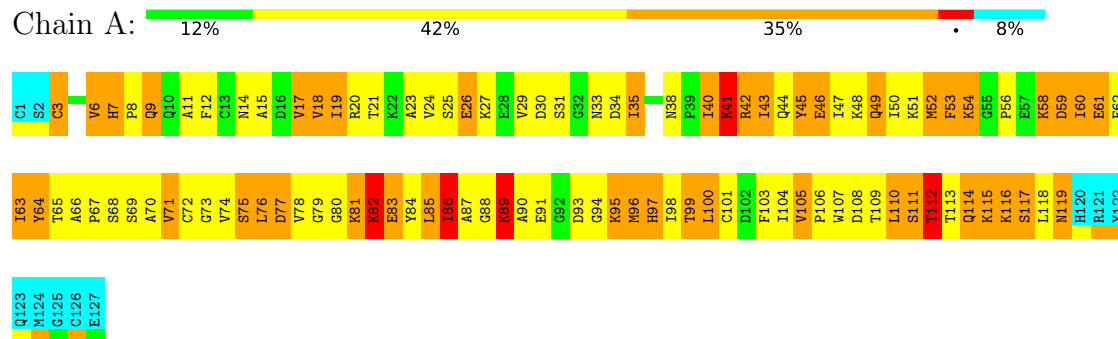
### 4.2.6 Score per residue for model 6

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



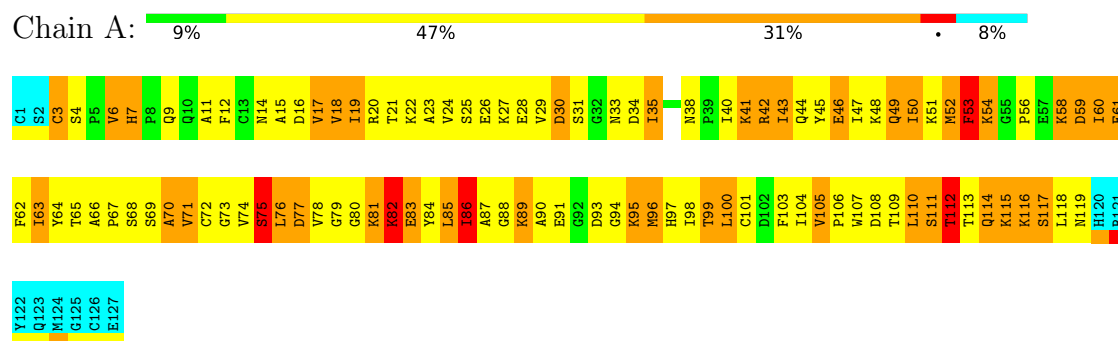
### 4.2.7 Score per residue for model 7

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



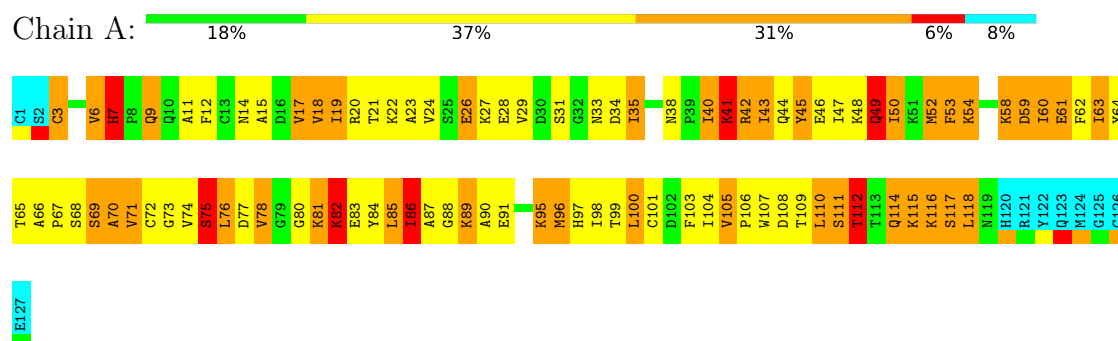
## 4.2.8 Score per residue for model 8

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



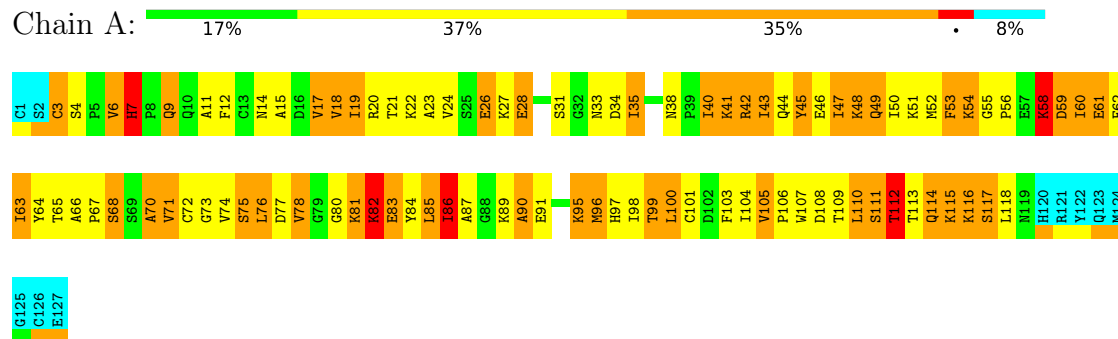
## 4.2.9 Score per residue for model 9

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



## 4.2.10 Score per residue for model 10

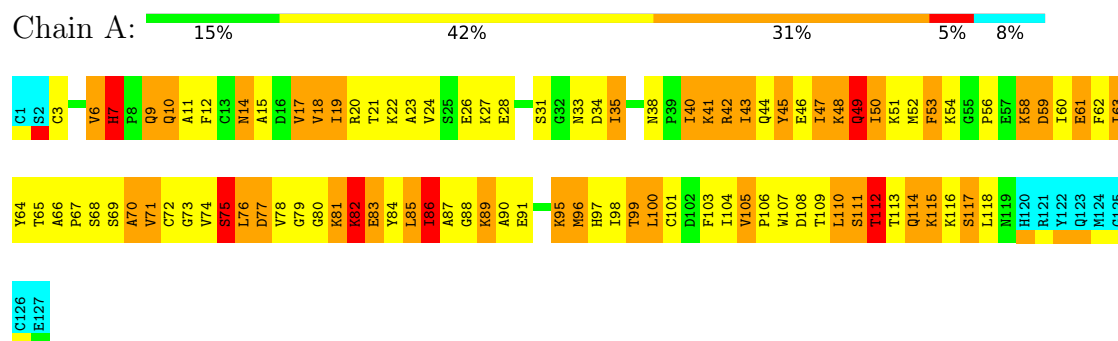
- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2





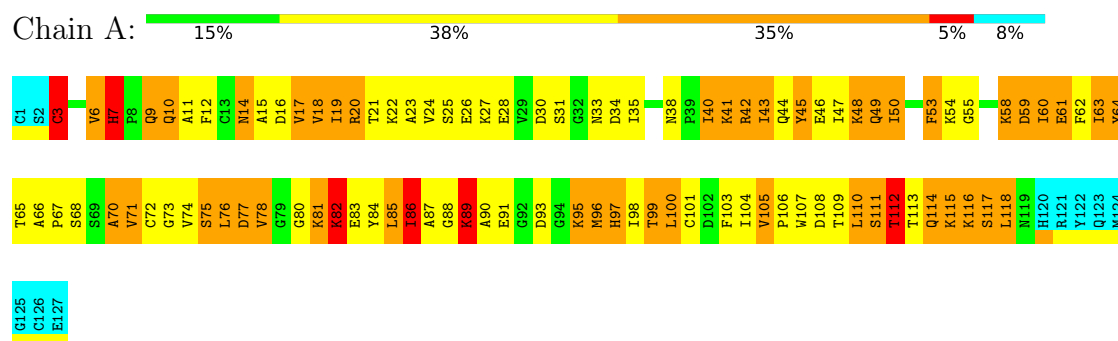
#### 4.2.11 Score per residue for model 11

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



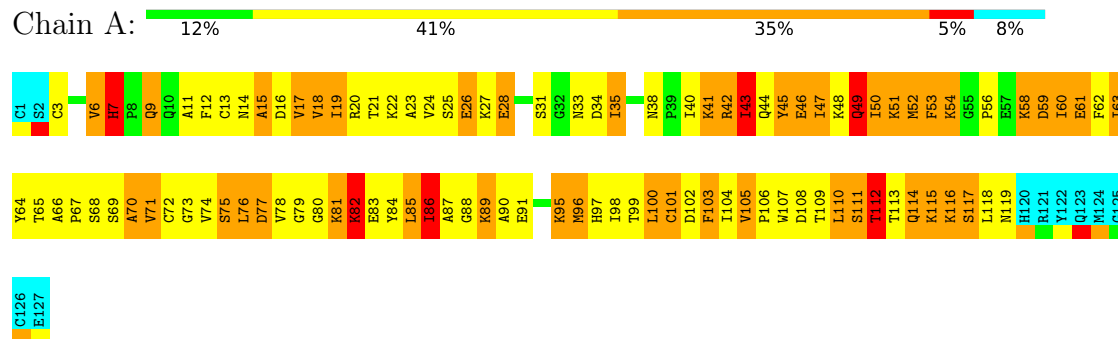
#### 4.2.12 Score per residue for model 12

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



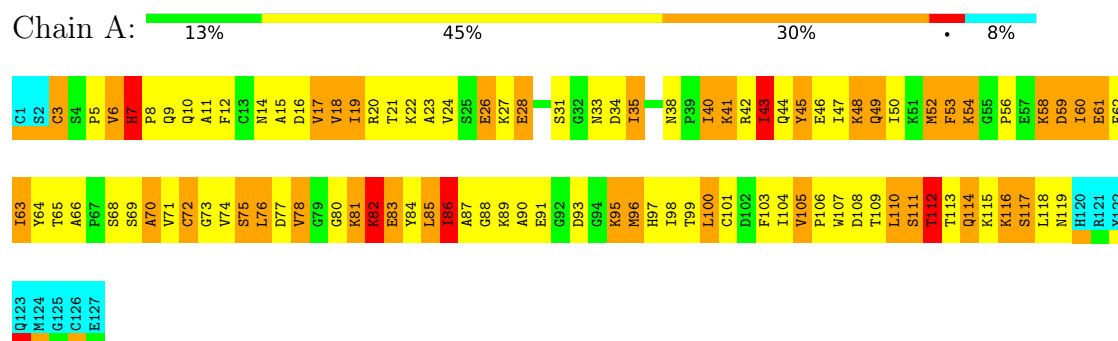
#### 4.2.13 Score per residue for model 13

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



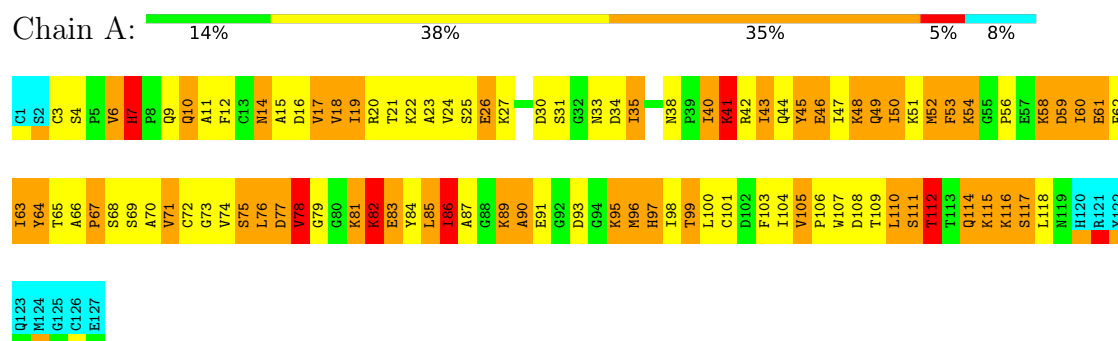
### 4.2.14 Score per residue for model 14

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



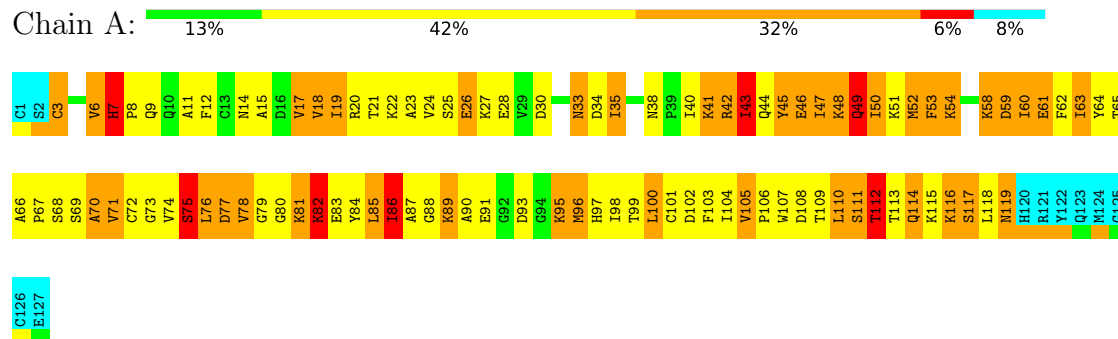
### 4.2.15 Score per residue for model 15

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



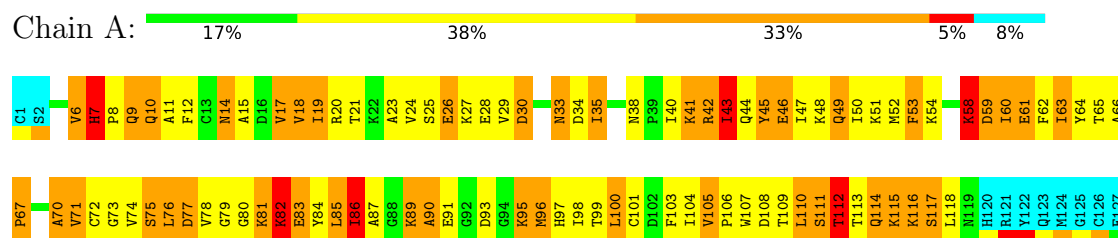
### 4.2.16 Score per residue for model 16

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



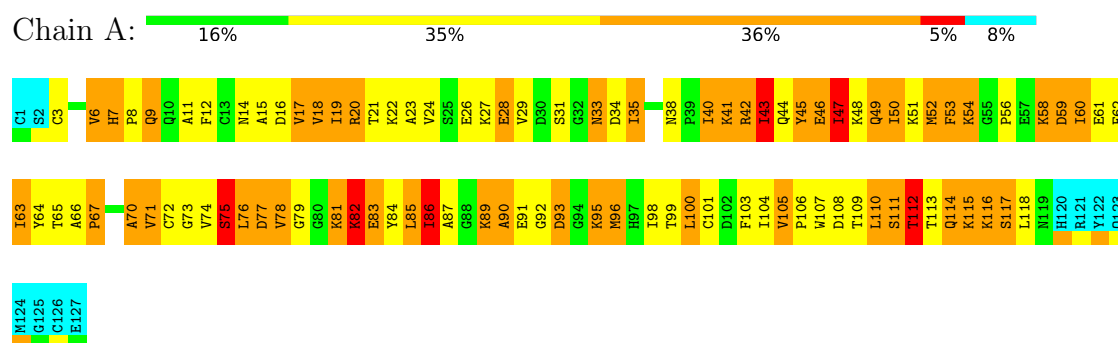
### 4.2.17 Score per residue for model 17

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



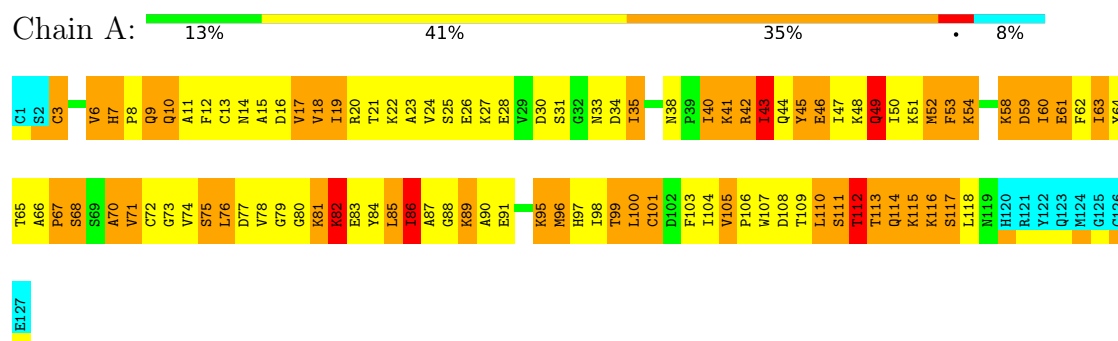
### 4.2.18 Score per residue for model 18

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



### 4.2.19 Score per residue for model 19

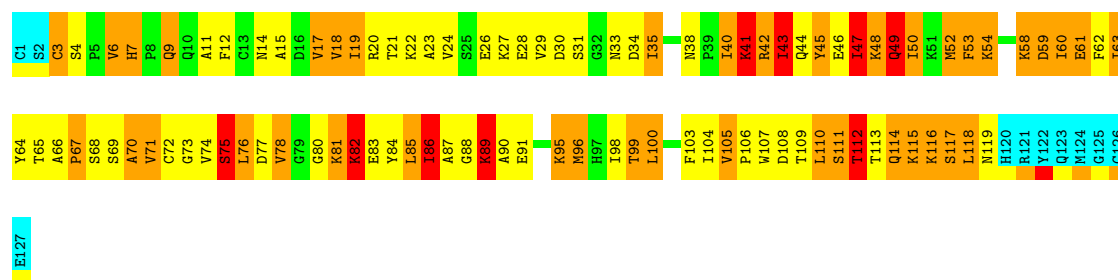
- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



### 4.2.20 Score per residue for model 20 (medoid)

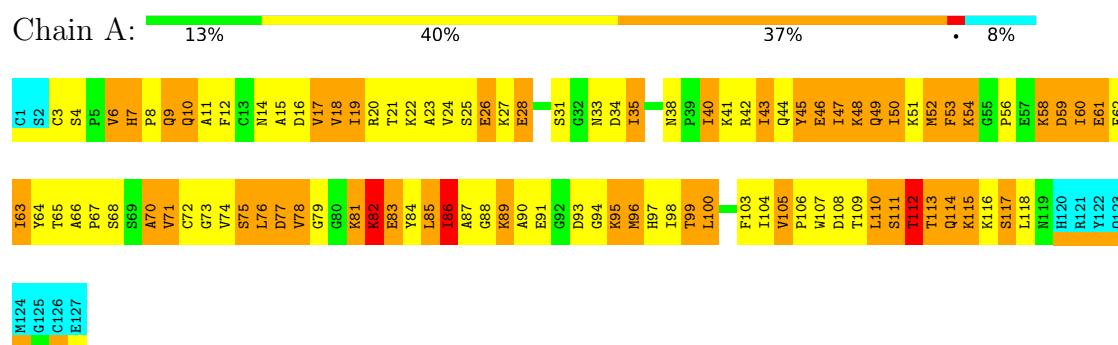
- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2





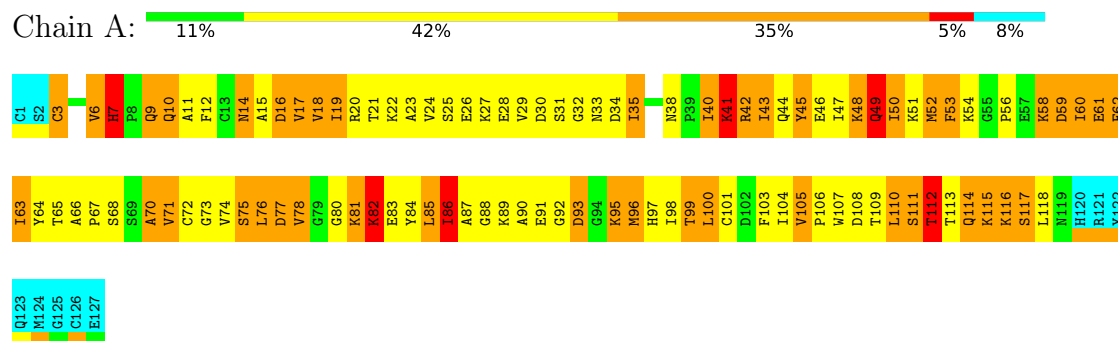
#### 4.2.21 Score per residue for model 21

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



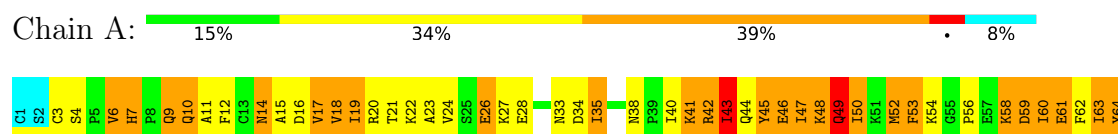
#### 4.2.22 Score per residue for model 22

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



#### 4.2.23 Score per residue for model 23

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2

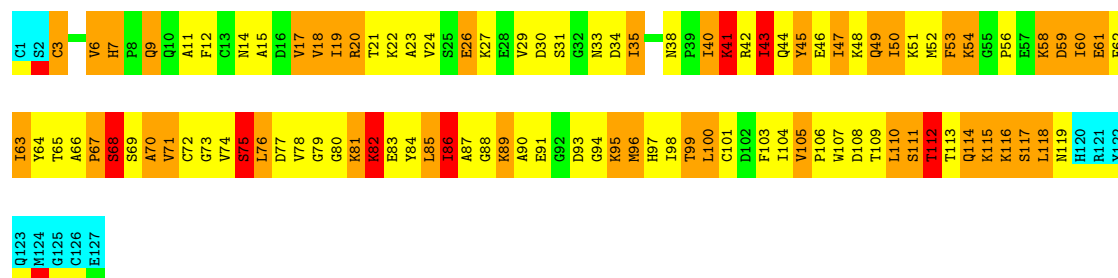




#### 4.2.24 Score per residue for model 24

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2

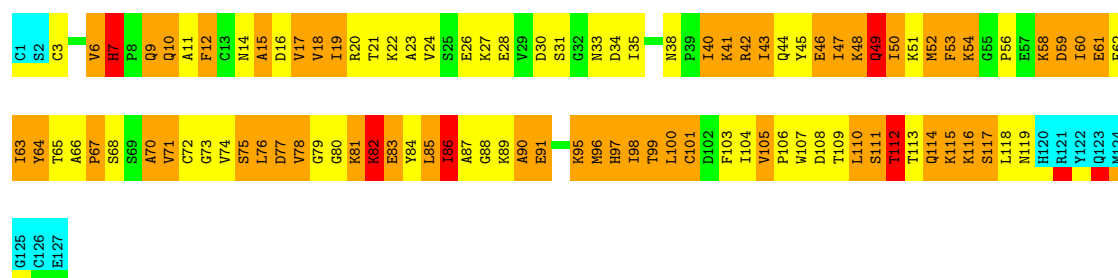
Chain A: 13% 42% 32% 6% 8%



#### 4.2.25 Score per residue for model 25

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2

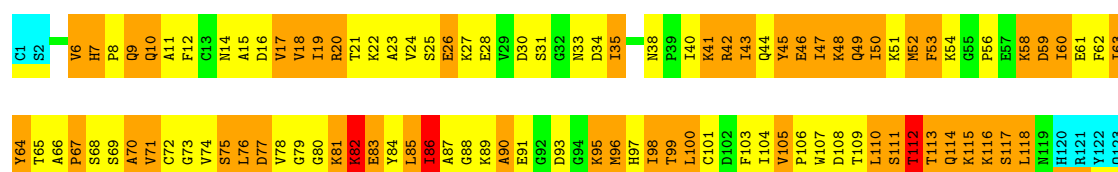
Chain A: 13% 35% 40% 8%



#### 4.2.26 Score per residue for model 26

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2

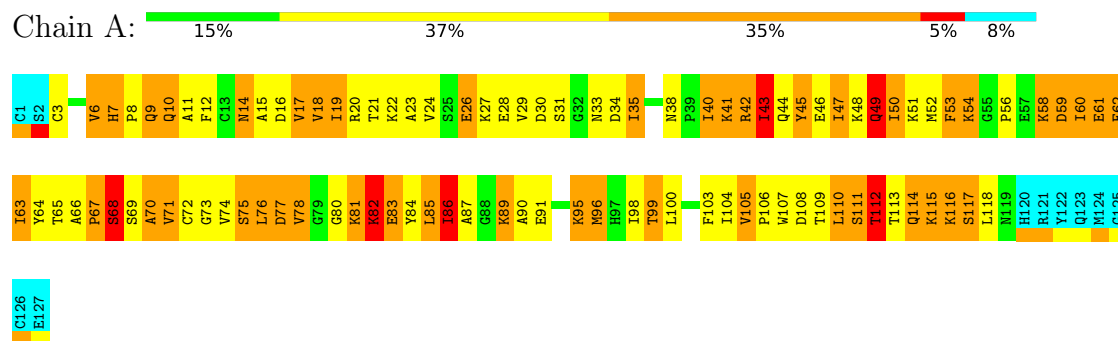
Chain A: 12% 39% 39% 8%





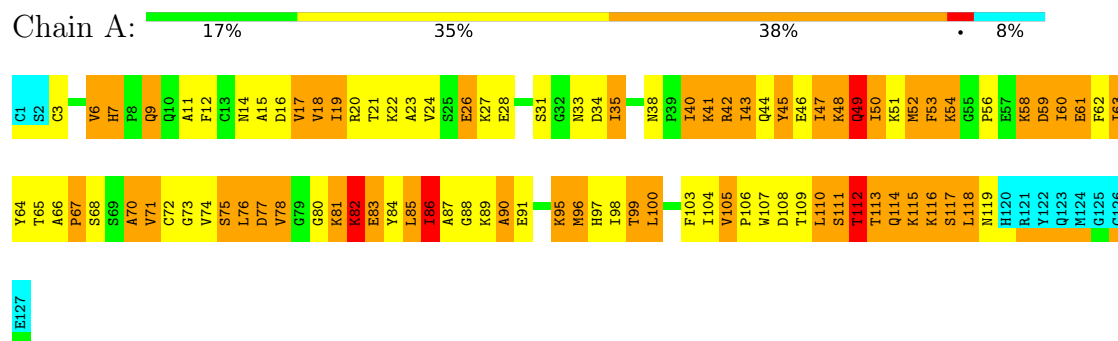
#### 4.2.27 Score per residue for model 27

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



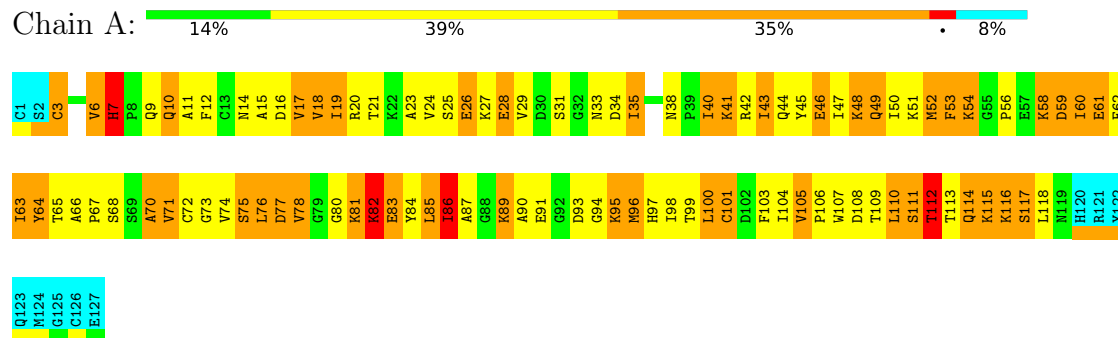
#### 4.2.28 Score per residue for model 28

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



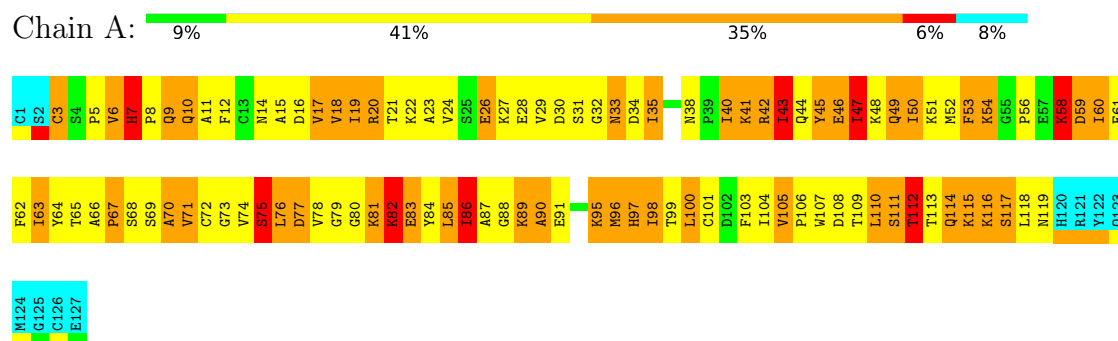
#### 4.2.29 Score per residue for model 29

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



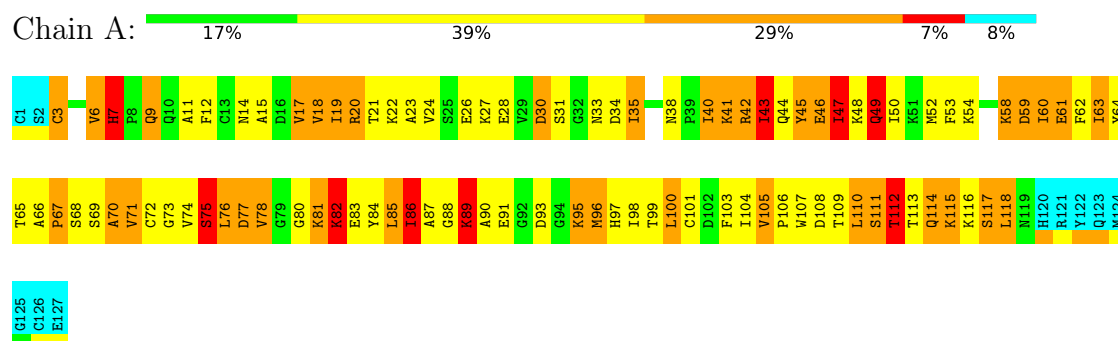
### 4.2.30 Score per residue for model 30

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



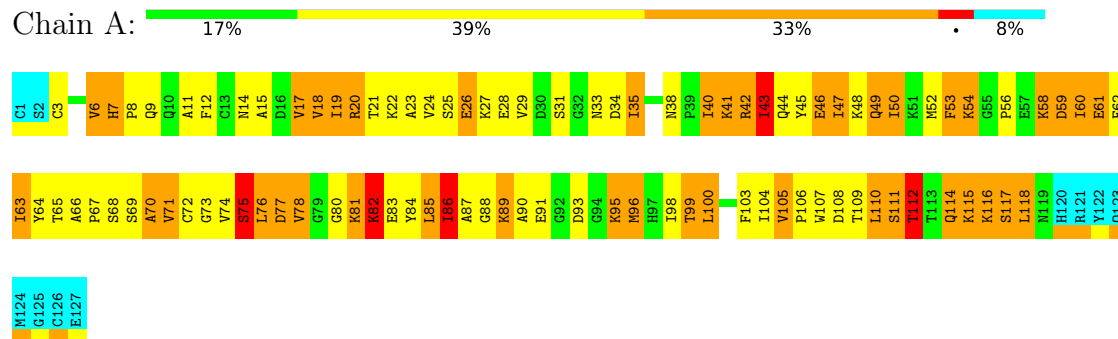
### 4.2.31 Score per residue for model 31

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



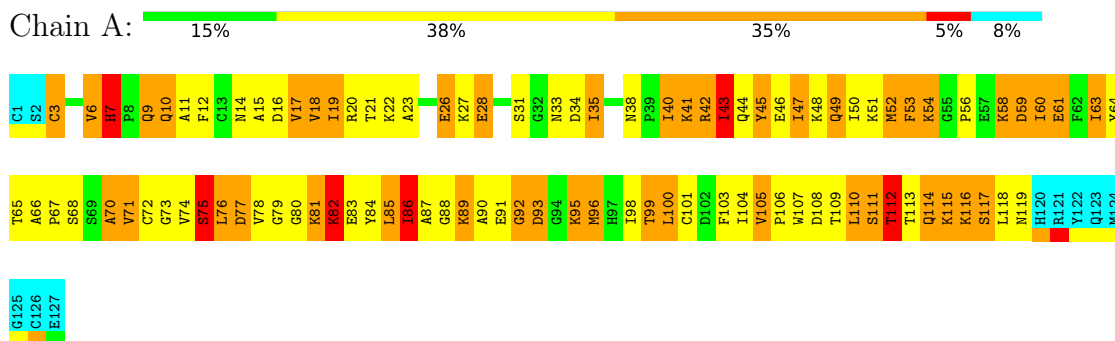
### 4.2.32 Score per residue for model 32

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



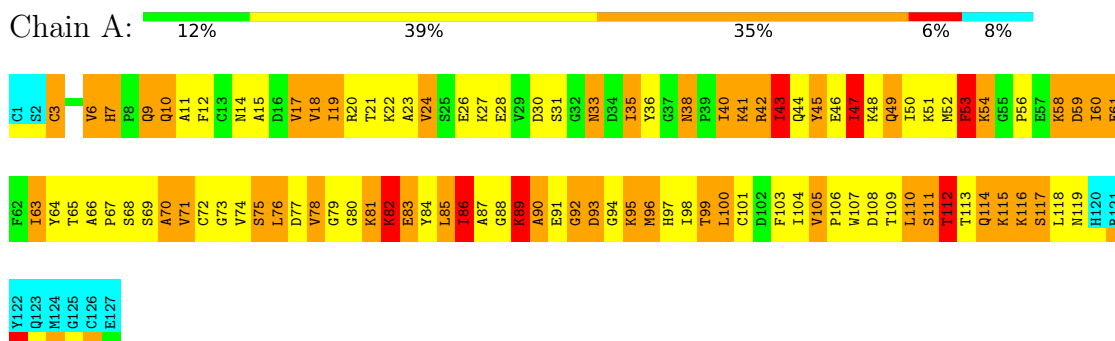
#### 4.2.33 Score per residue for model 33

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



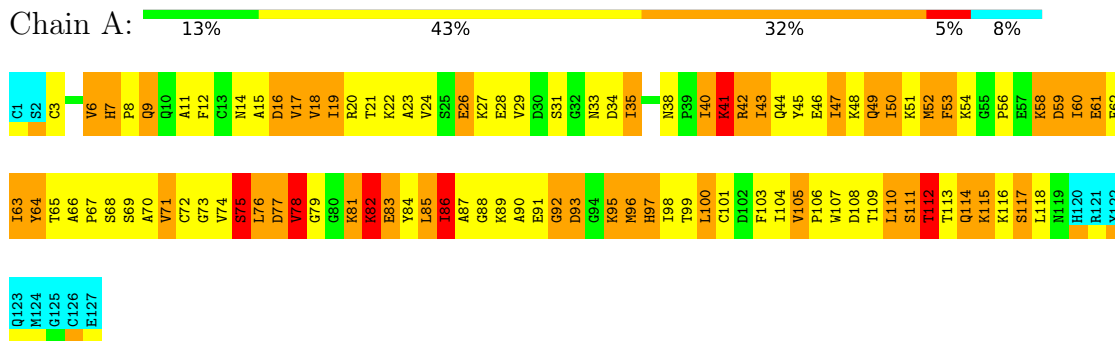
#### 4.2.34 Score per residue for model 34

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



#### 4.2.35 Score per residue for model 35

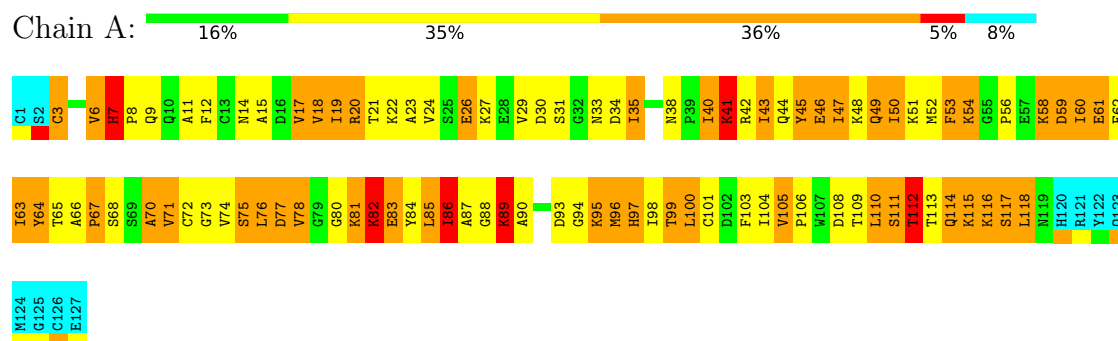
- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2





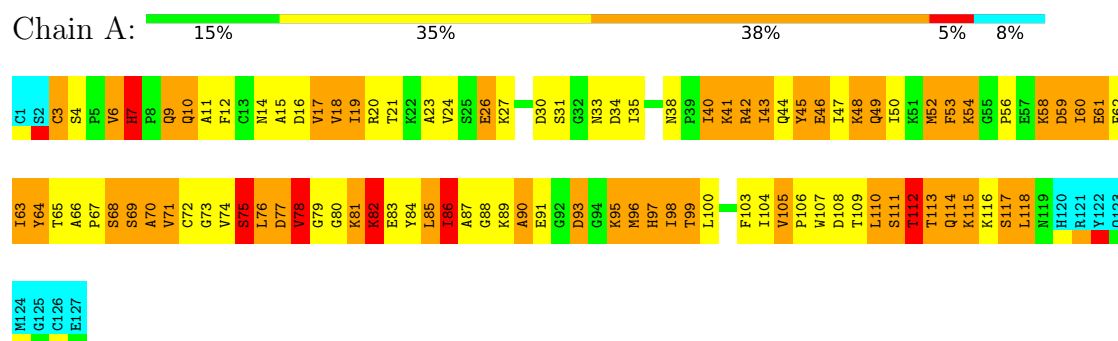
### 4.2.36 Score per residue for model 36

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



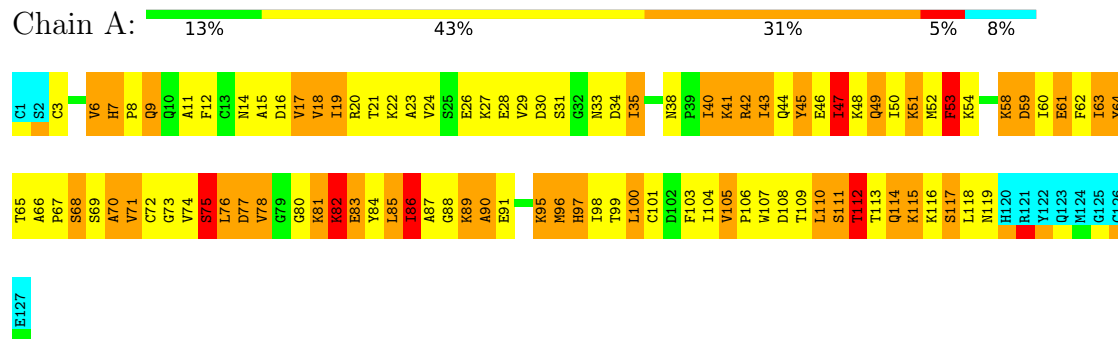
### 4.2.37 Score per residue for model 37

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



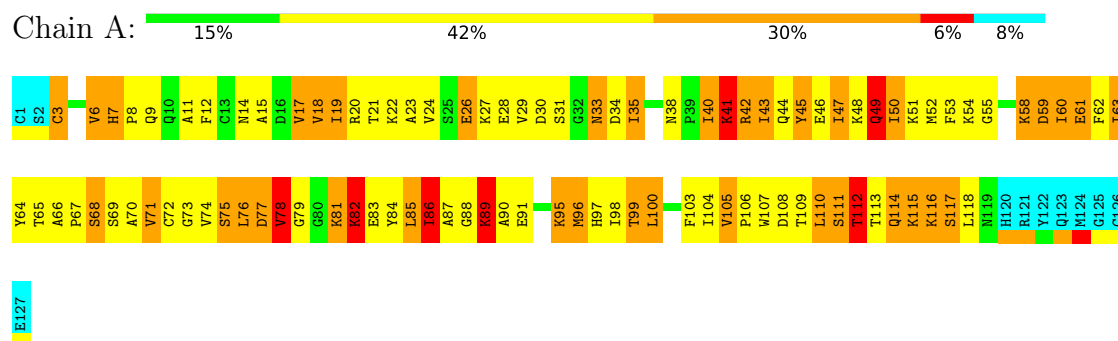
### 4.2.38 Score per residue for model 38

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



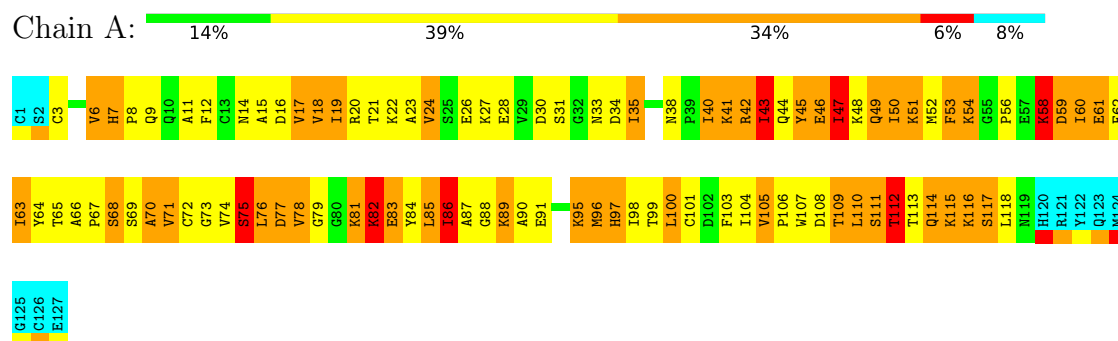
### 4.2.39 Score per residue for model 39

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



#### 4.2.42 Score per residue for model 42

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



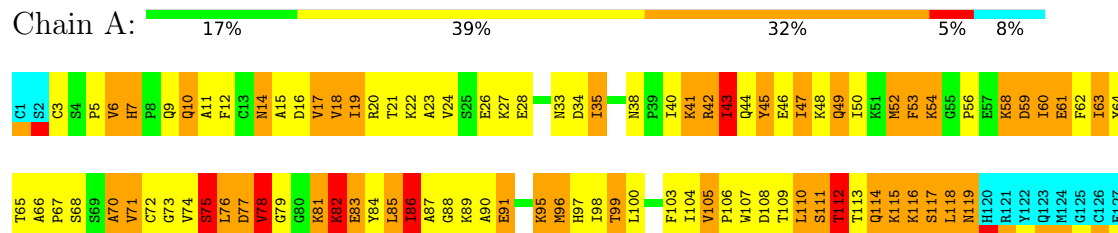
#### 4.2.43 Score per residue for model 43

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



#### 4.2.44 Score per residue for model 44

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



#### 4.2.45 Score per residue for model 45

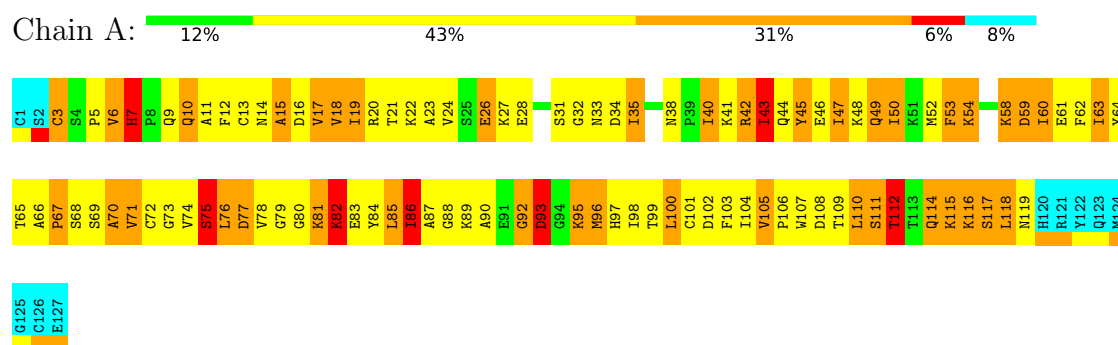
- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2





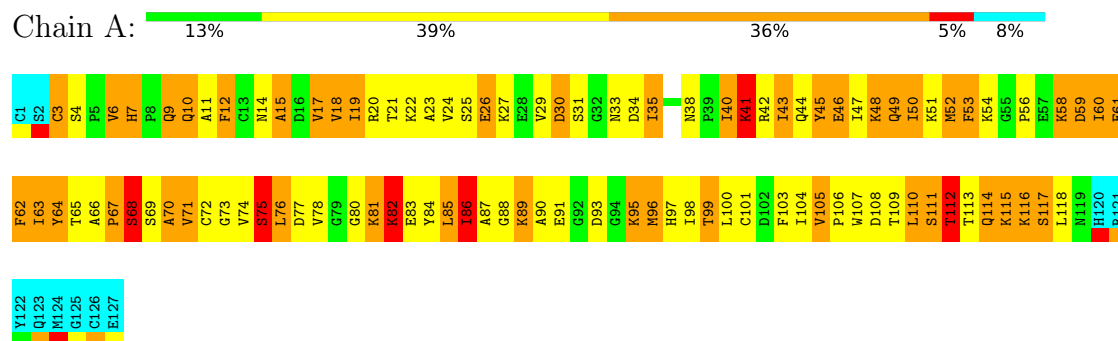
#### 4.2.46 Score per residue for model 46

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



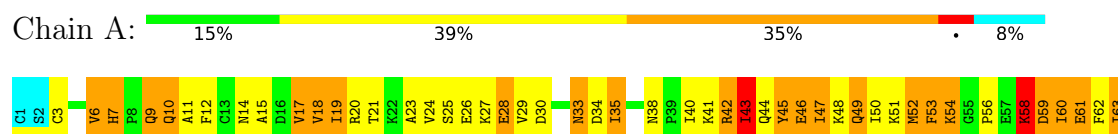
#### 4.2.47 Score per residue for model 47

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



#### 4.2.48 Score per residue for model 48

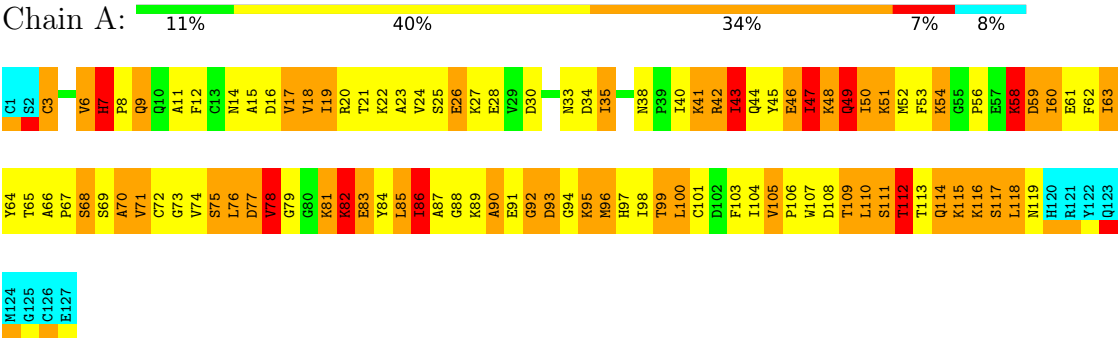
- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2





4.2.49 Score per residue for model 49

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING USING TORSION ANGLE DYNAMICS*.

Of the 100 calculated structures, 49 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
DYANA	refinement	1.4
DYANA	structure solution	

No chemical shift data was provided.

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	903	906	906	240±10
All	All	44247	44394	44394	11742

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 132.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:VAL:HG13	1:A:87:ALA:HB2	1.10	1.17	43	49
1:A:84:TYR:CG	1:A:86:ILE:HD13	1.06	1.85	41	49
1:A:84:TYR:CD1	1:A:86:ILE:HD13	1.05	1.85	31	49
1:A:76:LEU:HD13	1:A:84:TYR:CE2	1.05	1.85	20	49
1:A:63:ILE:CD1	1:A:96:MET:HE2	1.02	1.84	42	14
1:A:45:TYR:CZ	1:A:65:THR:HG21	1.02	1.89	22	49
1:A:53:PHE:CZ	1:A:118:LEU:HD13	1.01	1.90	6	25
1:A:53:PHE:CE2	1:A:118:LEU:HD22	1.01	1.91	48	22
1:A:87:ALA:HB3	1:A:103:PHE:CD2	1.00	1.92	35	49
1:A:78:VAL:HG22	1:A:82:LYS:O	0.98	1.58	2	38
1:A:74:VAL:HG23	1:A:104:ILE:HD12	0.93	1.40	48	49
1:A:12:PHE:CE1	1:A:103:PHE:CE1	0.93	2.56	8	49
1:A:60:ILE:HD13	1:A:93:ASP:O	0.93	1.63	18	1
1:A:45:TYR:CZ	1:A:76:LEU:HD12	0.92	2.00	10	49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:VAL:HG13	1:A:87:ALA:CB	0.92	1.95	25	34
1:A:47:ILE:HD11	1:A:60:ILE:O	0.91	1.66	49	7
1:A:63:ILE:HG21	1:A:98:ILE:HD13	0.91	1.42	29	49
1:A:12:PHE:CZ	1:A:103:PHE:CZ	0.91	2.59	29	49
1:A:18:VAL:CG1	1:A:87:ALA:HB2	0.90	1.96	49	49
1:A:24:VAL:HG12	1:A:78:VAL:HG11	0.90	1.40	45	39
1:A:21:THR:CG2	1:A:47:ILE:HD12	0.90	1.97	15	49
1:A:60:ILE:HG21	1:A:96:MET:HG2	0.90	1.41	42	34
1:A:86:ILE:HG13	1:A:98:ILE:HD12	0.89	1.44	26	49
1:A:53:PHE:CZ	1:A:118:LEU:HD11	0.89	2.02	45	3
1:A:60:ILE:HG21	1:A:96:MET:CG	0.89	1.98	18	41
1:A:21:THR:HG21	1:A:47:ILE:HD12	0.87	1.47	17	49
1:A:110:LEU:HD22	1:A:114:GLN:HB3	0.85	1.48	43	48
1:A:63:ILE:HD12	1:A:96:MET:HE2	0.85	1.46	42	4
1:A:53:PHE:CE2	1:A:118:LEU:HD11	0.85	2.07	45	1
1:A:12:PHE:CE1	1:A:103:PHE:CZ	0.84	2.66	35	49
1:A:43:ILE:HD13	1:A:67:PRO:HB3	0.84	1.50	25	46
1:A:53:PHE:CZ	1:A:118:LEU:HD22	0.84	2.07	42	26
1:A:86:ILE:CG1	1:A:98:ILE:HD12	0.84	2.01	41	49
1:A:45:TYR:CE2	1:A:65:THR:HG21	0.83	2.08	39	49
1:A:17:VAL:CG1	1:A:90:ALA:HB2	0.83	2.04	31	43
1:A:87:ALA:HB3	1:A:103:PHE:CE2	0.82	2.10	30	49
1:A:115:LYS:HA	1:A:118:LEU:HD12	0.82	1.49	47	15
1:A:103:PHE:O	1:A:104:ILE:HG23	0.82	1.74	13	49
1:A:86:ILE:HG22	1:A:96:MET:HE1	0.81	1.51	18	31
1:A:74:VAL:HG23	1:A:104:ILE:CD1	0.81	2.05	33	49
1:A:86:ILE:CG2	1:A:96:MET:HE1	0.80	2.06	18	27
1:A:23:ALA:CA	1:A:47:ILE:HG22	0.80	2.06	24	49
1:A:24:VAL:HG12	1:A:78:VAL:CG1	0.80	2.07	45	45
1:A:24:VAL:CG1	1:A:78:VAL:HG11	0.80	2.07	14	48
1:A:72:CYS:O	1:A:99:THR:HG22	0.79	1.77	43	29
1:A:12:PHE:CZ	1:A:103:PHE:CE1	0.79	2.70	13	49
1:A:53:PHE:CD2	1:A:118:LEU:HD22	0.79	2.13	30	21
1:A:64:TYR:CD1	1:A:97:HIS:CD2	0.78	2.70	38	13
1:A:66:ALA:HB1	1:A:71:VAL:HG22	0.78	1.54	41	6
1:A:76:LEU:HD22	1:A:84:TYR:CD2	0.78	2.13	20	49
1:A:12:PHE:CE2	1:A:103:PHE:CZ	0.78	2.72	13	49
1:A:21:THR:OG1	1:A:47:ILE:HD12	0.77	1.79	6	49
1:A:17:VAL:HG21	1:A:96:MET:SD	0.77	2.19	37	14
1:A:109:THR:O	1:A:110:LEU:C	0.76	2.28	12	49
1:A:84:TYR:CD1	1:A:86:ILE:HB	0.76	2.15	34	49

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:GLU:HG3	1:A:43:ILE:HD11	0.76	1.57	46	7
1:A:11:ALA:HB1	1:A:103:PHE:HB2	0.76	1.58	11	49
1:A:84:TYR:CD1	1:A:86:ILE:CD1	0.76	2.67	31	49
1:A:47:ILE:HG21	1:A:84:TYR:OH	0.75	1.81	17	49
1:A:85:LEU:O	1:A:86:ILE:C	0.75	2.30	32	49
1:A:45:TYR:OH	1:A:76:LEU:HD12	0.74	1.82	47	26
1:A:17:VAL:HG12	1:A:88:GLY:O	0.74	1.82	43	35
1:A:76:LEU:HD22	1:A:84:TYR:HD2	0.74	1.43	22	49
1:A:60:ILE:HG23	1:A:95:LYS:N	0.74	1.98	42	41
1:A:87:ALA:CB	1:A:103:PHE:CD2	0.73	2.71	38	49
1:A:69:SER:O	1:A:70:ALA:HB2	0.72	1.83	9	13
1:A:3:CYS:CB	1:A:101:CYS:SG	0.72	2.77	29	2
1:A:12:PHE:CE1	1:A:114:GLN:CG	0.72	2.72	15	48
1:A:35:ILE:HD12	1:A:35:ILE:N	0.72	2.00	20	49
1:A:64:TYR:CD1	1:A:64:TYR:C	0.72	2.67	35	15
1:A:60:ILE:HD13	1:A:93:ASP:C	0.72	2.09	18	1
1:A:42:ARG:O	1:A:44:GLN:NE2	0.72	2.23	26	49
1:A:3:CYS:O	1:A:100:LEU:HD11	0.72	1.85	4	16
1:A:6:VAL:HG13	1:A:7:HIS:N	0.72	2.00	38	49
1:A:21:THR:HG23	1:A:84:TYR:CE1	0.72	2.20	20	49
1:A:41:LYS:HZ3	1:A:43:ILE:HD12	0.72	1.45	22	2
1:A:60:ILE:HG21	1:A:96:MET:HG3	0.71	1.60	18	3
1:A:20:ARG:CD	1:A:53:PHE:CE2	0.71	2.74	49	9
1:A:45:TYR:CE2	1:A:65:THR:CG2	0.71	2.73	39	49
1:A:87:ALA:CB	1:A:103:PHE:CE2	0.71	2.74	46	49
1:A:69:SER:O	1:A:70:ALA:HB3	0.71	1.86	23	16
1:A:63:ILE:CG2	1:A:98:ILE:HD13	0.71	2.15	40	46
1:A:70:ALA:HB1	1:A:73:GLY:O	0.71	1.85	44	40
1:A:17:VAL:HG13	1:A:17:VAL:O	0.70	1.84	16	34
1:A:20:ARG:NH2	1:A:107:TRP:CH2	0.70	2.60	10	21
1:A:20:ARG:CZ	1:A:107:TRP:CZ2	0.70	2.74	8	27
1:A:53:PHE:CE1	1:A:118:LEU:HD11	0.70	2.21	28	3
1:A:12:PHE:CZ	1:A:114:GLN:HB3	0.69	2.23	37	49
1:A:52:MET:HE2	1:A:52:MET:O	0.69	1.86	30	1
1:A:8:PRO:O	1:A:113:THR:HG22	0.69	1.88	18	12
1:A:63:ILE:HG23	1:A:96:MET:SD	0.69	2.28	7	35
1:A:71:VAL:HG23	1:A:72:CYS:SG	0.69	2.28	36	39
1:A:102:ASP:O	1:A:103:PHE:C	0.69	2.35	13	1
1:A:21:THR:HG21	1:A:47:ILE:CD1	0.68	2.19	12	47
1:A:18:VAL:HG12	1:A:85:LEU:HB2	0.68	1.66	31	49
1:A:69:SER:O	1:A:70:ALA:CB	0.68	2.42	9	27

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ALA:HB1	1:A:103:PHE:CB	0.68	2.17	27	49
1:A:44:GLN:OE1	1:A:64:TYR:CZ	0.68	2.47	31	34
1:A:84:TYR:CE1	1:A:86:ILE:HB	0.68	2.24	37	49
1:A:59:ASP:OD1	1:A:60:ILE:N	0.68	2.27	12	40
1:A:20:ARG:CZ	1:A:107:TRP:CZ3	0.68	2.76	39	10
1:A:52:MET:HE2	1:A:56:PRO:HD2	0.67	1.66	36	1
1:A:12:PHE:CZ	1:A:114:GLN:CG	0.67	2.77	2	37
1:A:23:ALA:HA	1:A:47:ILE:HG22	0.67	1.65	24	49
1:A:17:VAL:CG2	1:A:96:MET:HE2	0.67	2.19	20	16
1:A:21:THR:CB	1:A:47:ILE:HD12	0.67	2.20	39	48
1:A:41:LYS:NZ	1:A:43:ILE:HD12	0.67	2.04	22	2
1:A:63:ILE:HD13	1:A:96:MET:HE2	0.67	1.67	37	12
1:A:53:PHE:CE2	1:A:118:LEU:CD2	0.67	2.77	48	21
1:A:74:VAL:CG2	1:A:104:ILE:HD12	0.67	2.18	48	49
1:A:110:LEU:O	1:A:111:SER:CB	0.67	2.43	23	49
1:A:64:TYR:CG	1:A:97:HIS:CD2	0.66	2.84	38	12
1:A:86:ILE:HA	1:A:104:ILE:HG22	0.66	1.67	7	49
1:A:52:MET:HE1	1:A:59:ASP:HA	0.66	1.67	38	2
1:A:66:ALA:CB	1:A:71:VAL:HG22	0.66	2.20	41	2
1:A:18:VAL:HG23	1:A:54:LYS:HB3	0.66	1.67	17	30
1:A:17:VAL:HG11	1:A:90:ALA:HB2	0.66	1.66	31	13
1:A:99:THR:O	1:A:104:ILE:HD11	0.66	1.91	48	49
1:A:6:VAL:O	1:A:7:HIS:CD2	0.66	2.48	10	43
1:A:48:LYS:O	1:A:49:GLN:O	0.66	2.13	46	49
1:A:89:LYS:O	1:A:90:ALA:HB3	0.66	1.90	49	40
1:A:20:ARG:CD	1:A:53:PHE:CZ	0.66	2.79	49	1
1:A:29:VAL:N	1:A:41:LYS:HZ2	0.65	1.88	39	2
1:A:58:LYS:O	1:A:59:ASP:CB	0.65	2.43	18	49
1:A:23:ALA:CB	1:A:47:ILE:HG22	0.65	2.22	45	49
1:A:47:ILE:CG2	1:A:84:TYR:OH	0.65	2.44	8	49
1:A:71:VAL:O	1:A:100:LEU:HD22	0.65	1.91	38	13
1:A:23:ALA:O	1:A:78:VAL:HG23	0.65	1.92	23	15
1:A:20:ARG:NH2	1:A:107:TRP:CZ2	0.65	2.65	40	17
1:A:20:ARG:NH1	1:A:107:TRP:CZ2	0.65	2.64	22	7
1:A:70:ALA:HB2	1:A:75:SER:OG	0.65	1.92	48	7
1:A:76:LEU:HD13	1:A:84:TYR:CD2	0.64	2.27	9	49
1:A:86:ILE:CG2	1:A:96:MET:CE	0.64	2.76	49	7
1:A:92:GLY:O	1:A:93:ASP:C	0.64	2.40	22	2
1:A:119:ASN:OD1	1:A:119:ASN:C	0.64	2.39	49	4
1:A:20:ARG:HD2	1:A:107:TRP:CE3	0.64	2.28	20	10
1:A:74:VAL:O	1:A:75:SER:C	0.63	2.41	35	47

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:SER:O	1:A:40:ILE:HD12	0.63	1.92	6	21
1:A:72:CYS:HA	1:A:100:LEU:HD22	0.63	1.67	2	26
1:A:63:ILE:HG23	1:A:96:MET:HG3	0.63	1.70	49	4
1:A:44:GLN:OE1	1:A:64:TYR:CE1	0.63	2.51	3	30
1:A:70:ALA:HB2	1:A:75:SER:CB	0.63	2.23	27	9
1:A:114:GLN:HE21	1:A:114:GLN:N	0.63	1.90	35	48
1:A:66:ALA:HB2	1:A:72:CYS:HB2	0.63	1.69	34	32
1:A:12:PHE:CE1	1:A:114:GLN:HG3	0.63	2.28	22	48
1:A:11:ALA:O	1:A:103:PHE:CD2	0.63	2.51	46	48
1:A:58:LYS:O	1:A:59:ASP:HB2	0.63	1.94	37	47
1:A:71:VAL:CG2	1:A:72:CYS:SG	0.63	2.87	8	37
1:A:111:SER:O	1:A:112:THR:CB	0.63	2.47	43	49
1:A:31:SER:OG	1:A:40:ILE:HG21	0.63	1.93	24	27
1:A:85:LEU:O	1:A:86:ILE:O	0.63	2.17	1	49
1:A:53:PHE:CE1	1:A:118:LEU:HD22	0.62	2.28	24	12
1:A:29:VAL:HG23	1:A:42:ARG:CD	0.62	2.24	32	1
1:A:44:GLN:OE1	1:A:64:TYR:CE2	0.62	2.53	43	18
1:A:108:ASP:O	1:A:109:THR:HG23	0.62	1.94	26	49
1:A:30:ASP:CG	1:A:41:LYS:HZ3	0.61	2.03	25	4
1:A:47:ILE:HG21	1:A:84:TYR:HH	0.61	1.54	2	5
1:A:113:THR:HG23	1:A:116:LYS:HE2	0.61	1.71	49	1
1:A:12:PHE:CE2	1:A:114:GLN:O	0.61	2.53	10	29
1:A:63:ILE:HD12	1:A:96:MET:SD	0.61	2.35	47	34
1:A:85:LEU:C	1:A:85:LEU:CD2	0.61	2.73	46	49
1:A:17:VAL:HG23	1:A:56:PRO:HD3	0.61	1.72	24	33
1:A:6:VAL:HG13	1:A:7:HIS:H	0.61	1.56	38	49
1:A:53:PHE:HZ	1:A:118:LEU:HD13	0.61	1.53	33	7
1:A:12:PHE:CD2	1:A:117:SER:HB3	0.61	2.30	4	46
1:A:103:PHE:CD1	1:A:103:PHE:C	0.61	2.78	14	48
1:A:12:PHE:CZ	1:A:114:GLN:CB	0.60	2.84	25	48
1:A:86:ILE:HG22	1:A:86:ILE:O	0.60	1.96	26	28
1:A:15:ALA:CB	1:A:87:ALA:HB1	0.60	2.26	45	49
1:A:12:PHE:CE2	1:A:103:PHE:HZ	0.60	2.12	44	49
1:A:23:ALA:HB2	1:A:47:ILE:HG22	0.60	1.73	45	48
1:A:53:PHE:CD2	1:A:118:LEU:CD2	0.60	2.85	39	20
1:A:106:PRO:HD2	1:A:109:THR:OG1	0.60	1.97	28	49
1:A:10:GLN:HE22	1:A:14:ASN:ND2	0.59	1.95	23	12
1:A:23:ALA:N	1:A:78:VAL:HG21	0.59	2.12	33	4
1:A:52:MET:HE3	1:A:56:PRO:O	0.59	1.97	22	3
1:A:92:GLY:O	1:A:95:LYS:O	0.59	2.20	45	2
1:A:21:THR:CG2	1:A:84:TYR:CE1	0.59	2.86	9	49

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:PHE:CE1	1:A:114:GLN:HG2	0.59	2.32	47	29
1:A:103:PHE:C	1:A:103:PHE:CD1	0.59	2.78	13	1
1:A:53:PHE:CE2	1:A:118:LEU:CD1	0.59	2.83	45	2
1:A:20:ARG:HD2	1:A:50:ILE:HD11	0.59	1.74	1	8
1:A:85:LEU:HD11	1:A:105:VAL:HG23	0.59	1.75	38	42
1:A:17:VAL:HG11	1:A:96:MET:SD	0.59	2.38	42	5
1:A:12:PHE:CG	1:A:103:PHE:CE2	0.59	2.91	16	46
1:A:110:LEU:HD22	1:A:114:GLN:CB	0.59	2.25	6	37
1:A:83:GLU:O	1:A:106:PRO:O	0.59	2.21	46	49
1:A:20:ARG:HD2	1:A:53:PHE:CE2	0.59	2.33	16	21
1:A:45:TYR:CZ	1:A:65:THR:CG2	0.59	2.82	32	8
1:A:9:GLN:NE2	1:A:116:LYS:HE3	0.59	2.13	49	8
1:A:54:LYS:C	1:A:54:LYS:CE	0.58	2.76	36	3
1:A:20:ARG:HD2	1:A:53:PHE:CZ	0.58	2.33	49	12
1:A:53:PHE:CE2	1:A:118:LEU:HD21	0.58	2.34	20	5
1:A:75:SER:OG	1:A:75:SER:O	0.58	2.21	24	5
1:A:18:VAL:N	1:A:54:LYS:O	0.58	2.37	1	15
1:A:27:LYS:HB3	1:A:44:GLN:HB2	0.58	1.75	40	49
1:A:99:THR:O	1:A:104:ILE:CD1	0.58	2.52	18	49
1:A:23:ALA:O	1:A:78:VAL:CG2	0.58	2.51	23	11
1:A:86:ILE:O	1:A:86:ILE:HG22	0.58	1.98	17	21
1:A:99:THR:C	1:A:104:ILE:HD11	0.58	2.24	10	36
1:A:49:GLN:CD	1:A:59:ASP:OD1	0.58	2.47	12	2
1:A:85:LEU:HD12	1:A:107:TRP:HD1	0.58	1.57	46	8
1:A:70:ALA:HB2	1:A:75:SER:HB3	0.58	1.76	35	5
1:A:45:TYR:O	1:A:47:ILE:N	0.58	2.37	41	49
1:A:17:VAL:HG12	1:A:90:ALA:HB2	0.57	1.75	1	9
1:A:71:VAL:CG2	1:A:72:CYS:N	0.57	2.66	19	5
1:A:30:ASP:CG	1:A:41:LYS:HZ1	0.57	2.07	49	2
1:A:56:PRO:HG3	1:A:60:ILE:HD11	0.57	1.76	49	2
1:A:87:ALA:O	1:A:103:PHE:O	0.57	2.22	31	46
1:A:21:THR:HA	1:A:50:ILE:HG23	0.57	1.76	11	12
1:A:9:GLN:OE1	1:A:116:LYS:CE	0.57	2.52	9	2
1:A:84:TYR:CD1	1:A:86:ILE:CB	0.57	2.88	34	49
1:A:20:ARG:CZ	1:A:51:LYS:CD	0.57	2.83	2	14
1:A:23:ALA:N	1:A:78:VAL:CG2	0.57	2.67	33	11
1:A:82:LYS:O	1:A:83:GLU:HG3	0.57	1.99	39	13
1:A:19:ILE:HD12	1:A:49:GLN:OE1	0.57	2.00	26	6
1:A:77:ASP:OD2	1:A:81:LYS:CE	0.57	2.53	46	7
1:A:67:PRO:O	1:A:68:SER:O	0.57	2.22	27	4
1:A:56:PRO:CB	1:A:93:ASP:CG	0.57	2.78	49	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ALA:CB	1:A:103:PHE:HB2	0.57	2.30	27	49
1:A:81:LYS:CD	1:A:81:LYS:N	0.56	2.68	23	42
1:A:72:CYS:O	1:A:99:THR:HA	0.56	2.00	24	48
1:A:60:ILE:HG13	1:A:96:MET:SD	0.56	2.40	49	12
1:A:53:PHE:CZ	1:A:118:LEU:CD1	0.56	2.81	38	8
1:A:6:VAL:O	1:A:7:HIS:C	0.56	2.48	29	47
1:A:63:ILE:CD1	1:A:96:MET:SD	0.56	2.93	15	34
1:A:22:LYS:O	1:A:47:ILE:HA	0.56	2.01	13	34
1:A:86:ILE:CG1	1:A:98:ILE:CD1	0.56	2.83	35	18
1:A:6:VAL:HG22	1:A:7:HIS:H	0.56	1.61	4	49
1:A:35:ILE:HD12	1:A:35:ILE:H	0.56	1.59	36	49
1:A:84:TYR:CE1	1:A:86:ILE:HG12	0.56	2.36	20	35
1:A:89:LYS:O	1:A:90:ALA:CB	0.56	2.54	26	34
1:A:108:ASP:O	1:A:109:THR:CG2	0.56	2.54	37	46
1:A:70:ALA:HB2	1:A:75:SER:HB2	0.56	1.78	6	8
1:A:20:ARG:HD3	1:A:53:PHE:CE2	0.56	2.36	22	6
1:A:20:ARG:NH1	1:A:107:TRP:CZ3	0.56	2.73	30	11
1:A:93:ASP:C	1:A:95:LYS:H	0.56	2.09	49	6
1:A:7:HIS:CB	1:A:10:GLN:CG	0.56	2.84	46	22
1:A:23:ALA:O	1:A:77:ASP:C	0.55	2.49	11	24
1:A:82:LYS:C	1:A:83:GLU:CD	0.55	2.74	25	13
1:A:18:VAL:O	1:A:54:LYS:N	0.55	2.39	17	47
1:A:115:LYS:HA	1:A:118:LEU:HD23	0.55	1.78	28	3
1:A:20:ARG:CD	1:A:107:TRP:CE3	0.55	2.90	43	10
1:A:59:ASP:O	1:A:93:ASP:O	0.55	2.25	18	1
1:A:84:TYR:CB	1:A:105:VAL:O	0.55	2.54	41	49
1:A:12:PHE:CZ	1:A:114:GLN:HG2	0.55	2.37	25	14
1:A:82:LYS:C	1:A:83:GLU:CG	0.55	2.79	7	22
1:A:19:ILE:HG21	1:A:52:MET:HE2	0.55	1.78	38	1
1:A:59:ASP:CG	1:A:60:ILE:N	0.55	2.64	22	42
1:A:85:LEU:HD21	1:A:103:PHE:CE1	0.55	2.36	9	49
1:A:72:CYS:HA	1:A:100:LEU:CD2	0.55	2.31	29	15
1:A:20:ARG:CZ	1:A:107:TRP:CH2	0.55	2.89	39	3
1:A:41:LYS:CG	1:A:67:PRO:HG3	0.55	2.32	3	24
1:A:53:PHE:CZ	1:A:118:LEU:CD2	0.55	2.90	20	7
1:A:84:TYR:CE1	1:A:86:ILE:CG1	0.55	2.90	20	49
1:A:12:PHE:N	1:A:12:PHE:CD1	0.55	2.74	25	23
1:A:20:ARG:HA	1:A:84:TYR:O	0.55	2.02	28	49
1:A:6:VAL:CG1	1:A:7:HIS:N	0.54	2.70	11	37
1:A:12:PHE:CD1	1:A:103:PHE:CZ	0.54	2.96	8	44
1:A:31:SER:OG	1:A:40:ILE:CG2	0.54	2.55	15	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:ASP:O	1:A:78:VAL:HB	0.54	2.02	37	43
1:A:86:ILE:O	1:A:86:ILE:CG2	0.54	2.54	23	42
1:A:17:VAL:HG22	1:A:96:MET:HE2	0.54	1.78	20	8
1:A:49:GLN:CD	1:A:59:ASP:CG	0.54	2.75	39	6
1:A:22:LYS:HG2	1:A:50:ILE:HG22	0.54	1.77	11	8
1:A:72:CYS:O	1:A:99:THR:CG2	0.54	2.53	23	14
1:A:63:ILE:HG21	1:A:98:ILE:CD1	0.54	2.28	35	10
1:A:81:LYS:O	1:A:82:LYS:CB	0.54	2.55	6	49
1:A:31:SER:O	1:A:31:SER:OG	0.54	2.26	43	10
1:A:102:ASP:O	1:A:104:ILE:HG12	0.54	2.01	13	1
1:A:72:CYS:O	1:A:99:THR:CB	0.54	2.55	41	6
1:A:65:THR:OG1	1:A:66:ALA:N	0.54	2.41	13	49
1:A:77:ASP:OD1	1:A:81:LYS:CE	0.54	2.56	35	19
1:A:35:ILE:N	1:A:35:ILE:CD1	0.54	2.71	4	49
1:A:19:ILE:C	1:A:85:LEU:HA	0.54	2.28	12	49
1:A:74:VAL:CG2	1:A:104:ILE:CD1	0.54	2.84	10	42
1:A:84:TYR:HB2	1:A:105:VAL:O	0.54	2.02	3	48
1:A:106:PRO:HG2	1:A:109:THR:CG2	0.54	2.32	49	49
1:A:83:GLU:OE1	1:A:83:GLU:C	0.54	2.50	42	4
1:A:26:GLU:C	1:A:26:GLU:OE1	0.54	2.50	49	2
1:A:20:ARG:HD3	1:A:53:PHE:CZ	0.54	2.37	17	5
1:A:77:ASP:CG	1:A:81:LYS:CE	0.54	2.81	19	10
1:A:46:GLU:HG3	1:A:62:PHE:CZ	0.54	2.38	23	18
1:A:54:LYS:C	1:A:54:LYS:HD2	0.54	2.27	48	1
1:A:103:PHE:O	1:A:104:ILE:CG2	0.54	2.55	13	49
1:A:82:LYS:C	1:A:83:GLU:HG3	0.54	2.28	21	19
1:A:17:VAL:CG2	1:A:96:MET:SD	0.54	2.96	28	14
1:A:77:ASP:C	1:A:79:GLY:H	0.54	2.11	41	15
1:A:53:PHE:CE1	1:A:118:LEU:CD2	0.54	2.91	20	4
1:A:75:SER:O	1:A:75:SER:OG	0.54	2.25	35	5
1:A:21:THR:OG1	1:A:47:ILE:CD1	0.53	2.56	31	27
1:A:92:GLY:O	1:A:93:ASP:O	0.53	2.26	46	9
1:A:16:ASP:N	1:A:88:GLY:O	0.53	2.39	46	9
1:A:53:PHE:CE2	1:A:118:LEU:HD13	0.53	2.39	14	5
1:A:113:THR:CG2	1:A:116:LYS:HE2	0.53	2.32	49	1
1:A:84:TYR:CD1	1:A:86:ILE:CG1	0.53	2.92	20	48
1:A:12:PHE:CD2	1:A:103:PHE:CZ	0.53	2.96	25	27
1:A:64:TYR:CE2	1:A:97:HIS:NE2	0.53	2.77	35	2
1:A:88:GLY:O	1:A:90:ALA:N	0.53	2.42	12	13
1:A:28:GLU:HA	1:A:43:ILE:CD1	0.53	2.34	14	3
1:A:17:VAL:HB	1:A:90:ALA:HB2	0.53	1.79	36	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ARG:HD3	1:A:107:TRP:CE3	0.53	2.39	30	9
1:A:10:GLN:CD	1:A:10:GLN:O	0.53	2.52	27	25
1:A:100:LEU:HD23	1:A:101:CYS:H	0.53	1.64	43	5
1:A:78:VAL:C	1:A:80:GLY:N	0.53	2.67	33	38
1:A:88:GLY:O	1:A:89:LYS:C	0.53	2.52	20	23
1:A:17:VAL:O	1:A:17:VAL:CG1	0.53	2.54	16	15
1:A:3:CYS:O	1:A:100:LEU:CD1	0.53	2.57	13	6
1:A:7:HIS:O	1:A:11:ALA:HB2	0.52	2.03	37	6
1:A:77:ASP:CG	1:A:81:LYS:NZ	0.52	2.67	23	10
1:A:29:VAL:HG23	1:A:29:VAL:O	0.52	2.04	22	10
1:A:77:ASP:OD1	1:A:79:GLY:N	0.52	2.42	13	9
1:A:68:SER:O	1:A:70:ALA:N	0.52	2.41	27	13
1:A:114:GLN:NE2	1:A:114:GLN:N	0.52	2.57	37	1
1:A:86:ILE:CG2	1:A:86:ILE:O	0.52	2.57	34	7
1:A:26:GLU:CG	1:A:44:GLN:O	0.52	2.58	17	47
1:A:17:VAL:CG1	1:A:96:MET:SD	0.52	2.97	42	2
1:A:64:TYR:CD2	1:A:97:HIS:NE2	0.52	2.77	35	3
1:A:30:ASP:N	1:A:41:LYS:NZ	0.52	2.57	5	4
1:A:49:GLN:NE2	1:A:59:ASP:CG	0.52	2.68	41	5
1:A:60:ILE:CG2	1:A:95:LYS:CA	0.52	2.87	42	7
1:A:17:VAL:HA	1:A:54:LYS:O	0.52	2.05	37	26
1:A:83:GLU:CD	1:A:83:GLU:N	0.52	2.68	40	15
1:A:108:ASP:C	1:A:109:THR:HG23	0.52	2.30	37	32
1:A:85:LEU:HD11	1:A:110:LEU:HD21	0.52	1.81	35	21
1:A:82:LYS:O	1:A:83:GLU:CD	0.52	2.53	17	9
1:A:46:GLU:CD	1:A:62:PHE:CZ	0.52	2.88	6	5
1:A:62:PHE:O	1:A:95:LYS:HA	0.52	2.05	25	46
1:A:6:VAL:O	1:A:7:HIS:O	0.52	2.28	22	22
1:A:53:PHE:CG	1:A:118:LEU:HD22	0.52	2.40	30	2
1:A:36:TYR:CD1	1:A:38:ASN:OD1	0.52	2.63	34	1
1:A:93:ASP:O	1:A:95:LYS:CE	0.52	2.58	37	5
1:A:53:PHE:CD2	1:A:118:LEU:HD21	0.51	2.40	1	4
1:A:87:ALA:O	1:A:103:PHE:HB3	0.51	2.05	20	14
1:A:10:GLN:O	1:A:10:GLN:CG	0.51	2.58	29	6
1:A:84:TYR:CD1	1:A:84:TYR:O	0.51	2.64	23	49
1:A:47:ILE:CG1	1:A:61:GLU:HA	0.51	2.35	19	44
1:A:77:ASP:CG	1:A:81:LYS:HZ1	0.51	2.12	41	11
1:A:52:MET:CG	1:A:52:MET:O	0.51	2.58	14	7
1:A:68:SER:HB2	1:A:71:VAL:CG1	0.51	2.35	43	5
1:A:19:ILE:O	1:A:84:TYR:O	0.51	2.28	8	49
1:A:63:ILE:CG2	1:A:96:MET:SD	0.51	2.98	18	35

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:GLY:HA2	1:A:100:LEU:N	0.51	2.21	15	46
1:A:3:CYS:SG	1:A:4:SER:N	0.51	2.83	40	12
1:A:49:GLN:CG	1:A:59:ASP:OD2	0.51	2.59	35	16
1:A:12:PHE:CD1	1:A:12:PHE:N	0.51	2.78	43	26
1:A:9:GLN:NE2	1:A:116:LYS:CE	0.51	2.74	36	16
1:A:77:ASP:OD1	1:A:80:GLY:N	0.51	2.43	19	7
1:A:60:ILE:CD1	1:A:93:ASP:O	0.51	2.50	18	1
1:A:3:CYS:SG	1:A:101:CYS:CB	0.51	2.98	48	2
1:A:81:LYS:O	1:A:82:LYS:CD	0.51	2.59	34	21
1:A:92:GLY:O	1:A:95:LYS:CE	0.51	2.59	45	2
1:A:19:ILE:HG13	1:A:21:THR:CG2	0.51	2.36	30	16
1:A:53:PHE:CG	1:A:118:LEU:HD23	0.51	2.40	1	7
1:A:53:PHE:CD1	1:A:118:LEU:CD2	0.51	2.94	5	6
1:A:29:VAL:HG23	1:A:42:ARG:HD3	0.51	1.83	32	1
1:A:91:GLU:CB	1:A:96:MET:HA	0.51	2.36	37	43
1:A:59:ASP:OD2	1:A:61:GLU:CD	0.51	2.54	8	6
1:A:52:MET:CE	1:A:56:PRO:O	0.51	2.59	37	3
1:A:110:LEU:HD13	1:A:115:LYS:HG3	0.51	1.82	43	33
1:A:19:ILE:HD11	1:A:96:MET:HE3	0.51	1.82	19	23
1:A:49:GLN:NE2	1:A:59:ASP:OD2	0.51	2.43	29	16
1:A:70:ALA:HB2	1:A:74:VAL:C	0.51	2.31	19	2
1:A:47:ILE:CD1	1:A:60:ILE:O	0.51	2.52	18	6
1:A:60:ILE:HG23	1:A:95:LYS:CA	0.51	2.36	18	5
1:A:69:SER:O	1:A:75:SER:CB	0.51	2.58	43	11
1:A:11:ALA:O	1:A:103:PHE:CB	0.51	2.59	12	40
1:A:77:ASP:OD2	1:A:81:LYS:NZ	0.51	2.44	2	35
1:A:66:ALA:HB3	1:A:72:CYS:H	0.51	1.66	48	17
1:A:49:GLN:NE2	1:A:59:ASP:OD1	0.51	2.44	39	13
1:A:56:PRO:CB	1:A:93:ASP:OD1	0.51	2.59	36	1
1:A:107:TRP:O	1:A:109:THR:N	0.50	2.42	30	25
1:A:86:ILE:HG13	1:A:98:ILE:CD1	0.50	2.35	35	9
1:A:60:ILE:HG13	1:A:96:MET:HE3	0.50	1.84	38	7
1:A:85:LEU:HD13	1:A:85:LEU:H	0.50	1.67	25	16
1:A:72:CYS:O	1:A:99:THR:CA	0.50	2.58	41	10
1:A:71:VAL:O	1:A:100:LEU:CD2	0.50	2.58	38	3
1:A:33:ASN:HA	1:A:38:ASN:O	0.50	2.05	22	49
1:A:20:ARG:HD3	1:A:107:TRP:CD2	0.50	2.42	43	10
1:A:42:ARG:O	1:A:43:ILE:C	0.50	2.52	4	44
1:A:60:ILE:CD1	1:A:96:MET:SD	0.50	2.99	44	7
1:A:50:ILE:CD1	1:A:83:GLU:OE2	0.50	2.60	15	1
1:A:52:MET:O	1:A:52:MET:CE	0.50	2.57	30	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:GLU:CG	1:A:43:ILE:HG23	0.50	2.37	49	2
1:A:53:PHE:CG	1:A:118:LEU:CD2	0.50	2.94	1	6
1:A:116:LYS:O	1:A:119:ASN:OD1	0.50	2.30	25	4
1:A:12:PHE:CB	1:A:117:SER:HB3	0.50	2.37	43	39
1:A:17:VAL:HG23	1:A:56:PRO:CD	0.50	2.36	10	3
1:A:28:GLU:HG2	1:A:41:LYS:NZ	0.50	2.22	38	4
1:A:23:ALA:C	1:A:78:VAL:HG23	0.50	2.32	26	7
1:A:68:SER:O	1:A:69:SER:C	0.50	2.54	24	3
1:A:88:GLY:C	1:A:90:ALA:N	0.49	2.68	28	13
1:A:116:LYS:NZ	1:A:116:LYS:O	0.49	2.45	3	9
1:A:29:VAL:CG2	1:A:42:ARG:O	0.49	2.60	24	10
1:A:26:GLU:OE1	1:A:28:GLU:N	0.49	2.45	40	2
1:A:15:ALA:CB	1:A:87:ALA:C	0.49	2.86	1	48
1:A:71:VAL:HG22	1:A:72:CYS:N	0.49	2.22	19	1
1:A:15:ALA:HB1	1:A:87:ALA:C	0.49	2.32	15	48
1:A:82:LYS:C	1:A:83:GLU:OE2	0.49	2.55	41	1
1:A:84:TYR:CE1	1:A:86:ILE:CB	0.49	2.95	37	47
1:A:12:PHE:CG	1:A:117:SER:HB3	0.49	2.42	17	25
1:A:112:THR:HG22	1:A:113:THR:N	0.49	2.22	45	18
1:A:45:TYR:CE1	1:A:76:LEU:HD12	0.49	2.43	7	13
1:A:9:GLN:OE1	1:A:116:LYS:NZ	0.49	2.46	10	2
1:A:6:VAL:HG22	1:A:7:HIS:N	0.49	2.22	20	49
1:A:45:TYR:OH	1:A:75:SER:CA	0.49	2.60	47	11
1:A:18:VAL:HG22	1:A:87:ALA:HB1	0.49	1.84	1	4
1:A:64:TYR:O	1:A:98:ILE:HG12	0.49	2.08	47	11
1:A:12:PHE:HA	1:A:103:PHE:CD2	0.49	2.43	16	10
1:A:19:ILE:HG22	1:A:52:MET:HG3	0.49	1.84	36	1
1:A:19:ILE:HG13	1:A:21:THR:HG22	0.49	1.82	30	9
1:A:74:VAL:O	1:A:74:VAL:HG12	0.49	2.08	6	33
1:A:12:PHE:CE1	1:A:114:GLN:HB3	0.49	2.43	37	1
1:A:24:VAL:CG1	1:A:78:VAL:CG1	0.48	2.90	11	10
1:A:23:ALA:C	1:A:78:VAL:CG2	0.48	2.86	26	9
1:A:83:GLU:OE1	1:A:83:GLU:O	0.48	2.32	42	1
1:A:83:GLU:O	1:A:106:PRO:C	0.48	2.56	6	33
1:A:84:TYR:CD1	1:A:84:TYR:C	0.48	2.91	37	49
1:A:10:GLN:O	1:A:10:GLN:NE2	0.48	2.46	19	1
1:A:9:GLN:CD	1:A:116:LYS:NZ	0.48	2.72	49	1
1:A:20:ARG:CG	1:A:53:PHE:CE2	0.48	2.97	42	9
1:A:20:ARG:O	1:A:50:ILE:CD1	0.48	2.61	9	2
1:A:6:VAL:C	1:A:7:HIS:CG	0.48	2.91	27	22
1:A:9:GLN:C	1:A:11:ALA:N	0.48	2.71	9	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ARG:O	1:A:50:ILE:HD13	0.48	2.09	9	9
1:A:52:MET:O	1:A:53:PHE:C	0.48	2.56	48	35
1:A:63:ILE:CD1	1:A:96:MET:CE	0.48	2.87	26	4
1:A:83:GLU:O	1:A:106:PRO:HA	0.48	2.09	23	22
1:A:91:GLU:CD	1:A:91:GLU:O	0.48	2.56	44	3
1:A:113:THR:O	1:A:116:LYS:CE	0.48	2.61	49	1
1:A:81:LYS:O	1:A:82:LYS:HB3	0.48	2.08	7	28
1:A:21:THR:OG1	1:A:47:ILE:HB	0.48	2.08	46	18
1:A:49:GLN:HG3	1:A:59:ASP:OD2	0.48	2.07	35	16
1:A:9:GLN:CD	1:A:116:LYS:CE	0.48	2.86	9	2
1:A:3:CYS:H	1:A:100:LEU:HD21	0.48	1.68	14	2
1:A:95:LYS:HD2	1:A:95:LYS:O	0.48	2.08	49	2
1:A:34:ASP:N	1:A:38:ASN:O	0.48	2.46	20	48
1:A:48:LYS:O	1:A:49:GLN:C	0.48	2.56	36	11
1:A:86:ILE:HG12	1:A:98:ILE:HD12	0.48	1.85	46	7
1:A:28:GLU:CG	1:A:41:LYS:HZ2	0.48	2.22	45	1
1:A:56:PRO:CG	1:A:60:ILE:HD11	0.48	2.39	49	1
1:A:19:ILE:HG22	1:A:52:MET:HA	0.48	1.86	19	8
1:A:49:GLN:HG3	1:A:59:ASP:OD1	0.48	2.09	8	2
1:A:9:GLN:NE2	1:A:113:THR:O	0.48	2.47	30	26
1:A:20:ARG:CZ	1:A:51:LYS:HD3	0.48	2.38	42	13
1:A:53:PHE:CE1	1:A:118:LEU:HB3	0.48	2.44	30	5
1:A:9:GLN:NE2	1:A:117:SER:OG	0.47	2.47	10	6
1:A:20:ARG:CZ	1:A:50:ILE:HD11	0.47	2.39	25	4
1:A:64:TYR:CZ	1:A:97:HIS:CE1	0.47	3.02	35	2
1:A:53:PHE:CD2	1:A:118:LEU:HD13	0.47	2.43	49	1
1:A:68:SER:C	1:A:70:ALA:N	0.47	2.70	43	2
1:A:91:GLU:HB3	1:A:95:LYS:O	0.47	2.09	49	4
1:A:21:THR:OG1	1:A:22:LYS:N	0.47	2.47	11	23
1:A:29:VAL:HG23	1:A:42:ARG:HD2	0.47	1.85	32	1
1:A:28:GLU:CG	1:A:41:LYS:NZ	0.47	2.77	45	1
1:A:94:GLY:C	1:A:95:LYS:HG3	0.47	2.35	49	1
1:A:22:LYS:O	1:A:47:ILE:CA	0.47	2.62	13	7
1:A:72:CYS:HA	1:A:100:LEU:HD23	0.47	1.85	13	3
1:A:11:ALA:CA	1:A:103:PHE:HB2	0.47	2.39	17	33
1:A:116:LYS:O	1:A:116:LYS:NZ	0.47	2.45	2	10
1:A:17:VAL:O	1:A:87:ALA:HA	0.47	2.08	5	17
1:A:113:THR:HA	1:A:116:LYS:HG2	0.47	1.85	22	8
1:A:20:ARG:HG2	1:A:53:PHE:CD2	0.47	2.45	21	2
1:A:90:ALA:HA	1:A:96:MET:CB	0.47	2.39	33	6
1:A:60:ILE:CG2	1:A:95:LYS:HA	0.47	2.40	42	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:ILE:HG23	1:A:98:ILE:HG21	0.47	1.86	48	24
1:A:28:GLU:CG	1:A:41:LYS:CE	0.47	2.93	6	12
1:A:38:ASN:N	1:A:38:ASN:OD1	0.47	2.48	27	17
1:A:25:SER:C	1:A:26:GLU:OE1	0.47	2.58	16	4
1:A:114:GLN:N	1:A:114:GLN:HE21	0.47	2.07	37	1
1:A:20:ARG:HB2	1:A:53:PHE:CE2	0.47	2.45	1	4
1:A:44:GLN:NE2	1:A:44:GLN:HA	0.47	2.24	38	29
1:A:27:LYS:O	1:A:44:GLN:N	0.47	2.47	24	12
1:A:53:PHE:CD1	1:A:118:LEU:HD23	0.47	2.45	5	3
1:A:17:VAL:HG21	1:A:96:MET:HE2	0.47	1.87	12	3
1:A:110:LEU:O	1:A:111:SER:OG	0.47	2.33	21	39
1:A:67:PRO:C	1:A:68:SER:O	0.47	2.58	27	4
1:A:9:GLN:HB2	1:A:113:THR:HG22	0.47	1.87	25	1
1:A:72:CYS:CA	1:A:100:LEU:HD22	0.46	2.37	2	2
1:A:78:VAL:C	1:A:80:GLY:H	0.46	2.17	33	26
1:A:91:GLU:OE2	1:A:97:HIS:ND1	0.46	2.48	5	1
1:A:9:GLN:NE2	1:A:116:LYS:HE2	0.46	2.26	39	15
1:A:50:ILE:CD1	1:A:83:GLU:CD	0.46	2.88	15	1
1:A:26:GLU:HG3	1:A:43:ILE:HG23	0.46	1.87	49	2
1:A:26:GLU:HG3	1:A:43:ILE:CG2	0.46	2.41	49	2
1:A:19:ILE:CD1	1:A:60:ILE:HG13	0.46	2.41	31	4
1:A:9:GLN:NE2	1:A:117:SER:CB	0.46	2.78	22	4
1:A:6:VAL:C	1:A:7:HIS:CD2	0.46	2.93	16	37
1:A:52:MET:O	1:A:52:MET:CG	0.46	2.63	3	3
1:A:31:SER:OG	1:A:31:SER:O	0.46	2.29	32	4
1:A:41:LYS:HE2	1:A:42:ARG:N	0.46	2.25	22	2
1:A:45:TYR:OH	1:A:75:SER:HA	0.46	2.10	24	10
1:A:8:PRO:O	1:A:114:GLN:NE2	0.46	2.49	32	10
1:A:10:GLN:NE2	1:A:14:ASN:ND2	0.46	2.62	23	6
1:A:93:ASP:C	1:A:95:LYS:N	0.46	2.73	49	5
1:A:8:PRO:CB	1:A:114:GLN:NE2	0.46	2.79	49	1
1:A:38:ASN:OD1	1:A:38:ASN:N	0.46	2.48	20	29
1:A:77:ASP:O	1:A:79:GLY:N	0.46	2.45	33	10
1:A:28:GLU:CG	1:A:41:LYS:HE3	0.46	2.41	31	6
1:A:85:LEU:HD12	1:A:107:TRP:CD1	0.46	2.45	43	3
1:A:78:VAL:CG2	1:A:82:LYS:O	0.46	2.50	32	3
1:A:30:ASP:CG	1:A:41:LYS:NZ	0.46	2.74	16	7
1:A:45:TYR:CE2	1:A:65:THR:HB	0.46	2.45	49	9
1:A:20:ARG:NH1	1:A:107:TRP:CE3	0.46	2.84	12	1
1:A:7:HIS:HB2	1:A:10:GLN:CG	0.46	2.41	17	6
1:A:95:LYS:N	1:A:95:LYS:HD3	0.46	2.26	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:PHE:CZ	1:A:107:TRP:NE1	0.46	2.84	44	4
1:A:114:GLN:NE2	1:A:114:GLN:H	0.46	2.07	37	1
1:A:119:ASN:C	1:A:119:ASN:ND2	0.45	2.73	13	1
1:A:12:PHE:HB2	1:A:117:SER:HB3	0.45	1.87	28	2
1:A:9:GLN:NE2	1:A:116:LYS:NZ	0.45	2.63	49	1
1:A:110:LEU:O	1:A:111:SER:HB2	0.45	2.10	23	42
1:A:7:HIS:NE2	1:A:101:CYS:O	0.45	2.49	5	3
1:A:59:ASP:O	1:A:94:GLY:N	0.45	2.49	24	6
1:A:86:ILE:HG12	1:A:98:ILE:CD1	0.45	2.42	13	4
1:A:9:GLN:OE1	1:A:117:SER:OG	0.45	2.34	14	8
1:A:28:GLU:HA	1:A:43:ILE:HD12	0.45	1.86	14	1
1:A:9:GLN:HE21	1:A:117:SER:CB	0.45	2.25	28	1
1:A:60:ILE:CD1	1:A:93:ASP:HA	0.45	2.41	49	3
1:A:20:ARG:CZ	1:A:51:LYS:HD2	0.45	2.41	2	13
1:A:22:LYS:HG2	1:A:50:ILE:CG2	0.45	2.42	26	8
1:A:25:SER:CB	1:A:46:GLU:HB3	0.45	2.41	40	15
1:A:41:LYS:NZ	1:A:41:LYS:HB2	0.45	2.27	35	8
1:A:17:VAL:CB	1:A:90:ALA:HB2	0.45	2.41	36	4
1:A:12:PHE:CZ	1:A:103:PHE:HZ	0.45	2.20	29	5
1:A:12:PHE:N	1:A:12:PHE:HD1	0.45	2.08	45	4
1:A:15:ALA:HB1	1:A:87:ALA:HB1	0.45	1.88	2	11
1:A:17:VAL:HG11	1:A:90:ALA:CB	0.45	2.38	31	5
1:A:78:VAL:O	1:A:80:GLY:N	0.45	2.49	46	10
1:A:86:ILE:HG22	1:A:96:MET:CE	0.45	2.41	49	1
1:A:21:THR:OG1	1:A:47:ILE:CG1	0.45	2.65	10	9
1:A:60:ILE:HD12	1:A:96:MET:SD	0.45	2.52	3	2
1:A:45:TYR:N	1:A:63:ILE:O	0.45	2.50	27	7
1:A:67:PRO:O	1:A:71:VAL:HG13	0.45	2.11	33	4
1:A:112:THR:O	1:A:115:LYS:N	0.45	2.49	2	12
1:A:23:ALA:N	1:A:78:VAL:HG23	0.45	2.27	6	6
1:A:67:PRO:O	1:A:68:SER:C	0.45	2.59	43	3
1:A:3:CYS:H	1:A:100:LEU:HD11	0.45	1.72	44	1
1:A:17:VAL:O	1:A:86:ILE:O	0.45	2.34	9	15
1:A:54:LYS:O	1:A:54:LYS:HG3	0.45	2.11	37	1
1:A:20:ARG:CG	1:A:53:PHE:CD2	0.45	3.00	42	1
1:A:60:ILE:CG2	1:A:95:LYS:N	0.45	2.76	42	2
1:A:93:ASP:O	1:A:95:LYS:HD2	0.45	2.11	49	2
1:A:114:GLN:N	1:A:114:GLN:NE2	0.45	2.63	29	11
1:A:46:GLU:HG3	1:A:62:PHE:CE2	0.45	2.46	5	2
1:A:91:GLU:OE1	1:A:97:HIS:ND1	0.45	2.50	23	2
1:A:29:VAL:CG2	1:A:42:ARG:HD3	0.45	2.42	32	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:PHE:CD2	1:A:118:LEU:CD1	0.45	3.00	45	2
1:A:81:LYS:O	1:A:82:LYS:CE	0.45	2.64	25	3
1:A:22:LYS:O	1:A:22:LYS:HG3	0.44	2.11	45	18
1:A:92:GLY:N	1:A:95:LYS:O	0.44	2.51	18	1
1:A:7:HIS:CG	1:A:10:GLN:HG3	0.44	2.47	30	2
1:A:18:VAL:HG22	1:A:87:ALA:CB	0.44	2.42	1	1
1:A:82:LYS:O	1:A:83:GLU:OE1	0.44	2.36	38	3
1:A:44:GLN:OE1	1:A:64:TYR:CD2	0.44	2.71	22	2
1:A:5:PRO:CB	1:A:100:LEU:O	0.44	2.65	46	2
1:A:30:ASP:N	1:A:41:LYS:HZ2	0.44	2.10	31	1
1:A:110:LEU:C	1:A:114:GLN:OE1	0.44	2.60	37	1
1:A:46:GLU:CG	1:A:62:PHE:CZ	0.44	3.00	23	4
1:A:29:VAL:N	1:A:41:LYS:NZ	0.44	2.61	39	1
1:A:106:PRO:O	1:A:108:ASP:N	0.44	2.48	49	22
1:A:12:PHE:CD1	1:A:103:PHE:CE2	0.44	3.05	16	11
1:A:50:ILE:CD1	1:A:83:GLU:HG2	0.44	2.43	46	4
1:A:12:PHE:HB2	1:A:117:SER:OG	0.44	2.13	13	3
1:A:102:ASP:O	1:A:103:PHE:O	0.44	2.34	13	1
1:A:32:GLY:O	1:A:40:ILE:N	0.44	2.36	46	2
1:A:116:LYS:HE3	1:A:116:LYS:C	0.44	2.38	48	3
1:A:19:ILE:N	1:A:85:LEU:O	0.44	2.47	17	7
1:A:85:LEU:C	1:A:85:LEU:HD22	0.44	2.37	46	5
1:A:106:PRO:HG2	1:A:109:THR:HG21	0.44	1.87	49	29
1:A:63:ILE:CG2	1:A:98:ILE:CD1	0.44	2.96	35	2
1:A:99:THR:OG1	1:A:102:ASP:HB2	0.44	2.11	40	1
1:A:56:PRO:CG	1:A:93:ASP:OD1	0.44	2.65	49	1
1:A:83:GLU:O	1:A:83:GLU:OE1	0.44	2.36	21	3
1:A:50:ILE:HD13	1:A:83:GLU:HG2	0.44	1.90	13	5
1:A:108:ASP:O	1:A:108:ASP:CG	0.44	2.60	30	3
1:A:73:GLY:O	1:A:100:LEU:HB3	0.44	2.12	40	2
1:A:26:GLU:HG2	1:A:27:LYS:N	0.44	2.27	49	2
1:A:19:ILE:O	1:A:85:LEU:HA	0.44	2.12	35	23
1:A:100:LEU:HG	1:A:101:CYS:N	0.44	2.28	3	7
1:A:99:THR:O	1:A:102:ASP:N	0.44	2.50	13	1
1:A:41:LYS:O	1:A:67:PRO:HD3	0.44	2.12	43	2
1:A:49:GLN:CG	1:A:59:ASP:OD1	0.44	2.66	8	2
1:A:81:LYS:N	1:A:81:LYS:HD3	0.44	2.28	48	19
1:A:10:GLN:O	1:A:10:GLN:OE1	0.44	2.36	29	1
1:A:52:MET:SD	1:A:56:PRO:O	0.44	2.76	36	2
1:A:11:ALA:O	1:A:103:PHE:HB2	0.43	2.13	21	8
1:A:20:ARG:CD	1:A:107:TRP:CD2	0.43	3.01	23	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LYS:CE	1:A:41:LYS:CA	0.43	2.96	39	2
1:A:23:ALA:HB2	1:A:47:ILE:CG2	0.43	2.42	45	4
1:A:119:ASN:ND2	1:A:119:ASN:C	0.43	2.76	25	1
1:A:35:ILE:O	1:A:35:ILE:HG22	0.43	2.13	39	39
1:A:45:TYR:CE2	1:A:65:THR:CB	0.43	3.02	22	7
1:A:5:PRO:HB3	1:A:100:LEU:O	0.43	2.14	14	1
1:A:60:ILE:HG21	1:A:96:MET:SD	0.43	2.53	49	1
1:A:63:ILE:HD12	1:A:86:ILE:HG21	0.43	1.90	28	6
1:A:99:THR:C	1:A:101:CYS:N	0.43	2.74	13	1
1:A:19:ILE:CG2	1:A:52:MET:CG	0.43	2.96	22	1
1:A:28:GLU:HG2	1:A:41:LYS:CE	0.43	2.43	5	2
1:A:30:ASP:HA	1:A:41:LYS:NZ	0.43	2.28	47	5
1:A:11:ALA:HB1	1:A:103:PHE:CG	0.43	2.48	17	2
1:A:77:ASP:CG	1:A:81:LYS:HE3	0.43	2.38	19	3
1:A:86:ILE:CG2	1:A:96:MET:SD	0.43	3.06	46	1
1:A:27:LYS:HB3	1:A:44:GLN:CB	0.43	2.44	30	10
1:A:19:ILE:C	1:A:21:THR:H	0.43	2.21	6	19
1:A:112:THR:C	1:A:114:GLN:N	0.43	2.76	25	8
1:A:44:GLN:NE2	1:A:44:GLN:CA	0.43	2.81	38	6
1:A:30:ASP:OD2	1:A:41:LYS:NZ	0.43	2.50	30	2
1:A:17:VAL:HA	1:A:55:GLY:CA	0.43	2.44	39	2
1:A:69:SER:O	1:A:70:ALA:O	0.43	2.37	14	1
1:A:28:GLU:CG	1:A:41:LYS:HD3	0.43	2.44	27	2
1:A:113:THR:HA	1:A:116:LYS:CG	0.43	2.43	49	2
1:A:82:LYS:HG3	1:A:83:GLU:CD	0.43	2.39	40	1
1:A:82:LYS:HB2	1:A:83:GLU:CD	0.43	2.38	37	8
1:A:69:SER:O	1:A:75:SER:OG	0.43	2.35	9	4
1:A:20:ARG:HG3	1:A:53:PHE:CD2	0.43	2.49	42	2
1:A:68:SER:C	1:A:70:ALA:H	0.43	2.22	39	2
1:A:116:LYS:HA	1:A:119:ASN:ND2	0.43	2.29	49	1
1:A:28:GLU:CG	1:A:41:LYS:HE2	0.43	2.43	13	12
1:A:74:VAL:O	1:A:75:SER:O	0.43	2.37	34	5
1:A:20:ARG:HD3	1:A:51:LYS:CD	0.43	2.44	38	1
1:A:116:LYS:O	1:A:119:ASN:ND2	0.42	2.52	5	1
1:A:12:PHE:HB2	1:A:117:SER:CB	0.42	2.42	28	1
1:A:54:LYS:C	1:A:54:LYS:HE3	0.42	2.38	44	2
1:A:84:TYR:CB	1:A:86:ILE:HD13	0.42	2.43	25	13
1:A:47:ILE:HG12	1:A:61:GLU:HA	0.42	1.91	41	7
1:A:111:SER:O	1:A:112:THR:OG1	0.42	2.37	33	8
1:A:42:ARG:HB3	1:A:64:TYR:CE2	0.42	2.50	36	2
1:A:89:LYS:O	1:A:89:LYS:CG	0.42	2.66	36	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:GLU:HG2	1:A:41:LYS:HZ2	0.42	1.73	4	2
1:A:107:TRP:C	1:A:109:THR:H	0.42	2.21	12	14
1:A:6:VAL:CG1	1:A:7:HIS:H	0.42	2.23	38	17
1:A:6:VAL:CG2	1:A:7:HIS:H	0.42	2.28	27	7
1:A:110:LEU:CD1	1:A:115:LYS:HG3	0.42	2.44	13	5
1:A:20:ARG:HG2	1:A:20:ARG:O	0.42	2.14	14	3
1:A:70:ALA:CB	1:A:74:VAL:C	0.42	2.93	19	1
1:A:92:GLY:C	1:A:93:ASP:O	0.42	2.62	46	3
1:A:114:GLN:O	1:A:118:LEU:HB3	0.42	2.14	45	1
1:A:45:TYR:CZ	1:A:76:LEU:CD1	0.42	2.97	47	1
1:A:7:HIS:CG	1:A:10:GLN:CG	0.42	3.03	30	2
1:A:91:GLU:OE1	1:A:97:HIS:CG	0.42	2.72	30	1
1:A:24:VAL:HG13	1:A:78:VAL:HG21	0.42	1.91	1	4
1:A:9:GLN:HB2	1:A:113:THR:CG2	0.42	2.45	26	5
1:A:109:THR:O	1:A:110:LEU:O	0.42	2.38	43	7
1:A:102:ASP:OD1	1:A:103:PHE:N	0.42	2.50	46	2
1:A:49:GLN:CG	1:A:61:GLU:HG3	0.42	2.45	17	1
1:A:63:ILE:CD1	1:A:96:MET:HE3	0.42	2.44	34	2
1:A:76:LEU:HD12	1:A:76:LEU:H	0.42	1.74	47	1
1:A:28:GLU:CG	1:A:41:LYS:HD2	0.42	2.45	34	5
1:A:81:LYS:C	1:A:82:LYS:CG	0.42	2.91	42	8
1:A:77:ASP:C	1:A:79:GLY:N	0.42	2.77	4	6
1:A:19:ILE:CD1	1:A:60:ILE:CG1	0.42	2.98	31	1
1:A:91:GLU:OE1	1:A:91:GLU:C	0.42	2.62	37	1
1:A:71:VAL:HG22	1:A:72:CYS:SG	0.42	2.55	8	1
1:A:9:GLN:CD	1:A:116:LYS:HE3	0.42	2.40	11	3
1:A:82:LYS:CG	1:A:83:GLU:H	0.42	2.28	46	5
1:A:19:ILE:HG22	1:A:52:MET:CG	0.42	2.45	24	2
1:A:3:CYS:HB2	1:A:101:CYS:SG	0.42	2.54	29	1
1:A:9:GLN:CD	1:A:117:SER:OG	0.42	2.63	43	1
1:A:40:ILE:HG22	1:A:41:LYS:N	0.41	2.30	18	3
1:A:76:LEU:HA	1:A:81:LYS:HZ2	0.41	1.74	36	2
1:A:36:TYR:HB3	1:A:38:ASN:OD1	0.41	2.14	34	1
1:A:60:ILE:C	1:A:62:PHE:H	0.41	2.22	38	6
1:A:107:TRP:C	1:A:109:THR:N	0.41	2.78	17	7
1:A:33:ASN:CA	1:A:38:ASN:O	0.41	2.68	22	2
1:A:63:ILE:HD13	1:A:96:MET:CE	0.41	2.43	28	1
1:A:64:TYR:CZ	1:A:97:HIS:NE2	0.41	2.88	35	1
1:A:9:GLN:OE1	1:A:116:LYS:HE2	0.41	2.16	48	1
1:A:93:ASP:O	1:A:95:LYS:CD	0.41	2.68	49	1
1:A:108:ASP:C	1:A:109:THR:CG2	0.41	2.93	37	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ILE:H	1:A:35:ILE:CD1	0.41	2.28	18	8
1:A:35:ILE:HG22	1:A:35:ILE:O	0.41	2.15	10	7
1:A:85:LEU:H	1:A:85:LEU:HD13	0.41	1.75	32	7
1:A:28:GLU:CG	1:A:43:ILE:HD11	0.41	2.44	48	2
1:A:45:TYR:HB2	1:A:63:ILE:C	0.41	2.40	27	1
1:A:68:SER:CB	1:A:71:VAL:CG1	0.41	2.98	43	1
1:A:27:LYS:HB3	1:A:44:GLN:CG	0.41	2.45	25	6
1:A:90:ALA:HA	1:A:96:MET:HB2	0.41	1.92	1	3
1:A:81:LYS:O	1:A:82:LYS:HE2	0.41	2.16	6	3
1:A:77:ASP:OD1	1:A:79:GLY:CA	0.41	2.68	46	2
1:A:28:GLU:HA	1:A:41:LYS:NZ	0.41	2.31	22	2
1:A:75:SER:O	1:A:81:LYS:NZ	0.41	2.54	22	2
1:A:45:TYR:OH	1:A:65:THR:HG21	0.41	2.11	32	3
1:A:89:LYS:C	1:A:90:ALA:O	0.41	2.63	43	1
1:A:20:ARG:NE	1:A:51:LYS:HD2	0.41	2.30	48	1
1:A:76:LEU:CD2	1:A:84:TYR:CD2	0.41	2.97	20	3
1:A:17:VAL:CG1	1:A:17:VAL:O	0.41	2.67	2	1
1:A:83:GLU:OE1	1:A:83:GLU:CA	0.41	2.69	8	2
1:A:69:SER:O	1:A:75:SER:HB2	0.41	2.16	32	2
1:A:54:LYS:HG3	1:A:54:LYS:O	0.41	2.15	38	1
1:A:116:LYS:C	1:A:116:LYS:HE3	0.41	2.41	25	5
1:A:80:GLY:C	1:A:81:LYS:HD3	0.41	2.41	5	1
1:A:9:GLN:CD	1:A:116:LYS:HE2	0.41	2.41	10	1
1:A:59:ASP:OD2	1:A:61:GLU:OE2	0.41	2.39	17	1
1:A:91:GLU:N	1:A:96:MET:HA	0.41	2.30	42	3
1:A:81:LYS:C	1:A:82:LYS:CE	0.41	2.94	27	3
1:A:9:GLN:C	1:A:11:ALA:H	0.41	2.21	9	2
1:A:49:GLN:CD	1:A:49:GLN:C	0.41	2.88	22	1
1:A:91:GLU:HB2	1:A:96:MET:C	0.41	2.41	37	2
1:A:69:SER:O	1:A:75:SER:HB3	0.41	2.16	9	1
1:A:9:GLN:NE2	1:A:117:SER:HB2	0.41	2.30	22	2
1:A:54:LYS:HG3	1:A:55:GLY:N	0.41	2.31	12	1
1:A:20:ARG:NH1	1:A:50:ILE:HD11	0.41	2.30	28	1
1:A:60:ILE:HD13	1:A:94:GLY:H	0.41	1.75	34	1
1:A:49:GLN:HB2	1:A:59:ASP:CG	0.41	2.41	42	1
1:A:45:TYR:OH	1:A:75:SER:N	0.41	2.54	43	2
1:A:89:LYS:O	1:A:90:ALA:O	0.41	2.38	43	1
1:A:22:LYS:O	1:A:47:ILE:HB	0.41	2.16	45	1
1:A:25:SER:OG	1:A:46:GLU:HB3	0.41	2.15	49	1
1:A:80:GLY:HA3	1:A:81:LYS:HE2	0.41	1.91	16	1
1:A:27:LYS:O	1:A:43:ILE:HA	0.41	2.15	27	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:VAL:O	1:A:17:VAL:HG13	0.41	2.16	34	1
1:A:49:GLN:HG3	1:A:59:ASP:CG	0.41	2.41	35	1
1:A:41:LYS:CE	1:A:41:LYS:HA	0.41	2.46	39	1
1:A:91:GLU:HB2	1:A:96:MET:HA	0.41	1.93	49	1
1:A:35:ILE:CD1	1:A:35:ILE:H	0.40	2.28	4	1
1:A:54:LYS:CE	1:A:54:LYS:HA	0.40	2.46	9	1
1:A:77:ASP:OD1	1:A:77:ASP:C	0.40	2.64	19	1
1:A:20:ARG:HD3	1:A:107:TRP:CE2	0.40	2.51	25	1
1:A:22:LYS:HE2	1:A:78:VAL:HG11	0.40	1.93	33	1
1:A:82:LYS:O	1:A:83:GLU:OE2	0.40	2.39	41	1
1:A:108:ASP:O	1:A:108:ASP:OD1	0.40	2.39	43	1
1:A:103:PHE:CD1	1:A:104:ILE:N	0.40	2.90	29	2
1:A:23:ALA:HA	1:A:47:ILE:HA	0.40	1.93	41	1
1:A:3:CYS:O	1:A:5:PRO:HD3	0.40	2.17	44	1
1:A:20:ARG:HG3	1:A:53:PHE:CE2	0.40	2.50	49	1
1:A:28:GLU:OE1	1:A:30:ASP:OD1	0.40	2.39	8	1
1:A:80:GLY:CA	1:A:81:LYS:HE2	0.40	2.46	23	1
1:A:43:ILE:CD1	1:A:67:PRO:HB3	0.40	2.46	27	1
1:A:27:LYS:HG2	1:A:29:VAL:HG13	0.40	1.93	38	2
1:A:5:PRO:CG	1:A:100:LEU:O	0.40	2.69	46	1
1:A:12:PHE:CB	1:A:117:SER:OG	0.40	2.69	6	1
1:A:20:ARG:O	1:A:20:ARG:HG2	0.40	2.17	23	1
1:A:22:LYS:HE2	1:A:24:VAL:CG1	0.40	2.47	24	1
1:A:84:TYR:CG	1:A:86:ILE:CD1	0.40	2.83	25	1
1:A:91:GLU:CD	1:A:91:GLU:C	0.40	2.89	3	1
1:A:63:ILE:HD13	1:A:96:MET:CG	0.40	2.47	33	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	117/127 (92%)	68±2 (58±2%)	30±2 (26±2%)	19±2 (16±2%)	0	4
All	All	5733/6223 (92%)	3316 (58%)	1492 (26%)	925 (16%)	0	4

All 31 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	6	VAL	49
1	A	17	VAL	49
1	A	40	ILE	49
1	A	41	LYS	49
1	A	46	GLU	49
1	A	49	GLN	49
1	A	59	ASP	49
1	A	75	SER	49
1	A	82	LYS	49
1	A	86	ILE	49
1	A	110	LEU	49
1	A	111	SER	49
1	A	112	THR	49
1	A	53	PHE	46
1	A	70	ALA	44
1	A	47	ILE	35
1	A	43	ILE	26
1	A	7	HIS	24
1	A	67	PRO	23
1	A	90	ALA	16
1	A	3	CYS	13
1	A	78	VAL	12
1	A	89	LYS	9
1	A	93	ASP	9
1	A	68	SER	9
1	A	58	LYS	7
1	A	92	GLY	7
1	A	15	ALA	4
1	A	69	SER	2
1	A	103	PHE	1
1	A	32	GLY	1

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	101/110 (92%)	58±2 (58±2%)	43±2 (42±2%)	0	4
All	All	4949/5390 (92%)	2860 (58%)	2089 (42%)	0	4

All 70 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	7	HIS	49
1	A	14	ASN	49
1	A	18	VAL	49
1	A	19	ILE	49
1	A	50	ILE	49
1	A	58	LYS	49
1	A	63	ILE	49
1	A	71	VAL	49
1	A	76	LEU	49
1	A	81	LYS	49
1	A	82	LYS	49
1	A	85	LEU	49
1	A	86	ILE	49
1	A	95	LYS	49
1	A	96	MET	49
1	A	105	VAL	49
1	A	112	THR	49
1	A	114	GLN	49
1	A	115	LYS	49
1	A	117	SER	49
1	A	43	ILE	48
1	A	61	GLU	48
1	A	116	LYS	47
1	A	60	ILE	46
1	A	35	ILE	44
1	A	100	LEU	43
1	A	42	ARG	41
1	A	77	ASP	41
1	A	97	HIS	41
1	A	45	TYR	40
1	A	68	SER	38
1	A	9	GLN	37
1	A	89	LYS	35
1	A	54	LYS	35
1	A	99	THR	34
1	A	26	GLU	32

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Mol	Chain	Res	Type	Models (Total)
1	A	78	VAL	31
1	A	101	CYS	30
1	A	52	MET	30
1	A	51	LYS	29
1	A	83	GLU	28
1	A	10	GLN	27
1	A	3	CYS	25
1	A	75	SER	25
1	A	49	GLN	22
1	A	16	ASP	21
1	A	93	ASP	21
1	A	48	LYS	19
1	A	118	LEU	18
1	A	64	TYR	15
1	A	30	ASP	13
1	A	28	GLU	12
1	A	47	ILE	11
1	A	119	ASN	10
1	A	41	LYS	10
1	A	20	ARG	9
1	A	98	ILE	7
1	A	33	ASN	7
1	A	113	THR	7
1	A	24	VAL	4
1	A	91	GLU	4
1	A	69	SER	4
1	A	62	PHE	4
1	A	53	PHE	3
1	A	72	CYS	3
1	A	12	PHE	3
1	A	109	THR	3
1	A	13	CYS	2
1	A	59	ASP	1
1	A	38	ASN	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided