



Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 02:20 am GMT

PDB ID : 2TMP
Title : N-TERMINAL DOMAIN OF TISSUE INHIBITOR OF
METALLOPROTEINASE-2 (N-TIMP-2), NMR, 49 STRUCTURES
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Williamson, R.A.
Deposited on : 1998-05-26

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

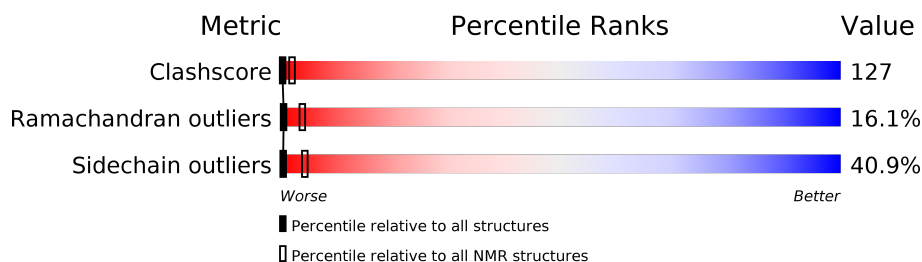
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	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)	0.19	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:

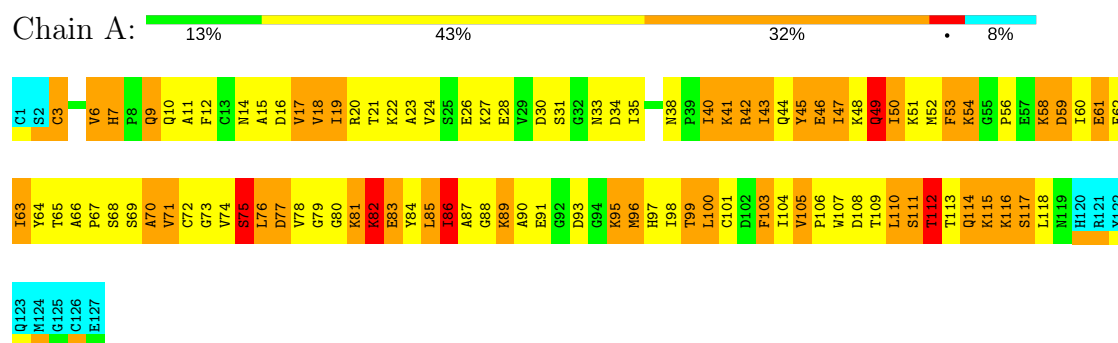
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	THR	ALA	CONFLICT	UNP P16035

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2

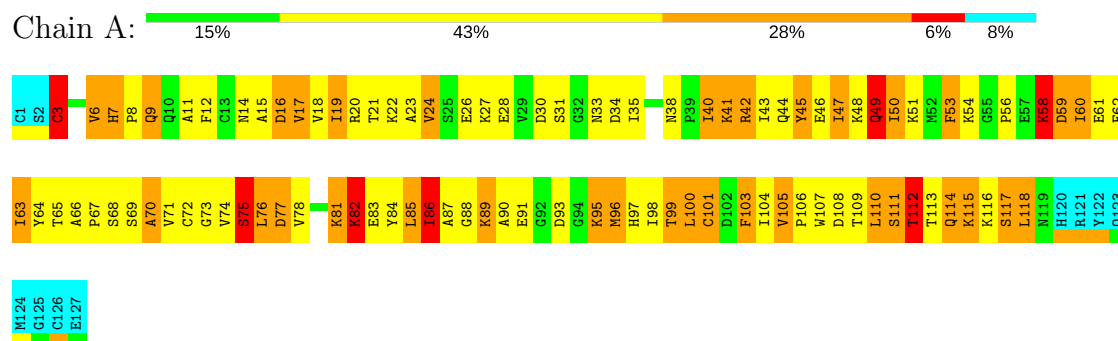


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

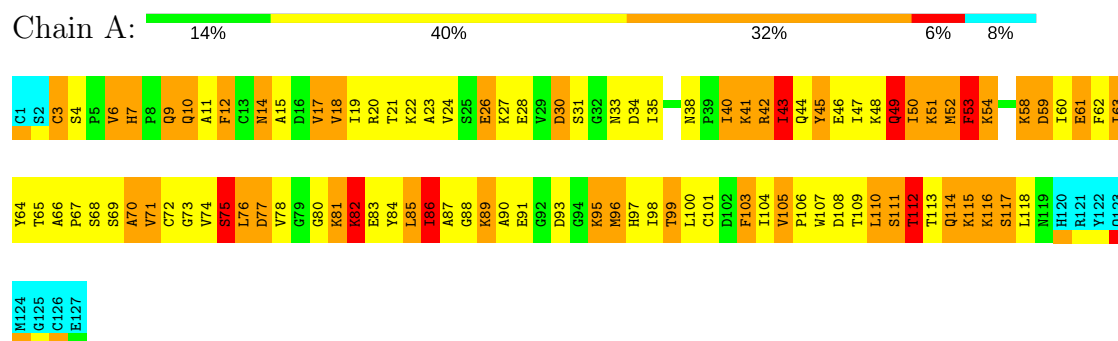
4.2.1 Score per residue for model 1

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



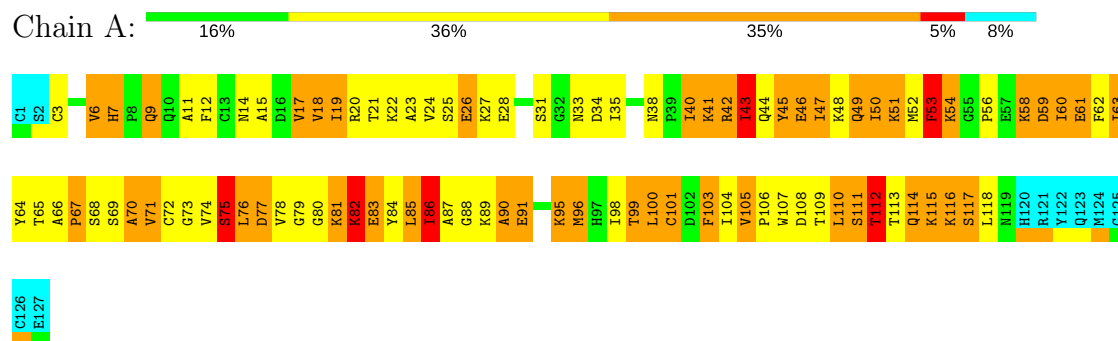
4.2.2 Score per residue for model 2

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



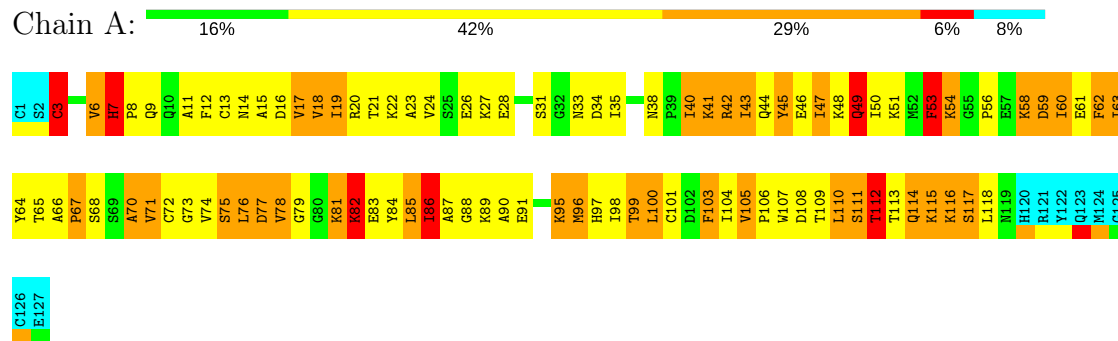
4.2.3 Score per residue for model 3

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



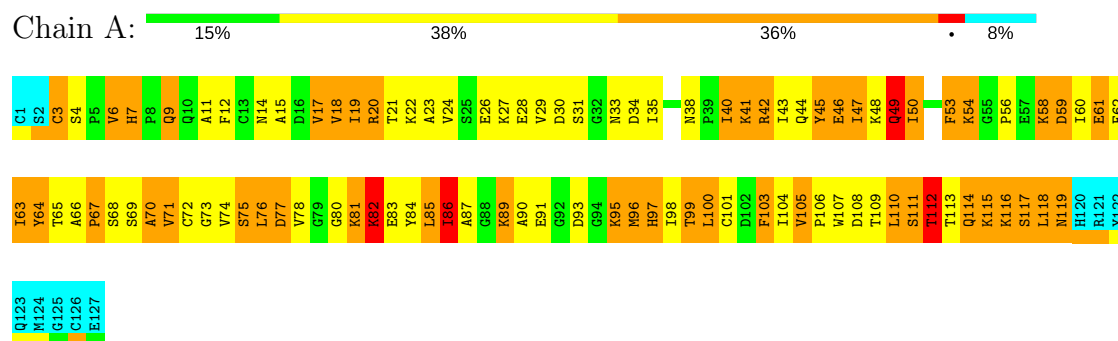
4.2.4 Score per residue for model 4

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



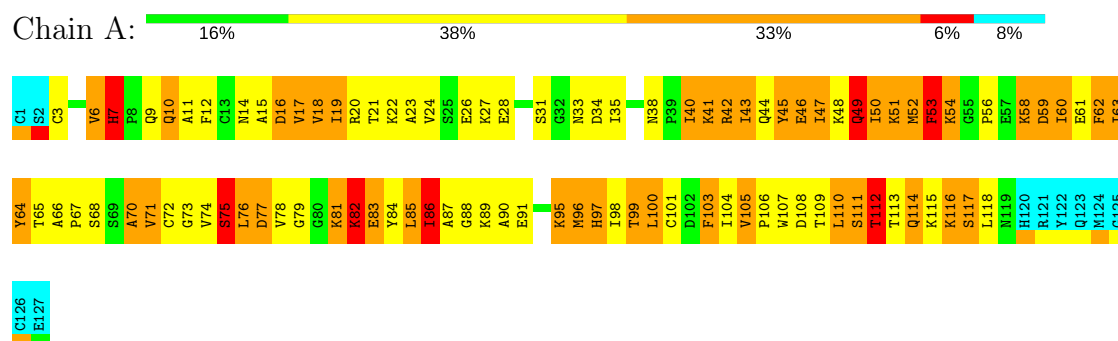
4.2.5 Score per residue for model 5

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



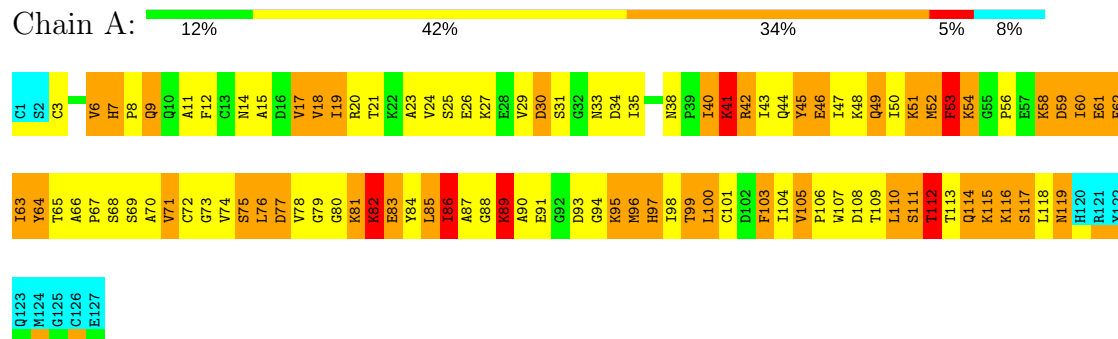
4.2.6 Score per residue for model 6

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



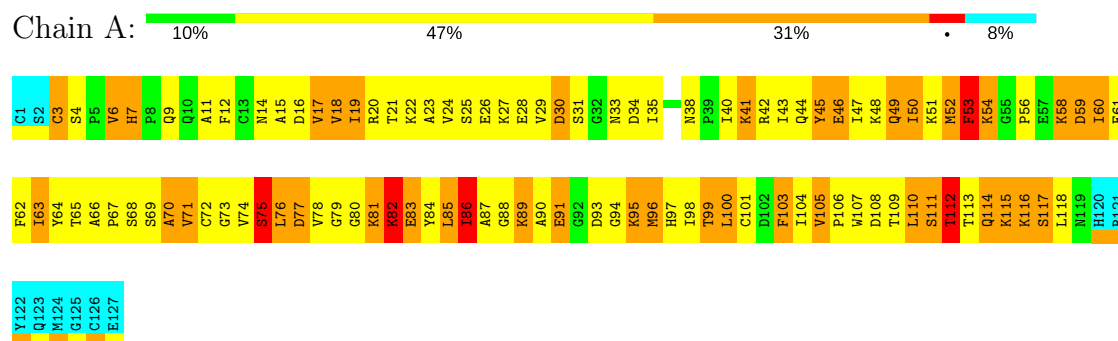
4.2.7 Score per residue for model 7

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



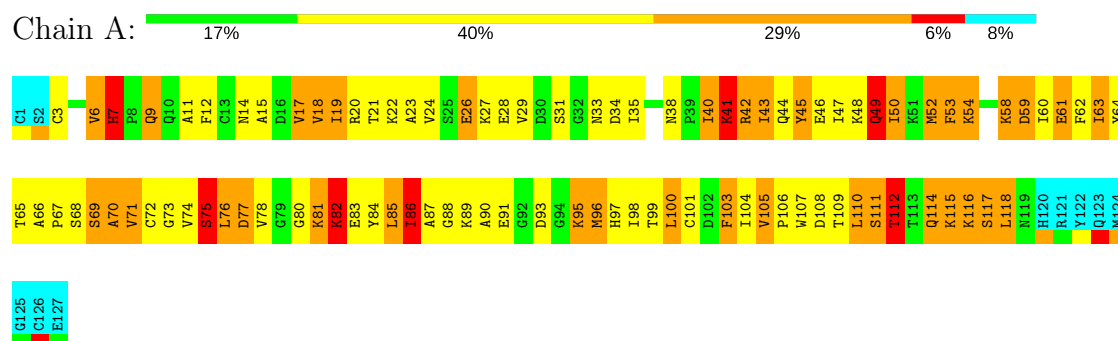
4.2.8 Score per residue for model 8

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



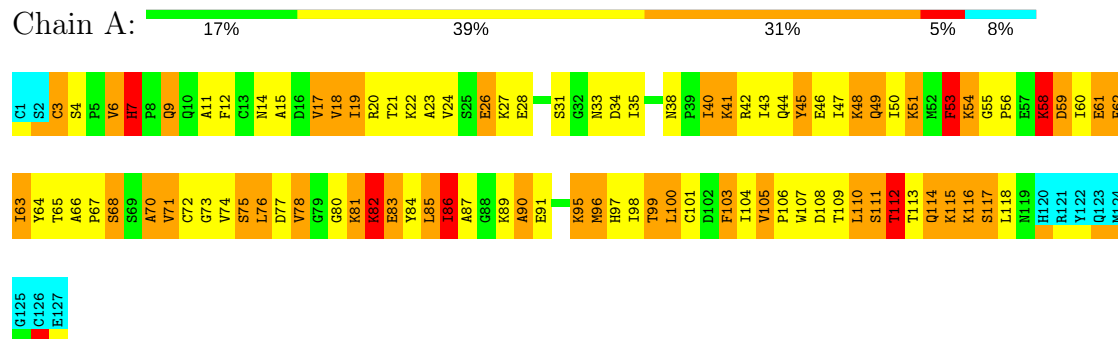
4.2.9 Score per residue for model 9

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



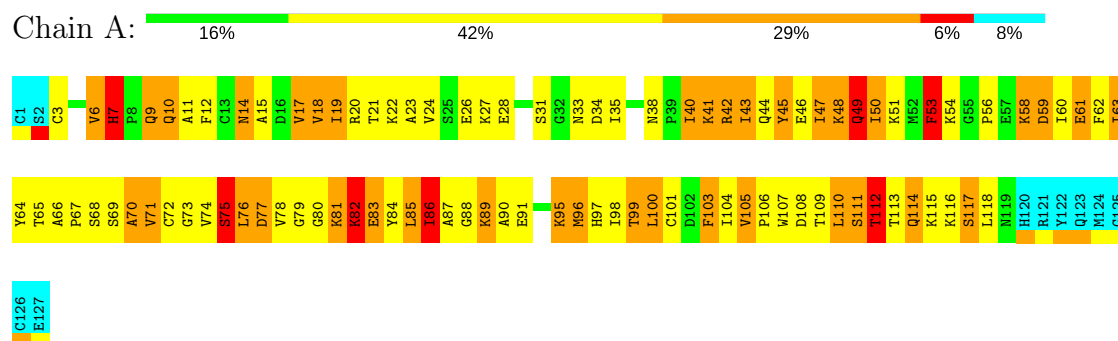
4.2.10 Score per residue for model 10

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



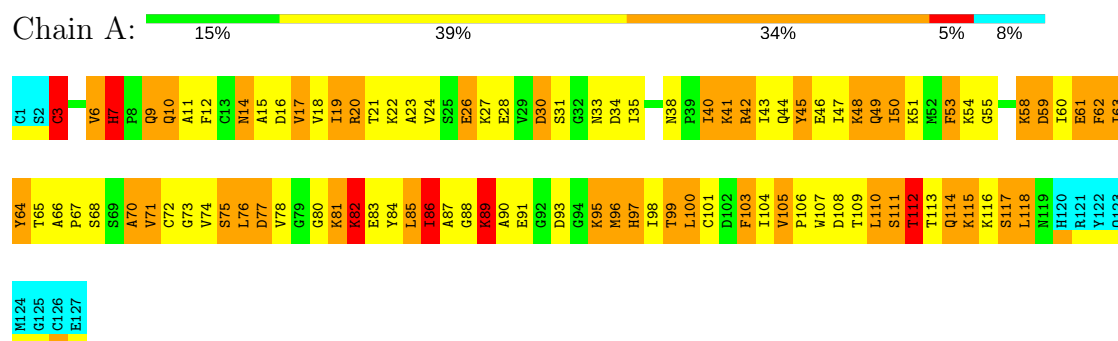
4.2.11 Score per residue for model 11

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



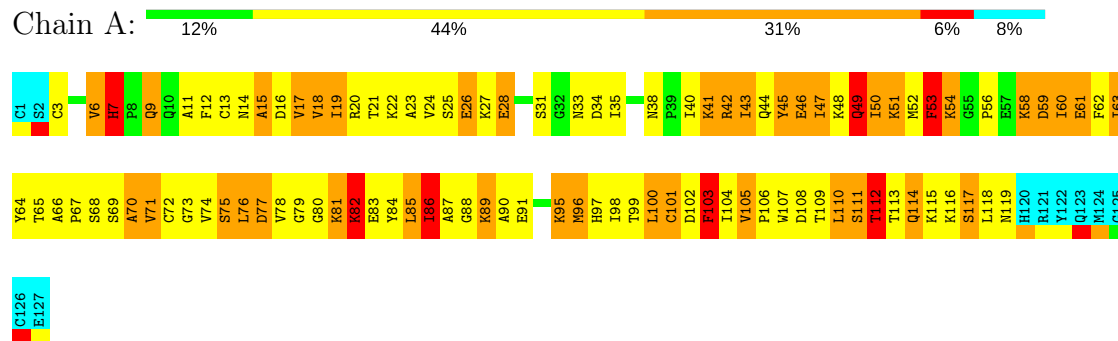
4.2.12 Score per residue for model 12

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



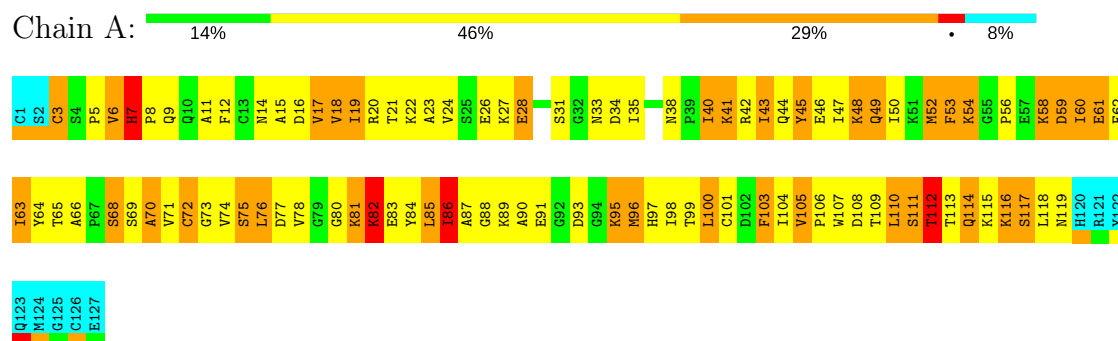
4.2.13 Score per residue for model 13

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



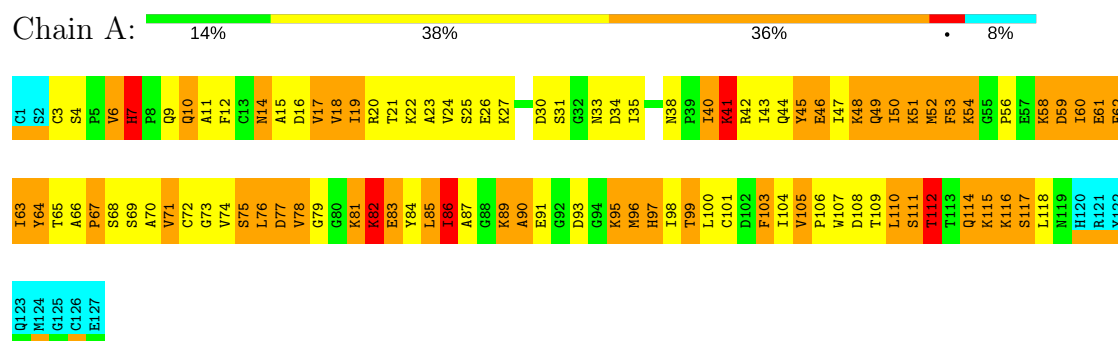
4.2.14 Score per residue for model 14

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



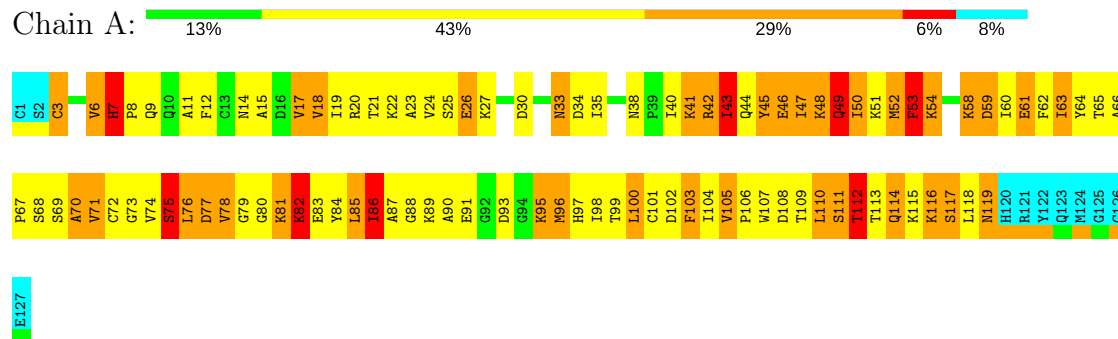
4.2.15 Score per residue for model 15

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



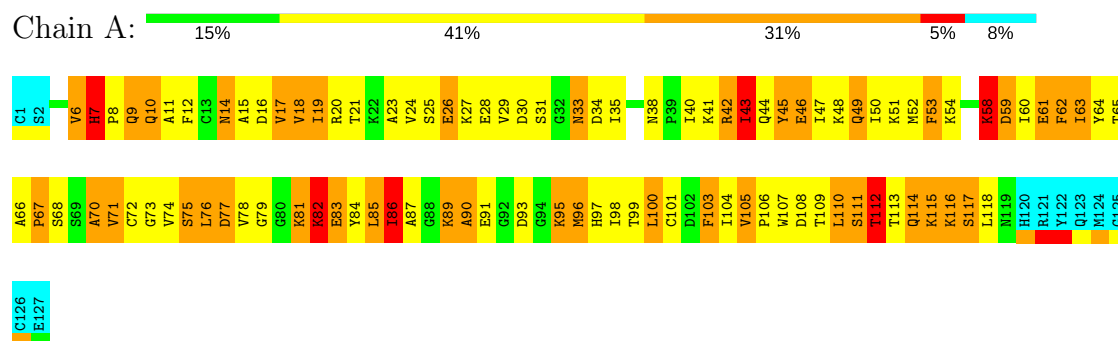
4.2.16 Score per residue for model 16

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



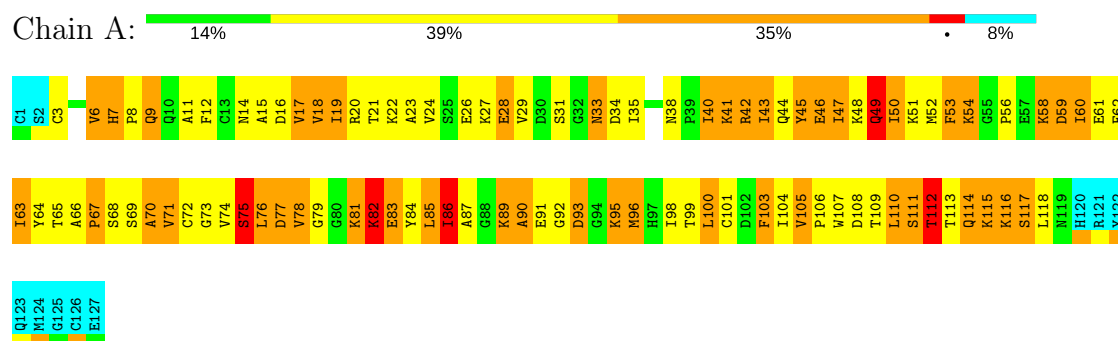
4.2.17 Score per residue for model 17

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



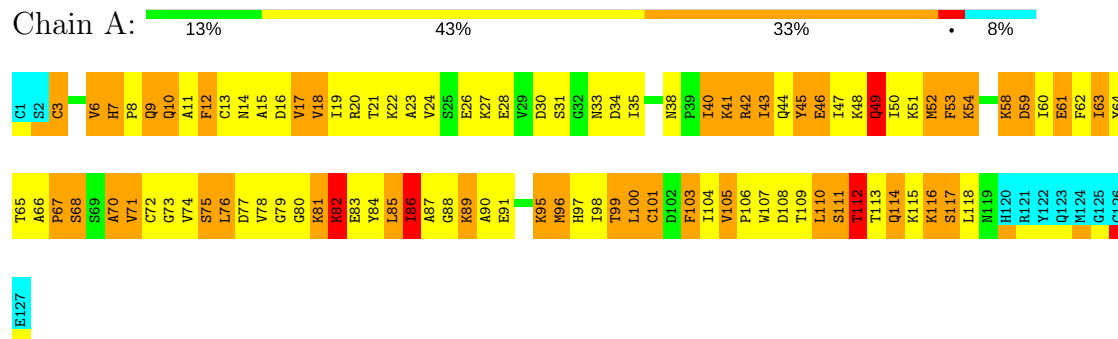
4.2.18 Score per residue for model 18

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



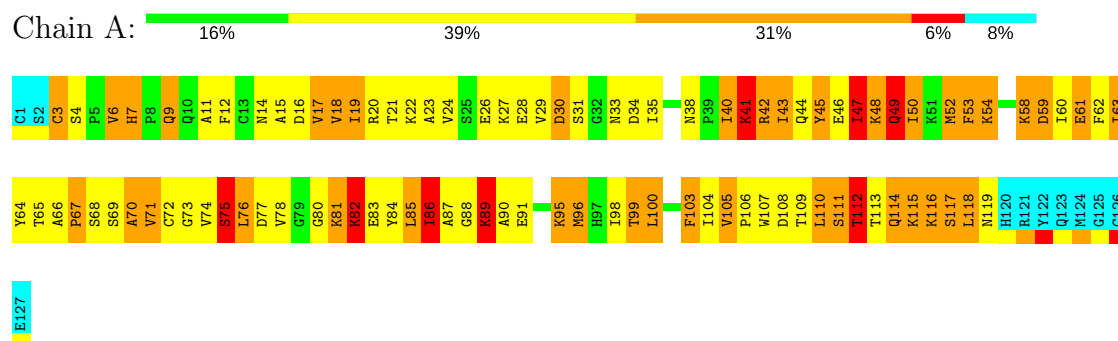
4.2.19 Score per residue for model 19

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



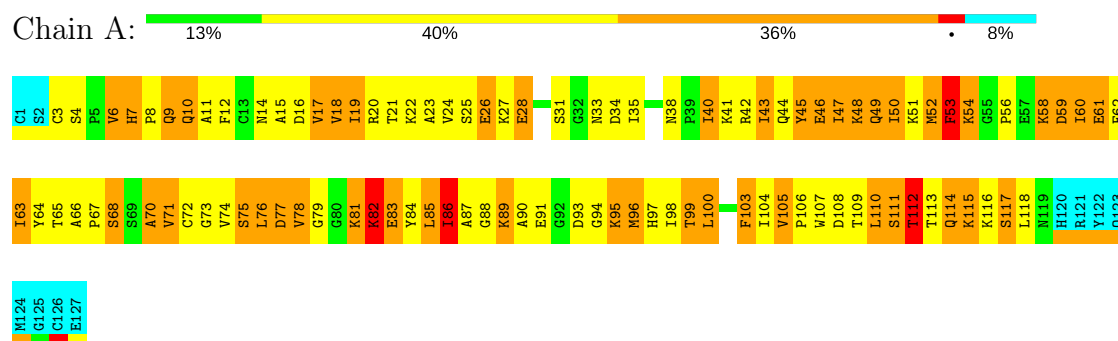
4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



4.2.21 Score per residue for model 21

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



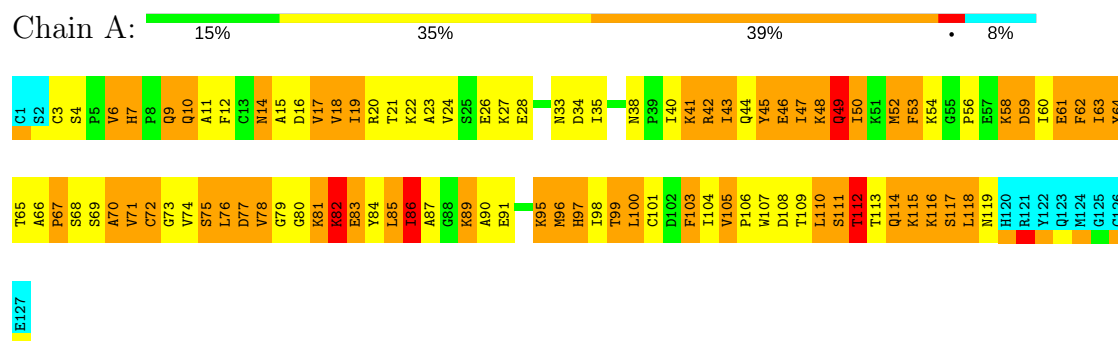
4.2.22 Score per residue for model 22

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



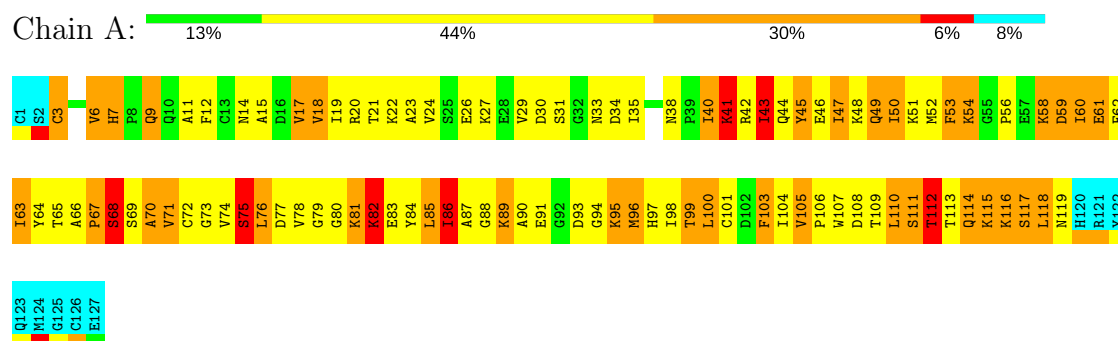
4.2.23 Score per residue for model 23

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



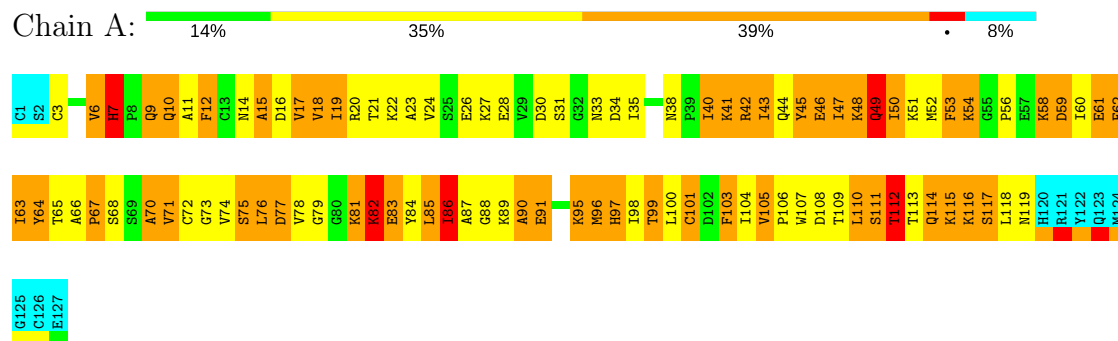
4.2.24 Score per residue for model 24

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



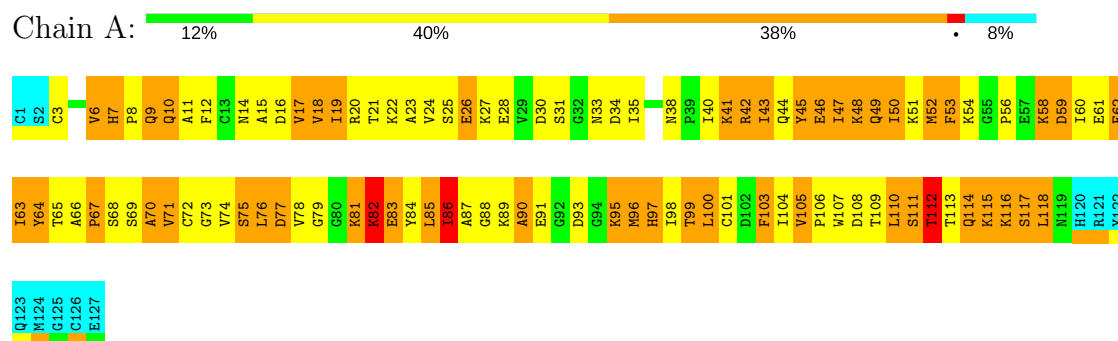
4.2.25 Score per residue for model 25

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



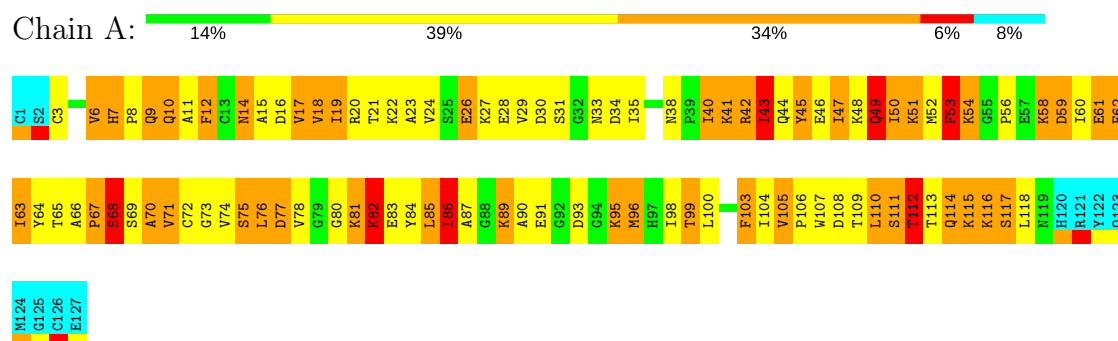
4.2.26 Score per residue for model 26

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



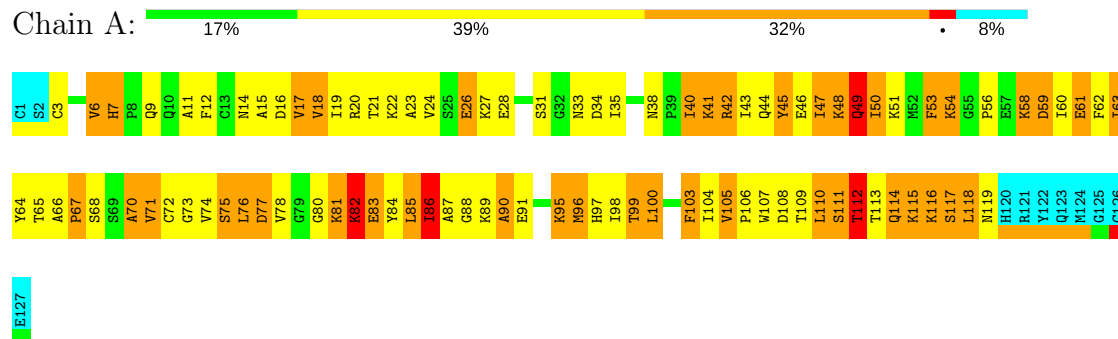
4.2.27 Score per residue for model 27

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



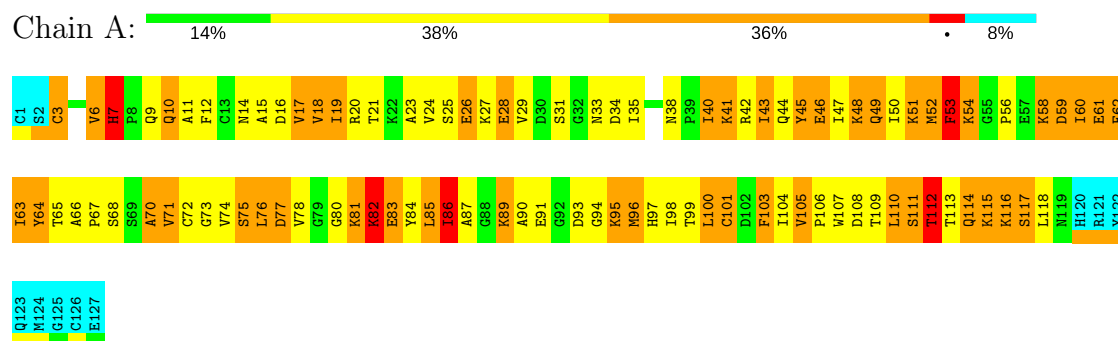
4.2.28 Score per residue for model 28

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



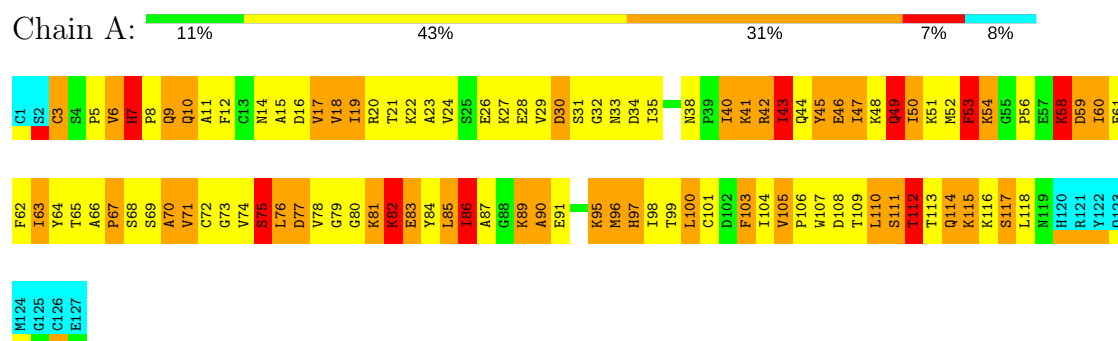
4.2.29 Score per residue for model 29

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



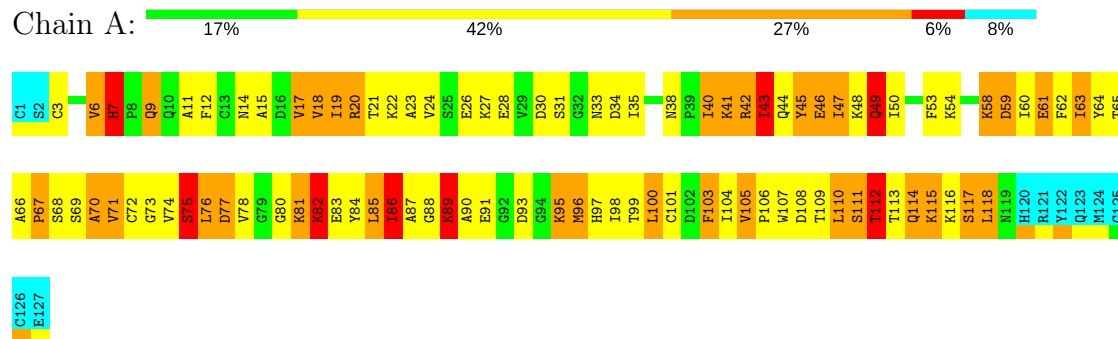
4.2.30 Score per residue for model 30

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



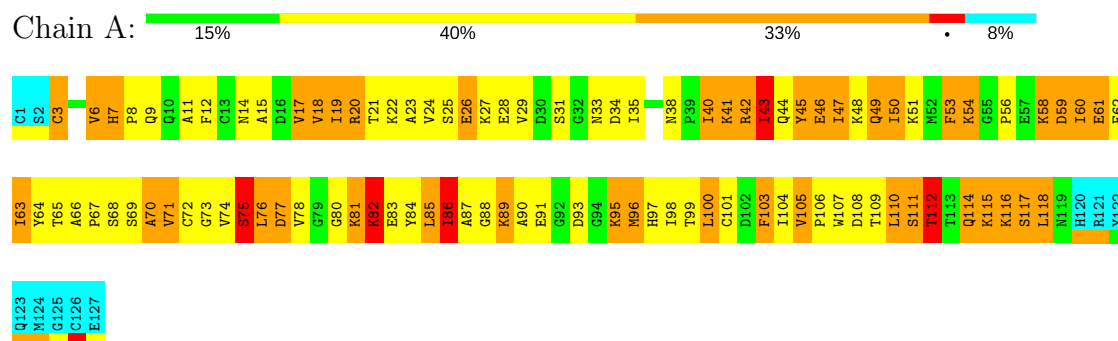
4.2.31 Score per residue for model 31

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



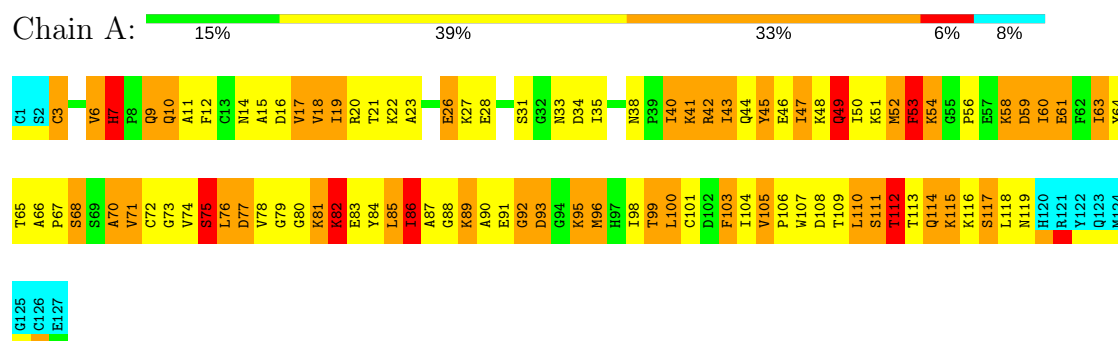
4.2.32 Score per residue for model 32

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



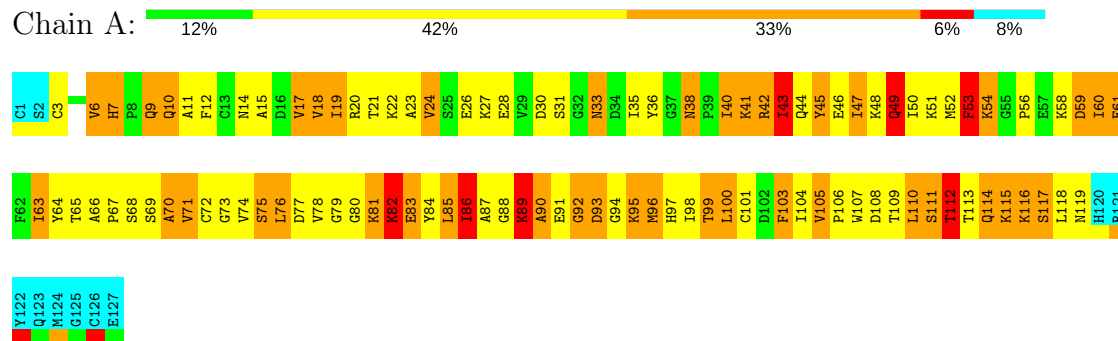
4.2.33 Score per residue for model 33

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



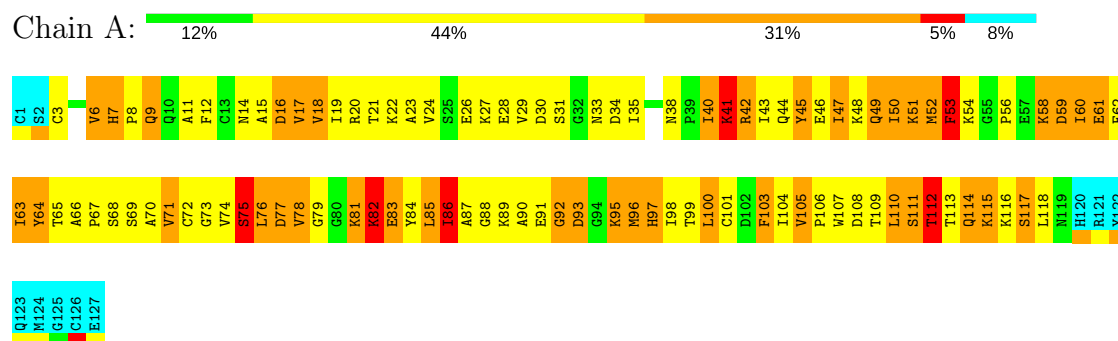
4.2.34 Score per residue for model 34

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



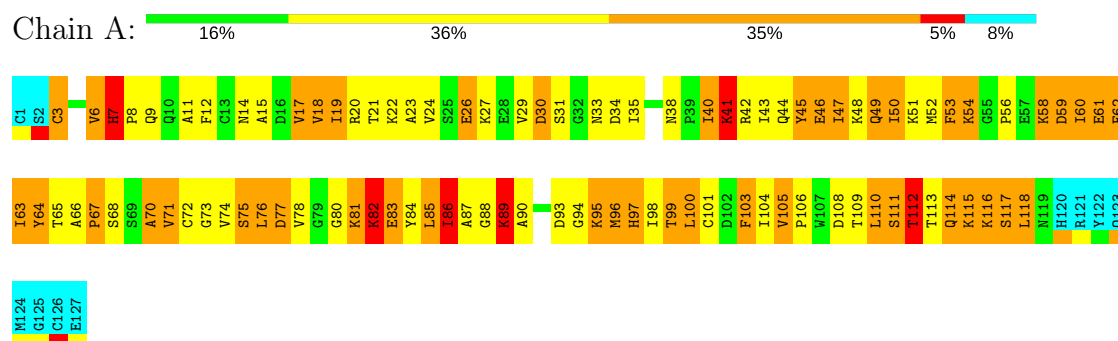
4.2.35 Score per residue for model 35

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



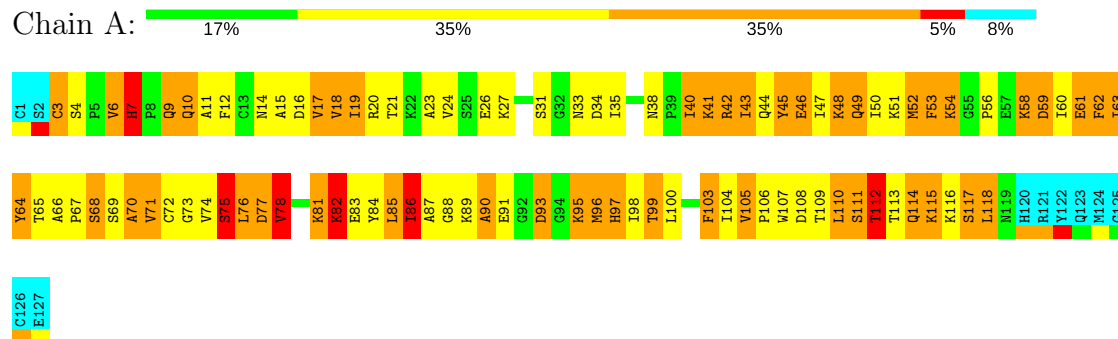
4.2.36 Score per residue for model 36

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



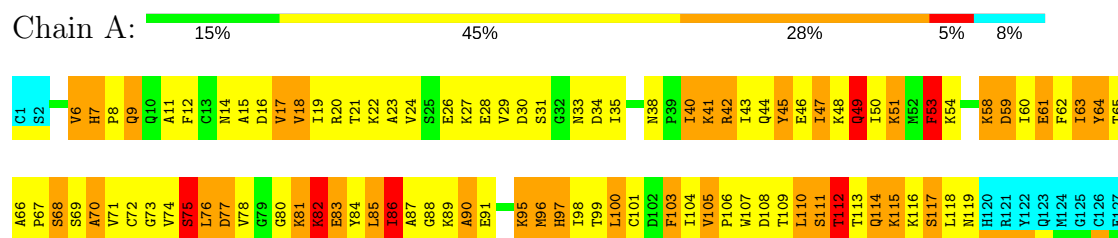
4.2.37 Score per residue for model 37

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



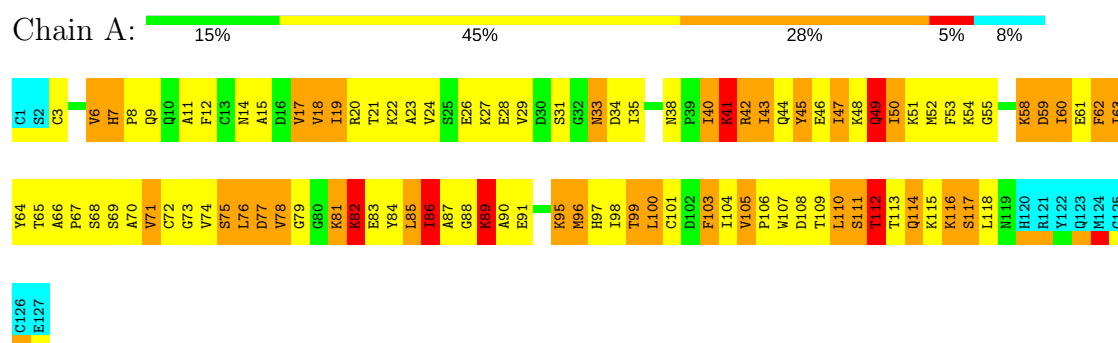
4.2.38 Score per residue for model 38

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



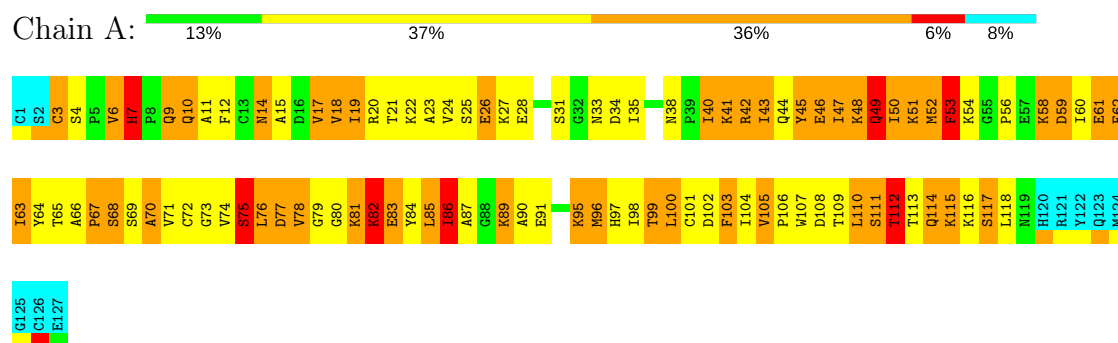
4.2.39 Score per residue for model 39

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



4.2.40 Score per residue for model 40

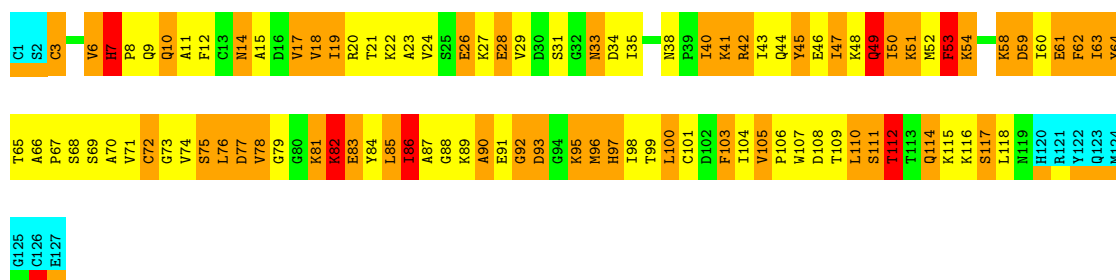
- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2



4.2.41 Score per residue for model 41

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2

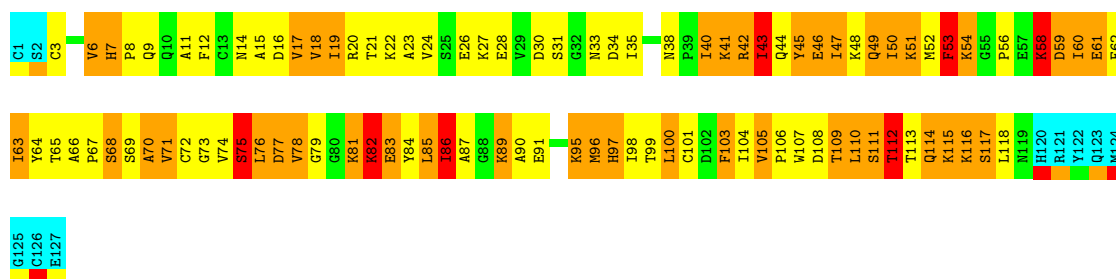




4.2.42 Score per residue for model 42

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2

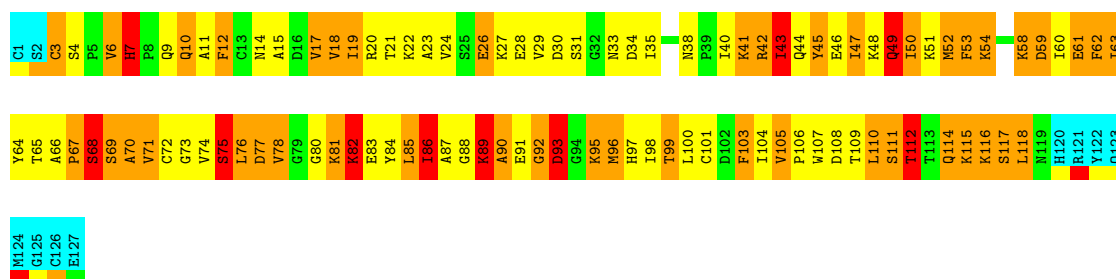
Chain A: 15% 39% 33% 6% 8%



4.2.43 Score per residue for model 43

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2

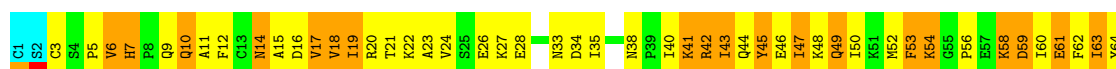
Chain A: 13% 36% 35% 8% 8%

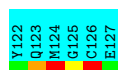


4.2.44 Score per residue for model 44

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2

Chain A: 16% 40% 33% 8%

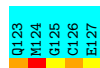
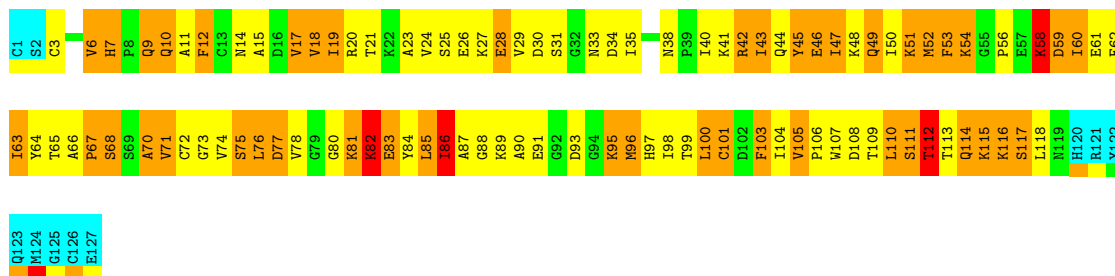




4.2.48 Score per residue for model 48

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2

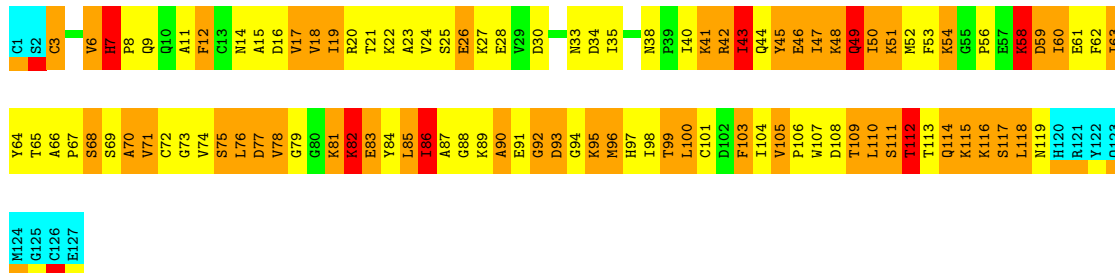
Chain A: 14% 40% 35% 8%



4.2.49 Score per residue for model 49

- Molecule 1: TISSUE INHIBITOR OF METALLOPROTEINASES-2

Chain A: 11% 39% 36% 6% 8%



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	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 4214
Number of chemical shift lists	1
Total number of shifts	1328
Number of shifts mapped to atoms	1328
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	903	906	906	229±9
All	All	44247	44394	44394	11214

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 127.

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: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
1:A:18:VAL:HG13	1:A:87:ALA:CB	0.92	1.95	25	34

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:74:VAL:HG23	1:A:104:ILE:CD1	0.81	2.05	33	49
1:A:41:LYS:HZ3	1:A:43:ILE:HD12	0.80	1.36	22	2
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:84:TYR:CD1	1:A:86:ILE:HB	0.76	2.15	34	49
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:17:VAL:O	1:A:17:VAL:HG13	0.72	1.84	16	15
1:A:3:CYS:CB	1:A:101:CYS:SG	0.72	2.77	29	2
1:A:35:ILE:HD12	1:A:35:ILE:N	0.72	2.00	20	21
1:A:12:PHE:CE1	1:A:114:GLN:CG	0.72	2.72	15	48
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:35:ILE:N	1:A:35:ILE:HD12	0.72	2.00	29	28
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:109:THR:O	1:A:110:LEU:C	0.71	2.28	12	49
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:85:LEU:O	1:A:86:ILE:C	0.70	2.30	32	49
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: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	2.26	47	35
1:A:71:VAL:HG23	1:A:72:CYS:SG	0.69	2.28	36	39
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
1:A:11:ALA:HB1	1:A:103:PHE:CB	0.68	2.17	27	49
1:A:84:TYR:CE1	1:A:86:ILE:HB	0.68	2.24	37	49
1:A:44:GLN:OE1	1:A:64:TYR:CZ	0.68	2.47	31	34
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:89:LYS:O	1:A:90:ALA:HB3	0.67	1.89	26	40
1:A:64:TYR:CD1	1:A:64:TYR:C	0.67	2.67	35	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ILE:HD13	1:A:93:ASP:C	0.67	2.09	18	1
1:A:12:PHE:CZ	1:A:114:GLN:CG	0.67	2.77	25	37
1:A:63:ILE:CD1	1:A:96:MET:HE2	0.67	2.20	5	11
1:A:23:ALA:HA	1:A:47:ILE:HG22	0.67	1.65	24	49
1:A:21:THR:CB	1:A:47:ILE:HD12	0.67	2.20	39	48
1:A:53:PHE:CE2	1:A:118:LEU:CD2	0.67	2.77	48	21
1:A:110:LEU:O	1:A:111:SER:CB	0.67	2.43	23	49
1:A:74:VAL:CG2	1:A:104:ILE:HD12	0.67	2.18	48	49
1:A:41:LYS:NZ	1:A:43:ILE:HD12	0.66	2.04	22	2
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: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:64:TYR:C	1:A:64:TYR:CD1	0.66	2.69	7	6
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:20:ARG:CD	1:A:53:PHE:CZ	0.66	2.79	49	1
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: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:20:ARG:NH2	1:A:107:TRP:CZ2	0.65	2.65	40	17
1:A:30:ASP:CG	1:A:41:LYS:HZ3	0.64	1.95	25	1
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:102:ASP:O	1:A:103:PHE:C	0.64	2.35	13	1
1:A:20:ARG:HD2	1:A:107:TRP:CE3	0.64	2.28	20	10
1:A:72:CYS:HA	1:A:100:LEU:HD22	0.63	1.67	2	26
1:A:31:SER:O	1:A:40:ILE:HD12	0.63	1.92	6	21
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:66:ALA:HB2	1:A:72:CYS:HB2	0.63	1.69	34	32
1:A:114:GLN:N	1:A:114:GLN:HE21	0.63	1.90	35	28
1:A:114:GLN:HE21	1:A:114:GLN:N	0.63	1.91	4	21
1:A:12:PHE:CE1	1:A:114:GLN:HG3	0.63	2.28	22	48

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:85:LEU:O	1:A:86:ILE:O	0.63	2.17	1	49
1:A:31:SER:OG	1:A:40:ILE:HG21	0.63	1.93	24	27
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:17:VAL:HG13	1:A:17:VAL:O	0.61	1.95	18	20
1:A:113:THR:HG23	1:A:116:LYS:HE2	0.61	1.71	49	1
1:A:63:ILE:HD12	1:A:96:MET:SD	0.61	2.35	47	34
1:A:12:PHE:CE2	1:A:114:GLN:O	0.61	2.53	10	29
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:12:PHE:CZ	1:A:114:GLN:CB	0.60	2.84	25	48
1:A:86:ILE:O	1:A:86:ILE:HG22	0.60	1.96	26	27
1:A:15:ALA:CB	1:A:87:ALA:HB1	0.60	2.26	45	49
1:A:86:ILE:HG22	1:A:86:ILE:O	0.60	1.95	23	22
1:A:23:ALA:HB2	1:A:47:ILE:HG22	0.60	1.73	45	48
1:A:12:PHE:CE2	1:A:103:PHE:HZ	0.60	2.12	44	49
1:A:53:PHE:CD2	1:A:118:LEU:CD2	0.60	2.85	39	20
1:A:63:ILE:CD1	1:A:96:MET:HE1	0.60	2.26	42	3
1:A:106:PRO:HD2	1:A:109:THR:OG1	0.60	1.97	28	49
1:A:23:ALA:N	1:A:78:VAL:HG21	0.59	2.12	33	4
1:A:92:GLY:O	1:A:95:LYS:O	0.59	2.20	45	2
1:A:10:GLN:HE22	1:A:14:ASN:ND2	0.59	1.95	23	12
1:A:63:ILE:CD1	1:A:96:MET:CE	0.59	2.80	42	14
1:A:21:THR:CG2	1:A:84:TYR:CE1	0.59	2.86	9	49
1:A:12:PHE:CE1	1:A:114:GLN:HG2	0.59	2.32	47	29
1:A:92:GLY:O	1:A:93:ASP:C	0.59	2.40	22	2
1:A:53:PHE:CE2	1:A:118:LEU:CD1	0.59	2.83	45	2
1:A:85:LEU:HD11	1:A:105:VAL:HG23	0.59	1.75	38	42
1:A:20:ARG:HD2	1:A:50:ILE:HD11	0.59	1.74	39	8
1:A:17:VAL:HG11	1:A:96:MET:SD	0.59	2.38	42	5
1:A:119:ASN:OD1	1:A:119:ASN:C	0.59	2.39	49	1
1:A:110:LEU:HD22	1:A:114:GLN:CB	0.59	2.25	6	37
1:A:12:PHE:CG	1:A:103:PHE:CE2	0.59	2.91	16	46

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:VAL:N	1:A:41:LYS:HZ2	0.59	1.94	39	2
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:74:VAL:O	1:A:75:SER:C	0.59	2.41	35	47
1:A:9:GLN:NE2	1:A:116:LYS:HE3	0.59	2.13	49	8
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	7
1:A:99:THR:O	1:A:104:ILE:CD1	0.58	2.52	18	49
1:A:27:LYS:HB3	1:A:44:GLN:HB2	0.58	1.75	40	49
1:A:23:ALA:O	1:A:78:VAL:CG2	0.58	2.51	23	11
1:A:18:VAL:N	1:A:54:LYS:O	0.58	2.37	1	15
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:75:SER:O	1:A:75:SER:OG	0.57	2.19	11	5
1:A:71:VAL:CG2	1:A:72:CYS:N	0.57	2.66	19	5
1:A:17:VAL:HG12	1:A:90:ALA:HB2	0.57	1.75	1	9
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:77:ASP:OD2	1:A:81:LYS:CE	0.57	2.53	46	7
1:A:19:ILE:HD12	1:A:49:GLN:OE1	0.57	2.00	26	6
1:A:67:PRO:O	1:A:68:SER:O	0.57	2.22	27	4
1:A:11:ALA:CB	1:A:103:PHE:HB2	0.57	2.30	27	49
1:A:81:LYS:N	1:A:81:LYS:CD	0.56	2.68	23	23
1:A:72:CYS:O	1:A:99:THR:HA	0.56	2.00	24	48
1:A:53:PHE:CZ	1:A:118:LEU:CD1	0.56	2.81	38	8
1:A:60:ILE:HG13	1:A:96:MET:SD	0.56	2.40	49	12
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:20:ARG:HD3	1:A:53:PHE:CE2	0.56	2.36	22	6
1:A:35:ILE:HD12	1:A:35:ILE:H	0.56	1.59	36	24
1:A:108:ASP:O	1:A:109:THR:CG2	0.56	2.54	37	46

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:VAL:HG22	1:A:7:HIS:H	0.56	1.61	4	49
1:A:89:LYS:O	1:A:90:ALA:CB	0.56	2.54	26	34
1:A:103:PHE:CD1	1:A:103:PHE:C	0.56	2.78	14	20
1:A:84:TYR:CE1	1:A:86:ILE:HG12	0.56	2.36	20	35
1:A:70:ALA:HB2	1:A:75:SER:HB2	0.56	1.78	6	8
1:A:103:PHE:C	1:A:103:PHE:CD1	0.56	2.77	10	29
1:A:20:ARG:NH1	1:A:107:TRP:CZ3	0.56	2.73	30	11
1:A:85:LEU:C	1:A:85:LEU:CD2	0.56	2.73	46	26
1:A:81:LYS:CD	1:A:81:LYS:N	0.56	2.69	35	19
1:A:7:HIS:CB	1:A:10:GLN:CG	0.56	2.84	46	22
1:A:85:LEU:CD2	1:A:85:LEU:C	0.56	2.74	12	23
1:A:35:ILE:H	1:A:35:ILE:HD12	0.56	1.60	33	25
1:A:18:VAL:O	1:A:54:LYS:N	0.55	2.39	17	47
1:A:77:ASP:O	1:A:78:VAL:HB	0.55	2.01	21	43
1:A:115:LYS:HA	1:A:118:LEU:HD23	0.55	1.78	28	3
1:A:77:ASP:CG	1:A:81:LYS:HZ1	0.55	2.04	39	12
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:19:ILE:HD11	1:A:96:MET:HE3	0.55	1.79	16	28
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:12:PHE:CD1	1:A:12:PHE:N	0.55	2.74	25	29
1:A:84:TYR:CE1	1:A:86:ILE:CG1	0.55	2.90	20	49
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: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	43
1:A:86:ILE:O	1:A:86:ILE:CG2	0.54	2.54	45	25
1:A:12:PHE:CD1	1:A:103:PHE:CZ	0.54	2.96	8	44
1:A:86:ILE:CG2	1:A:86:ILE:O	0.54	2.54	23	24
1:A:31:SER:OG	1:A:40:ILE:CG2	0.54	2.55	15	16
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:119:ASN:C	1:A:119:ASN:OD1	0.54	2.46	44	2
1:A:72:CYS:O	1:A:99:THR:CB	0.54	2.55	41	6
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	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ASP:O	1:A:104:ILE:HG12	0.54	2.01	13	1
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:CD1	1:A:35:ILE:N	0.54	2.71	4	26
1:A:74:VAL:CG2	1:A:104:ILE:CD1	0.54	2.84	10	42
1:A:106:PRO:HG2	1:A:109:THR:CG2	0.54	2.32	49	49
1:A:84:TYR:HB2	1:A:105:VAL:O	0.54	2.02	3	48
1:A:20:ARG:HD3	1:A:53:PHE:CZ	0.54	2.37	17	5
1:A:54:LYS:C	1:A:54:LYS:CE	0.54	2.76	36	2
1:A:46:GLU:HG3	1:A:62:PHE:CZ	0.54	2.38	23	18
1:A:103:PHE:O	1:A:104:ILE:CG2	0.54	2.55	13	49
1:A:12:PHE:N	1:A:12:PHE:CD1	0.54	2.74	45	20
1:A:17:VAL:CG2	1:A:96:MET:SD	0.54	2.96	28	14
1:A:53:PHE:CE1	1:A:118:LEU:CD2	0.54	2.91	20	4
1:A:92:GLY:O	1:A:93:ASP:O	0.53	2.26	46	9
1:A:21:THR:OG1	1:A:47:ILE:CD1	0.53	2.56	31	27
1:A:35:ILE:N	1:A:35:ILE:CD1	0.53	2.71	27	23
1:A:16:ASP:N	1:A:88:GLY:O	0.53	2.39	46	9
1:A:99:THR:C	1:A:104:ILE:HD11	0.53	2.24	10	27
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:49:GLN:CD	1:A:59:ASP:OD1	0.53	2.47	12	2
1:A:28:GLU:HA	1:A:43:ILE:CD1	0.53	2.34	14	3
1:A:88:GLY:O	1:A:90:ALA:N	0.53	2.42	12	13
1:A:17:VAL:HB	1:A:90:ALA:HB2	0.53	1.79	36	3
1:A:100:LEU:HD23	1:A:101:CYS:H	0.53	1.64	43	5
1:A:20:ARG:HD3	1:A:107:TRP:CE3	0.53	2.39	30	9
1:A:30:ASP:CG	1:A:41:LYS:HZ1	0.53	2.07	49	1
1:A:17:VAL:O	1:A:17:VAL:CG1	0.53	2.54	16	10
1:A:3:CYS:O	1:A:100:LEU:CD1	0.53	2.57	13	6
1:A:52:MET:O	1:A:52:MET:CE	0.53	2.57	30	1
1:A:7:HIS:O	1:A:11:ALA:HB2	0.52	2.03	37	6
1:A:77:ASP:OD1	1:A:79:GLY:N	0.52	2.42	13	9
1:A:29:VAL:HG23	1:A:29:VAL:O	0.52	2.04	22	5
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	8
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:PRO:CB	1:A:93:ASP:CG	0.52	2.78	49	1
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:17:VAL:HA	1:A:54:LYS:O	0.52	2.05	37	26
1:A:60:ILE:CG2	1:A:95:LYS:CA	0.52	2.87	42	7
1:A:85:LEU:HD11	1:A:110:LEU:HD21	0.52	1.81	35	21
1:A:6:VAL:O	1:A:7:HIS:C	0.52	2.48	29	36
1:A:62:PHE:O	1:A:95:LYS:HA	0.52	2.05	25	46
1:A:31:SER:OG	1:A:31:SER:O	0.52	2.28	8	10
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: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	4
1:A:53:PHE:CD2	1:A:118:LEU:HD21	0.51	2.40	1	4
1:A:47:ILE:CG1	1:A:61:GLU:HA	0.51	2.35	19	44
1:A:84:TYR:O	1:A:84:TYR:CD1	0.51	2.64	23	27
1:A:68:SER:HB2	1:A:71:VAL:CG1	0.51	2.35	43	5
1:A:52:MET:CG	1:A:52:MET:O	0.51	2.58	14	7
1:A:54:LYS:CE	1:A:54:LYS:C	0.51	2.78	42	1
1:A:63:ILE:CG2	1:A:96:MET:SD	0.51	2.98	18	35
1:A:73:GLY:HA2	1:A:100:LEU:N	0.51	2.21	15	46
1:A:19:ILE:O	1:A:84:TYR:O	0.51	2.28	8	49
1:A:49:GLN:CG	1:A:59:ASP:OD2	0.51	2.59	35	16
1:A:3:CYS:SG	1:A:4:SER:N	0.51	2.83	40	12
1:A:77:ASP:OD1	1:A:80:GLY:N	0.51	2.43	19	7
1:A:9:GLN:NE2	1:A:116:LYS:CE	0.51	2.74	36	16
1:A:93:ASP:C	1:A:95:LYS:H	0.51	2.09	49	5
1:A:3:CYS:SG	1:A:101:CYS:CB	0.51	2.98	48	2
1:A:60:ILE:CD1	1:A:93:ASP:O	0.51	2.50	18	1
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:84:TYR:CD1	1:A:84:TYR:O	0.51	2.64	30	22
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:GLN:NE2	1:A:59:ASP:OD2	0.51	2.43	29	16
1:A:23:ALA:O	1:A:77:ASP:C	0.51	2.49	11	15
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:63:ILE:HD12	1:A:96:MET:CE	0.51	2.35	42	3
1:A:11:ALA:O	1:A:103:PHE:CB	0.51	2.59	12	40
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:69:SER:O	1:A:75:SER:CB	0.51	2.58	43	11
1:A:19:ILE:HD11	1:A:96:MET:HE2	0.51	1.83	28	7
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:72:CYS:O	1:A:99:THR:CA	0.50	2.58	41	10
1:A:77:ASP:OD2	1:A:81:LYS:NZ	0.50	2.44	41	35
1:A:85:LEU:HD13	1:A:85:LEU:H	0.50	1.67	25	10
1:A:82:LYS:C	1:A:83:GLU:CG	0.50	2.79	7	4
1:A:71:VAL:O	1:A:100:LEU:CD2	0.50	2.58	38	3
1:A:59:ASP:CG	1:A:60:ILE:N	0.50	2.64	22	30
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: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:10:GLN:CG	1:A:10:GLN:O	0.50	2.60	44	5
1:A:26:GLU:CG	1:A:43:ILE:HG23	0.50	2.37	49	2
1:A:116:LYS:O	1:A:119:ASN:OD1	0.50	2.30	25	4
1:A:53:PHE:CG	1:A:118:LEU:CD2	0.50	2.94	1	6
1:A:12:PHE:CB	1:A:117:SER:HB3	0.50	2.37	43	39
1:A:28:GLU:HG2	1:A:41:LYS:NZ	0.50	2.22	38	4
1:A:17:VAL:HG23	1:A:56:PRO:CD	0.50	2.36	10	3
1:A:116:LYS:NZ	1:A:116:LYS:O	0.49	2.45	3	8
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:71:VAL:HG22	1:A:72:CYS:N	0.49	2.22	19	1
1:A:83:GLU:OE1	1:A:83:GLU:C	0.49	2.50	42	1
1:A:84:TYR:CE1	1:A:86:ILE:CB	0.49	2.95	37	47
1:A:26:GLU:OE1	1:A:26:GLU:C	0.49	2.50	49	1
1:A:19:ILE:C	1:A:85:LEU:HA	0.49	2.28	12	49
1:A:12:PHE:CG	1:A:117:SER:HB3	0.49	2.42	17	25
1:A:82:LYS:C	1:A:83:GLU:HG3	0.49	2.28	21	13
1:A:112:THR:HG22	1:A:113:THR:N	0.49	2.22	45	21

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:TYR:CE1	1:A:76:LEU:HD12	0.49	2.43	7	13
1:A:54:LYS:HD2	1:A:54:LYS:C	0.49	2.27	48	1
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	2.23	30	49
1:A:45:TYR:OH	1:A:75:SER:CA	0.49	2.60	47	11
1:A:77:ASP:C	1:A:79:GLY:H	0.49	2.11	41	12
1:A:52:MET:O	1:A:52:MET:CG	0.49	2.60	47	3
1:A:77:ASP:CG	1:A:81:LYS:CE	0.49	2.81	19	6
1:A:78:VAL:C	1:A:80:GLY:N	0.49	2.67	33	32
1:A:18:VAL:HG22	1:A:87:ALA:HB1	0.49	1.84	1	4
1:A:12:PHE:HA	1:A:103:PHE:CD2	0.49	2.43	16	10
1:A:64:TYR:O	1:A:98:ILE:HG12	0.49	2.08	47	11
1:A:19:ILE:HG22	1:A:52:MET:HG3	0.49	1.84	36	1
1:A:74:VAL:O	1:A:74:VAL:HG12	0.49	2.08	6	21
1:A:29:VAL:N	1:A:41:LYS:NZ	0.49	2.61	39	1
1:A:19:ILE:HG13	1:A:21:THR:HG22	0.49	1.82	30	9
1:A:12:PHE:CE1	1:A:114:GLN:HB3	0.49	2.43	37	1
1:A:74:VAL:HG12	1:A:74:VAL:O	0.48	2.08	8	12
1:A:24:VAL:CG1	1:A:78:VAL:CG1	0.48	2.90	11	10
1:A:83:GLU:OE1	1:A:83:GLU:O	0.48	2.32	42	2
1:A:10:GLN:NE2	1:A:10:GLN:O	0.48	2.46	19	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:83:GLU:O	1:A:106:PRO:HA	0.48	2.09	23	22
1:A:20:ARG:O	1:A:50:ILE:HD13	0.48	2.09	9	9
1:A:113:THR:O	1:A:116:LYS:CE	0.48	2.61	49	1
1:A:10:GLN:O	1:A:10:GLN:CD	0.48	2.52	27	11
1:A:49:GLN:HG3	1:A:59:ASP:OD2	0.48	2.07	35	16
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:116:LYS:O	1:A:116:LYS:NZ	0.48	2.46	20	9
1:A:3:CYS:H	1:A:100:LEU:HD21	0.48	1.68	14	2
1:A:95:LYS:O	1:A:95:LYS:HD2	0.48	2.08	49	1
1:A:34:ASP:N	1:A:38:ASN:O	0.48	2.46	20	48
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:88:GLY:O	1:A:89:LYS:C	0.48	2.52	20	17
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	2.46	39	26

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:ASP:CG	1:A:81:LYS:NZ	0.48	2.67	23	10
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	41	5
1:A:9:GLN:NE2	1:A:117:SER:OG	0.47	2.47	10	6
1:A:64:TYR:CZ	1:A:97:HIS:CE1	0.47	3.02	35	2
1:A:20:ARG:CZ	1:A:50:ILE:HD11	0.47	2.39	25	4
1:A:53:PHE:CD2	1:A:118:LEU:HD13	0.47	2.43	49	1
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: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:82:LYS:O	1:A:83:GLU:CD	0.47	2.53	17	7
1:A:17:VAL:O	1:A:87:ALA:HA	0.47	2.08	5	17
1:A:95:LYS:HD2	1:A:95:LYS:O	0.47	2.09	37	1
1:A:90:ALA:HA	1:A:96:MET:CB	0.47	2.39	33	6
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:49:GLN:NE2	1:A:59:ASP:CG	0.47	2.68	41	3
1:A:46:GLU:CD	1:A:62:PHE:CZ	0.47	2.88	6	4
1:A:38:ASN:OD1	1:A:38:ASN:N	0.47	2.48	27	25
1:A:83:GLU:N	1:A:83:GLU:CD	0.47	2.68	40	4
1:A:10:GLN:CD	1:A:10:GLN:O	0.47	2.53	37	14
1:A:60:ILE:CG2	1:A:95:LYS:HA	0.47	2.40	42	5
1:A:86:ILE:HG23	1:A:98:ILE:HG21	0.47	1.86	48	24
1:A:108:ASP:C	1:A:109:THR:HG23	0.47	2.30	37	21
1:A:28:GLU:CG	1:A:41:LYS:CE	0.47	2.93	6	12
1:A:85:LEU:H	1:A:85:LEU:HD13	0.47	1.70	45	13
1:A:27:LYS:O	1:A:44:GLN:N	0.47	2.47	24	12
1:A:44:GLN:NE2	1:A:44:GLN:HA	0.47	2.24	38	12
1:A:26:GLU:C	1:A:26:GLU:OE1	0.47	2.53	40	1
1:A:20:ARG:HB2	1:A:53:PHE:CE2	0.47	2.45	1	4
1:A:53:PHE:CD1	1:A:118:LEU:HD23	0.47	2.45	5	3
1:A:9:GLN:HB2	1:A:113:THR:HG22	0.47	1.87	25	1
1:A:9:GLN:NE2	1:A:116:LYS:HE2	0.46	2.26	39	15
1:A:29:VAL:O	1:A:29:VAL:HG23	0.46	2.11	17	5
1:A:72:CYS:CA	1:A:100:LEU:HD22	0.46	2.37	2	2
1:A:91:GLU:OE2	1:A:97:HIS:ND1	0.46	2.48	5	1
1:A:110:LEU:O	1:A:111:SER:OG	0.46	2.33	21	37

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:GLY:C	1:A:90:ALA:N	0.46	2.68	28	6
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:9:GLN:NE2	1:A:117:SER:CB	0.46	2.78	22	4
1:A:19:ILE:CD1	1:A:60:ILE:HG13	0.46	2.41	31	4
1:A:70:ALA:HB2	1:A:74:VAL:C	0.46	2.31	19	1
1:A:41:LYS:HE2	1:A:42:ARG:N	0.46	2.25	39	2
1:A:59:ASP:OD2	1:A:61:GLU:CD	0.46	2.54	8	6
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:82:LYS:C	1:A:83:GLU:CD	0.46	2.74	25	7
1:A:8:PRO:CB	1:A:114:GLN:NE2	0.46	2.79	49	1
1:A:77:ASP:O	1:A:79:GLY:N	0.46	2.45	33	10
1:A:78:VAL:CG2	1:A:82:LYS:O	0.46	2.50	32	3
1:A:38:ASN:N	1:A:38:ASN:OD1	0.46	2.48	20	21
1:A:85:LEU:HD12	1:A:107:TRP:CD1	0.46	2.45	43	3
1:A:28:GLU:CG	1:A:41:LYS:HE3	0.46	2.41	31	6
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:95:LYS:N	1:A:95:LYS:HD3	0.46	2.26	18	2
1:A:7:HIS:HB2	1:A:10:GLN:CG	0.46	2.41	17	6
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:63:ILE:HD12	1:A:96:MET:HE1	0.46	1.87	42	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:60:ILE:CD1	1:A:93:ASP:HA	0.45	2.41	49	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:9:GLN:HE21	1:A:117:SER:CB	0.45	2.25	28	1
1:A:28:GLU:HA	1:A:43:ILE:HD12	0.45	1.86	14	1
1:A:7:HIS:NE2	1:A:101:CYS:O	0.45	2.49	5	3
1:A:42:ARG:O	1:A:43:ILE:C	0.45	2.52	4	32
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:17:VAL:CB	1:A:90:ALA:HB2	0.45	2.41	36	4
1:A:20:ARG:CZ	1:A:51:LYS:HD2	0.45	2.41	2	13
1:A:83:GLU:CD	1:A:83:GLU:N	0.45	2.69	44	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:PHE:CZ	1:A:103:PHE:HZ	0.45	2.20	29	5
1:A:41:LYS:NZ	1:A:41:LYS:HB2	0.45	2.27	35	5
1:A:78:VAL:O	1:A:80:GLY:N	0.45	2.49	46	10
1:A:15:ALA:HB1	1:A:87:ALA:HB1	0.45	1.88	2	11
1:A:49:GLN:CD	1:A:59:ASP:CG	0.45	2.75	39	1
1:A:17:VAL:HG11	1:A:90:ALA:CB	0.45	2.38	31	5
1:A:12:PHE:N	1:A:12:PHE:HD1	0.45	2.08	45	3
1:A:86:ILE:HG22	1:A:96:MET:CE	0.45	2.41	49	2
1:A:67:PRO:O	1:A:71:VAL:HG13	0.45	2.11	33	4
1:A:21:THR:OG1	1:A:47:ILE:CG1	0.45	2.65	10	9
1:A:82:LYS:C	1:A:83:GLU:OE2	0.45	2.55	41	1
1:A:45:TYR:N	1:A:63:ILE:O	0.45	2.50	27	7
1:A:60:ILE:HD12	1:A:96:MET:SD	0.45	2.52	3	2
1:A:44:GLN:HA	1:A:44:GLN:NE2	0.45	2.26	1	17
1:A:112:THR:O	1:A:115:LYS:N	0.45	2.49	37	12
1:A:68:SER:O	1:A:69:SER:C	0.45	2.54	24	3
1:A:23:ALA:N	1:A:78:VAL:HG23	0.45	2.27	6	6
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:15:ALA:CB	1:A:87:ALA:C	0.45	2.86	1	21
1:A:41:LYS:HB2	1:A:41:LYS:NZ	0.45	2.27	15	3
1:A:17:VAL:CG1	1:A:17:VAL:O	0.45	2.62	28	6
1:A:54:LYS:O	1:A:54:LYS:HG3	0.45	2.11	37	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:20:ARG:CG	1:A:53:PHE:CD2	0.45	3.00	42	1
1:A:15:ALA:HB1	1:A:87:ALA:C	0.45	2.32	15	30
1:A:91:GLU:OE1	1:A:97:HIS:ND1	0.45	2.50	23	2
1:A:46:GLU:HG3	1:A:62:PHE:CE2	0.45	2.46	5	2
1:A:29:VAL:CG2	1:A:42:ARG:HD3	0.45	2.42	32	1
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:19:ILE:CD1	1:A:96:MET:HE3	0.44	2.43	15	6
1:A:22:LYS:HG3	1:A:22:LYS:O	0.44	2.11	45	10
1:A:7:HIS:CG	1:A:10:GLN:HG3	0.44	2.47	30	2
1:A:86:ILE:CG2	1:A:96:MET:HE3	0.44	2.41	30	2
1:A:92:GLY:N	1:A:95:LYS:O	0.44	2.51	18	1
1:A:44:GLN:OE1	1:A:64:TYR:CD2	0.44	2.71	22	2
1:A:82:LYS:O	1:A:83:GLU:OE1	0.44	2.36	38	3
1:A:5:PRO:CB	1:A:100:LEU:O	0.44	2.65	46	2
1:A:18:VAL:HG22	1:A:87:ALA:CB	0.44	2.42	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:GLU:C	1:A:83:GLU:OE1	0.44	2.56	21	1
1:A:46:GLU:CG	1:A:62:PHE:CZ	0.44	3.00	23	4
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:102:ASP:O	1:A:103:PHE:O	0.44	2.34	13	1
1:A:12:PHE:HB2	1:A:117:SER:OG	0.44	2.13	13	3
1:A:50:ILE:CD1	1:A:83:GLU:HG2	0.44	2.43	46	4
1:A:12:PHE:HD1	1:A:12:PHE:N	0.44	2.09	25	1
1:A:32:GLY:O	1:A:40:ILE:N	0.44	2.36	46	2
1:A:106:PRO:HG2	1:A:109:THR:HG21	0.44	1.87	49	29
1:A:69:SER:O	1:A:75:SER:OG	0.44	2.35	24	3
1:A:19:ILE:N	1:A:85:LEU:O	0.44	2.47	17	7
1:A:99:THR:OG1	1:A:102:ASP:HB2	0.44	2.11	40	1
1:A:63:ILE:CG2	1:A:98:ILE:CD1	0.44	2.96	35	2
1:A:56:PRO:CG	1:A:93:ASP:OD1	0.44	2.65	49	1
1:A:50:ILE:HD13	1:A:83:GLU:HG2	0.44	1.90	39	5
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	47	23
1:A:99:THR:O	1:A:102:ASP:N	0.44	2.50	13	1
1:A:100:LEU:HG	1:A:101:CYS:N	0.44	2.28	3	7
1:A:41:LYS:O	1:A:67:PRO:HD3	0.44	2.12	43	2
1:A:84:TYR:C	1:A:84:TYR:CD1	0.44	2.91	37	22
1:A:81:LYS:N	1:A:81:LYS:HD3	0.44	2.28	48	13
1:A:83:GLU:O	1:A:106:PRO:C	0.44	2.56	6	18
1:A:23:ALA:C	1:A:78:VAL:CG2	0.44	2.86	26	5
1:A:52:MET:SD	1:A:56:PRO:O	0.44	2.76	36	2
1:A:49:GLN:CG	1:A:59:ASP:OD1	0.44	2.66	8	2
1:A:10:GLN:O	1:A:10:GLN:OE1	0.44	2.36	29	1
1:A:9:GLN:CD	1:A:116:LYS:NZ	0.44	2.72	49	1
1:A:23:ALA:HB2	1:A:47:ILE:CG2	0.43	2.42	45	4
1:A:11:ALA:O	1:A:103:PHE:HB2	0.43	2.13	21	8
1:A:41:LYS:CA	1:A:41:LYS:CE	0.43	2.96	39	2
1:A:76:LEU:HA	1:A:81:LYS:HZ2	0.43	1.72	22	2
1:A:20:ARG:CD	1:A:107:TRP:CD2	0.43	3.01	23	6
1:A:84:TYR:CD1	1:A:84:TYR:C	0.43	2.91	30	21
1:A:52:MET:O	1:A:53:PHE:C	0.43	2.56	48	17
1:A:35:ILE:HG22	1:A:35:ILE:O	0.43	2.13	39	31
1:A:45:TYR:CE2	1:A:65:THR:CB	0.43	3.02	22	7
1:A:6:VAL:C	1:A:7:HIS:CG	0.43	2.91	27	4
1:A:23:ALA:C	1:A:78:VAL:HG23	0.43	2.32	26	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:GLU:O	1:A:91:GLU:CD	0.43	2.56	44	1
1:A:52:MET:HE2	1:A:52:MET:O	0.43	2.12	30	1
1:A:5:PRO:HB3	1:A:100:LEU:O	0.43	2.14	14	1
1:A:9:GLN:CD	1:A:116:LYS:CE	0.43	2.86	9	1
1:A:60:ILE:HG21	1:A:96:MET:SD	0.43	2.53	49	1
1:A:19:ILE:CG2	1:A:52:MET:CG	0.43	2.96	22	1
1:A:63:ILE:HD12	1:A:86:ILE:HG21	0.43	1.90	28	6
1:A:48:LYS:O	1:A:49:GLN:C	0.43	2.56	36	5
1:A:63:ILE:HD13	1:A:96:MET:CE	0.43	2.43	28	1
1:A:28:GLU:HG2	1:A:41:LYS:CE	0.43	2.43	5	2
1:A:81:LYS:HD3	1:A:81:LYS:N	0.43	2.28	19	6
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:86:ILE:CG2	1:A:96:MET:SD	0.43	3.06	46	1
1:A:68:SER:C	1:A:70:ALA:N	0.43	2.70	43	2
1:A:27:LYS:HB3	1:A:44:GLN:CB	0.43	2.44	30	10
1:A:17:VAL:HA	1:A:55:GLY:CA	0.43	2.44	39	2
1:A:113:THR:HA	1:A:116:LYS:CG	0.43	2.43	49	2
1:A:30:ASP:OD2	1:A:41:LYS:NZ	0.43	2.50	30	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:44:GLN:NE2	1:A:44:GLN:CA	0.43	2.81	38	3
1:A:35:ILE:O	1:A:35:ILE:HG22	0.43	2.14	11	15
1:A:28:GLU:HG2	1:A:41:LYS:HZ2	0.43	1.74	26	1
1:A:20:ARG:HG3	1:A:53:PHE:CD2	0.43	2.49	42	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:12:PHE:HB2	1:A:117:SER:CB	0.42	2.42	28	1
1:A:89:LYS:O	1:A:89:LYS:CG	0.42	2.66	36	1
1:A:116:LYS:O	1:A:119:ASN:ND2	0.42	2.52	5	1
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	7
1:A:84:TYR:CB	1:A:86:ILE:HD13	0.42	2.43	25	13
1:A:42:ARG:HB3	1:A:64:TYR:CE2	0.42	2.50	36	2
1:A:9:GLN:C	1:A:11:ALA:N	0.42	2.71	9	2
1:A:94:GLY:C	1:A:95:LYS:HG3	0.42	2.35	49	1
1:A:6:VAL:CG1	1:A:7:HIS:H	0.42	2.23	38	17
1:A:114:GLN:N	1:A:114:GLN:NE2	0.42	2.65	38	4
1:A:78:VAL:C	1:A:80:GLY:H	0.42	2.17	33	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:LYS:O	1:A:22:LYS:HG3	0.42	2.13	4	8
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	4
1:A:45:TYR:CZ	1:A:76:LEU:CD1	0.42	2.97	47	1
1:A:25:SER:C	1:A:26:GLU:OE1	0.42	2.58	16	1
1:A:114:GLN:O	1:A:118:LEU:HB3	0.42	2.14	45	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:44:GLN:CA	1:A:44:GLN:NE2	0.42	2.82	12	3
1:A:50:ILE:CD1	1:A:83:GLU:CD	0.42	2.88	15	1
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:24:VAL:HG13	1:A:78:VAL:HG21	0.42	1.91	1	4
1:A:63:ILE:CD1	1:A:96:MET:HE3	0.42	2.45	38	5
1:A:83:GLU:O	1:A:83:GLU:OE1	0.42	2.38	23	2
1:A:76:LEU:H	1:A:76:LEU:HD12	0.42	1.74	47	1
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:28:GLU:CG	1:A:41:LYS:HD2	0.42	2.45	34	5
1:A:95:LYS:HD3	1:A:95:LYS:N	0.42	2.30	45	1
1:A:19:ILE:CD1	1:A:60:ILE:CG1	0.42	2.98	31	1
1:A:67:PRO:C	1:A:68:SER:O	0.42	2.58	27	2
1:A:28:GLU:CD	1:A:41:LYS:HZ3	0.42	2.18	43	1
1:A:119:ASN:C	1:A:119:ASN:ND2	0.42	2.73	13	1
1:A:91:GLU:CD	1:A:91:GLU:O	0.42	2.58	25	1
1:A:86:ILE:CG2	1:A:96:MET:HE2	0.42	2.43	49	1
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:71:VAL:HG22	1:A:72:CYS:SG	0.42	2.55	8	1
1:A:3:CYS:HB2	1:A:101:CYS:SG	0.42	2.54	29	1
1:A:6:VAL:C	1:A:7:HIS:CD2	0.41	2.93	16	5
1:A:99:THR:C	1:A:101:CYS:N	0.41	2.74	13	1
1:A:40:ILE:HG22	1:A:41:LYS:N	0.41	2.30	18	3
1:A:36:TYR:HB3	1:A:38:ASN:OD1	0.41	2.14	34	1
1:A:33:ASN:CA	1:A:38:ASN:O	0.41	2.68	22	2
1:A:9:GLN:OE1	1:A:116:LYS:HE2	0.41	2.16	48	1
1:A:64:TYR:CZ	1:A:97:HIS:NE2	0.41	2.88	35	1
1:A:93:ASP:O	1:A:95:LYS:CD	0.41	2.68	49	1
1:A:28:GLU:CG	1:A:43:ILE:HD11	0.41	2.44	48	2
1:A:35:ILE:CD1	1:A:35:ILE:H	0.41	2.28	18	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:ASP:C	1:A:95:LYS:N	0.41	2.73	49	2
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: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:90:ALA:HA	1:A:96:MET:HB2	0.41	1.91	13	3
1:A:77:ASP:OD1	1:A:79:GLY:CA	0.41	2.68	46	2
1:A:20:ARG:NE	1:A:51:LYS:HD2	0.41	2.30	48	1
1:A:81:LYS:O	1:A:82:LYS:HE2	0.41	2.16	6	3
1:A:45:TYR:OH	1:A:65:THR:HG21	0.41	2.11	32	3
1:A:35:ILE:H	1:A:35:ILE:CD1	0.41	2.27	33	3
1:A:76:LEU:CD2	1:A:84:TYR:CD2	0.41	2.97	20	3
1:A:83:GLU:CA	1:A:83:GLU:OE1	0.41	2.69	8	1
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:30:ASP:CG	1:A:41:LYS:NZ	0.41	2.74	16	2
1:A:91:GLU:N	1:A:96:MET:HA	0.41	2.30	42	3
1:A:59:ASP:OD2	1:A:61:GLU:OE2	0.41	2.39	17	1
1:A:108:ASP:O	1:A:108:ASP:CG	0.41	2.59	22	1
1:A:9:GLN:NE2	1:A:117:SER:HB2	0.41	2.30	22	2
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:54:LYS:HG3	1:A:55:GLY:N	0.41	2.31	12	1
1:A:83:GLU:OE1	1:A:83:GLU:CA	0.41	2.68	23	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:69:SER:O	1:A:75:SER:HB3	0.41	2.16	9	1
1:A:25:SER:OG	1:A:46:GLU:HB3	0.41	2.15	49	1
1:A:41:LYS:HA	1:A:41:LYS:CE	0.41	2.46	39	1
1:A:27:LYS:O	1:A:43:ILE:HA	0.41	2.15	27	2
1:A:60:ILE:O	1:A:61:GLU:HB2	0.41	2.15	37	1
1:A:80:GLY:HA3	1:A:81:LYS:HE2	0.41	1.91	16	1
1:A:91:GLU:HB2	1:A:96:MET:HA	0.41	1.93	49	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:20:ARG:HD3	1:A:107:TRP:CE2	0.40	2.51	25	1
1:A:108:ASP:OD1	1:A:108:ASP:O	0.40	2.39	43	1
1:A:54:LYS:CE	1:A:54:LYS:HA	0.40	2.46	9	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:OE2	1:A:41:LYS:NZ	0.40	2.49	8	1
1:A:28:GLU:OE1	1:A:30:ASP:OD1	0.40	2.39	8	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:80:GLY:CA	1:A:81:LYS:HE2	0.40	2.46	23	1
1:A:5:PRO:CG	1:A:100:LEU:O	0.40	2.69	46	1
1:A:67:PRO:O	1:A:68:SER:C	0.40	2.59	43	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:12:PHE:CB	1:A:117:SER:OG	0.40	2.69	6	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	59	ASP	49
1	A	110	LEU	49
1	A	112	THR	49
1	A	82	LYS	49
1	A	41	LYS	49
1	A	75	SER	49
1	A	6	VAL	49
1	A	40	ILE	49
1	A	49	GLN	49

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Mol	Chain	Res	Type	Models (Total)
1	A	111	SER	49
1	A	46	GLU	49
1	A	17	VAL	49
1	A	86	ILE	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	93	ASP	9
1	A	68	SER	9
1	A	89	LYS	9
1	A	92	GLY	7
1	A	58	LYS	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%)	60±3 (59±3%)	41±3 (41±3%)	<div>04</div>
All	All	4949/5390 (92%)	2927 (59%)	2022 (41%)	<div>04</div>

All 67 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	112	THR	49
1	A	82	LYS	49

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Mol	Chain	Res	Type	Models (Total)
1	A	81	LYS	49
1	A	96	MET	49
1	A	114	GLN	49
1	A	63	ILE	49
1	A	95	LYS	49
1	A	103	PHE	49
1	A	105	VAL	49
1	A	76	LEU	49
1	A	50	ILE	49
1	A	14	ASN	49
1	A	45	TYR	49
1	A	117	SER	49
1	A	85	LEU	49
1	A	86	ILE	49
1	A	58	LYS	48
1	A	18	VAL	47
1	A	71	VAL	46
1	A	68	SER	46
1	A	116	LYS	44
1	A	97	HIS	44
1	A	61	GLU	43
1	A	77	ASP	42
1	A	115	LYS	42
1	A	100	LEU	41
1	A	51	LYS	41
1	A	19	ILE	40
1	A	42	ARG	40
1	A	54	LYS	36
1	A	9	GLN	35
1	A	99	THR	33
1	A	101	CYS	33
1	A	89	LYS	29
1	A	52	MET	28
1	A	49	GLN	28
1	A	10	GLN	26
1	A	83	GLU	26
1	A	75	SER	25
1	A	43	ILE	25
1	A	3	CYS	24
1	A	93	ASP	24
1	A	60	ILE	24
1	A	53	PHE	23

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Mol	Chain	Res	Type	Models (Total)
1	A	16	ASP	23
1	A	62	PHE	21
1	A	26	GLU	21
1	A	30	ASP	19
1	A	48	LYS	18
1	A	118	LEU	18
1	A	64	TYR	15
1	A	41	LYS	10
1	A	12	PHE	9
1	A	119	ASN	9
1	A	28	GLU	8
1	A	33	ASN	6
1	A	78	VAL	5
1	A	91	GLU	5
1	A	69	SER	4
1	A	20	ARG	4
1	A	72	CYS	3
1	A	109	THR	2
1	A	24	VAL	2
1	A	13	CYS	2
1	A	47	ILE	1
1	A	38	ASN	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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4214

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1328
Number of shifts mapped to atoms	1328
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	13

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	126	0.04 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	112	-0.17 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	116	0.87 ± 0.33	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 1105 atoms were assigned a chemical shift out of a possible 1406. 14 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	450/573 (79%)	225/228 (99%)	117/234 (50%)	108/111 (97%)
Sidechain	634/739 (86%)	397/434 (91%)	227/277 (82%)	10/28 (36%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	21/94 (22%)	20/50 (40%)	0/41 (0%)	1/3 (33%)
Overall	1105/1406 (79%)	642/712 (90%)	344/552 (62%)	119/142 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1184 atoms were assigned a chemical shift out of a possible 1529. 14 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	484/623 (78%)	242/248 (98%)	126/254 (50%)	116/121 (96%)
Sidechain	679/797 (85%)	427/470 (91%)	241/295 (82%)	11/32 (34%)
Aromatic	21/109 (19%)	20/58 (34%)	0/47 (0%)	1/4 (25%)
Overall	1184/1529 (77%)	689/776 (89%)	367/596 (62%)	128/157 (82%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	49	GLN	CG	13.43	39.38 – 28.18	-18.2
1	A	69	SER	CB	40.39	71.24 – 56.34	-15.7
1	A	85	LEU	CG	44.19	32.55 – 21.05	15.1
1	A	20	ARG	NE	108.32	92.63 – 76.73	14.9
1	A	26	GLU	CA	82.05	67.86 – 46.86	11.8
1	A	83	GLU	CA	82.05	67.86 – 46.86	11.8
1	A	41	LYS	CA	82.05	67.97 – 45.97	11.4
1	A	22	LYS	CA	81.83	67.97 – 45.97	11.3
1	A	60	ILE	CD1	30.21	21.91 – 5.01	9.9
1	A	20	ARG	CB	44.80	39.81 – 21.51	7.7
1	A	58	LYS	HD3	2.92	2.75 – 0.45	5.7
1	A	115	LYS	HE3	1.88	3.86 – 1.96	-5.4
1	A	39	PRO	HG3	3.67	3.56 – 0.26	5.3

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

