



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 01:51 PM UTC

PDB ID : 9GRK / pdb_00009grk
BMRB ID : 34956
Title : Cdc42 Binding peptide (W14A)
Authors : Mott, H.R.; Murphy, N.P.; Owen, D.
Deposited on : 2024-09-11

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

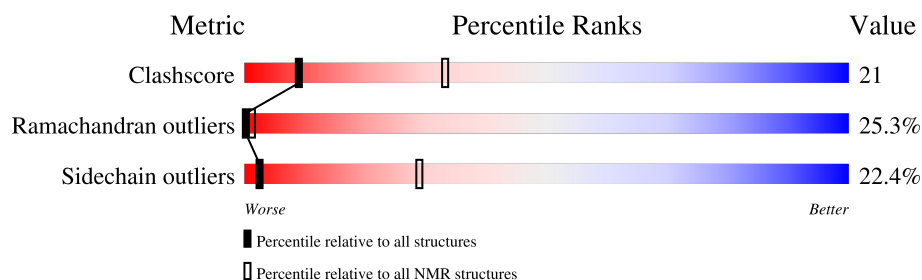
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 46%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	16	<div> <div></div> <div>38%</div> <div>31%</div> <div>12%</div> <div>19%</div> </div>

2 Ensemble composition and analysis

This entry contains 35 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:15 (13)	0.36	8

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 5 clusters and 8 single-model clusters were found.

Cluster number	Models
1	3, 4, 8, 9, 10, 13, 14, 25, 28, 29, 30, 31, 35
2	11, 17, 20, 27, 34
3	19, 22, 23, 26
4	7, 15, 21
5	1, 33
Single-model clusters	2; 5; 6; 12; 16; 18; 24; 32

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 262 atoms, of which 126 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG.

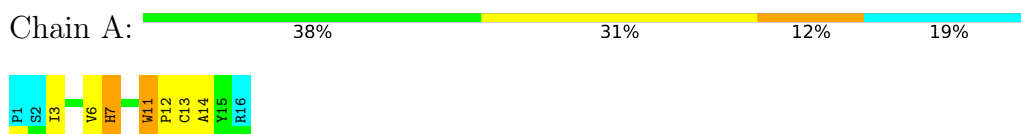
Mol	Chain	Residues	Atoms						Trace
1	A	16	Total	C	H	N	O	S	0
			262	86	126	27	21	2	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG

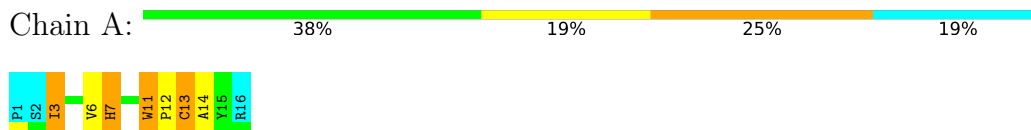


4.2 Scores per residue for each member of the ensemble

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

4.2.1 Score per residue for model 1

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



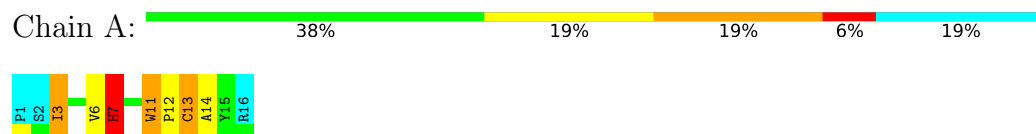
4.2.2 Score per residue for model 2

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



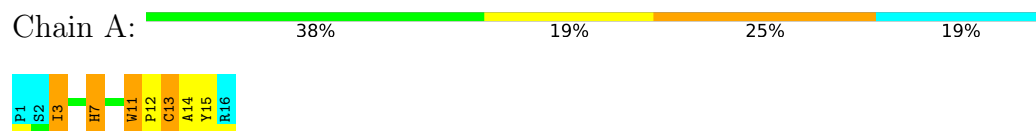
4.2.3 Score per residue for model 3

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



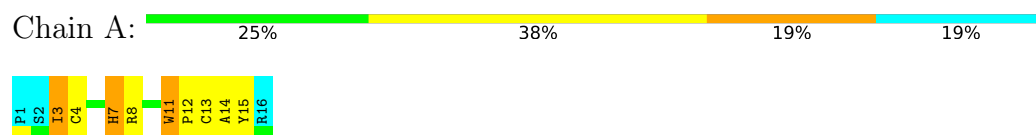
4.2.4 Score per residue for model 4

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



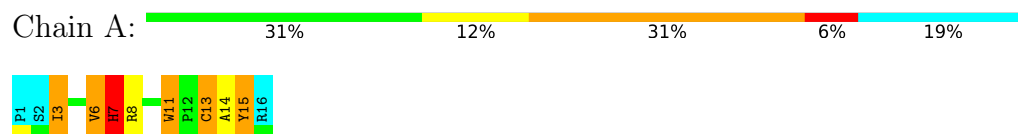
4.2.5 Score per residue for model 5

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



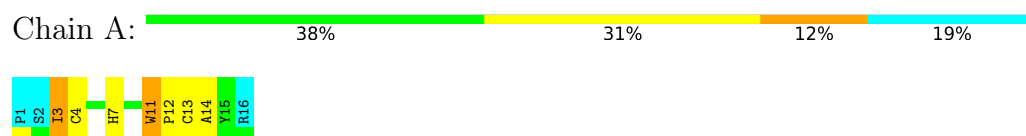
4.2.6 Score per residue for model 6

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



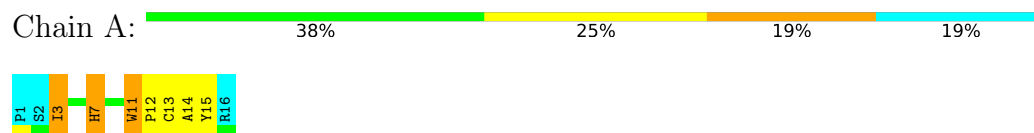
4.2.7 Score per residue for model 7

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



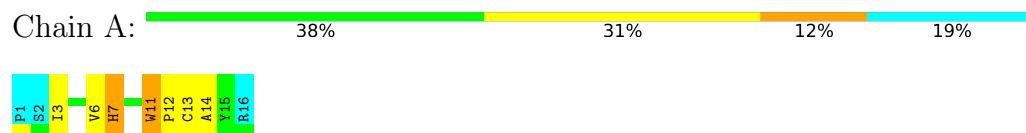
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



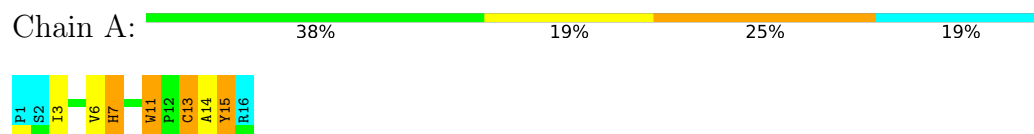
4.2.9 Score per residue for model 9

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



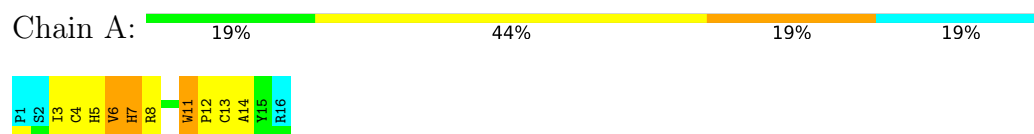
4.2.10 Score per residue for model 10

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



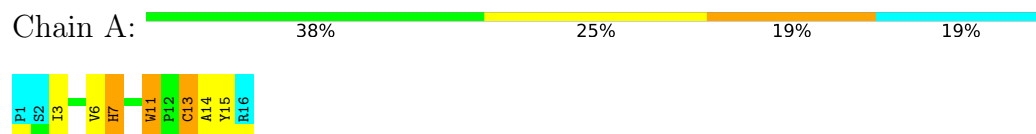
4.2.11 Score per residue for model 11

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



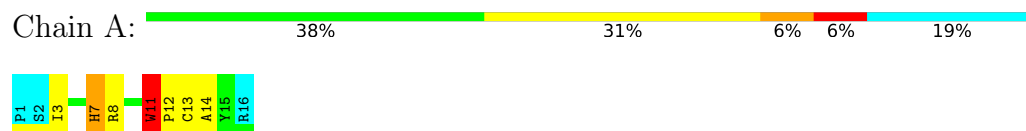
4.2.12 Score per residue for model 12

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



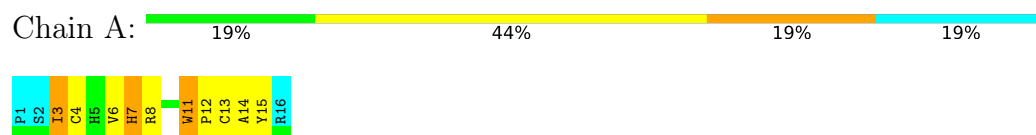
4.2.13 Score per residue for model 13

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



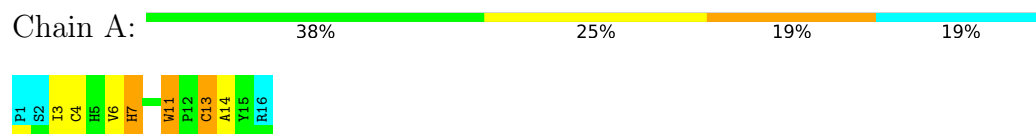
4.2.14 Score per residue for model 14

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



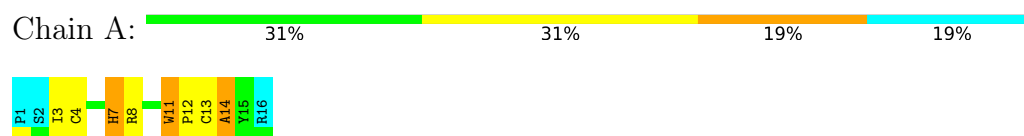
4.2.15 Score per residue for model 15

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



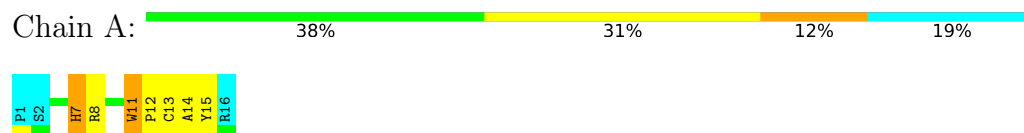
4.2.16 Score per residue for model 16

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



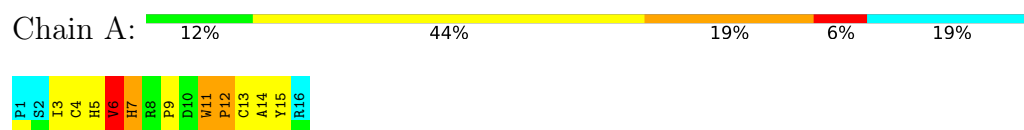
4.2.17 Score per residue for model 17

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



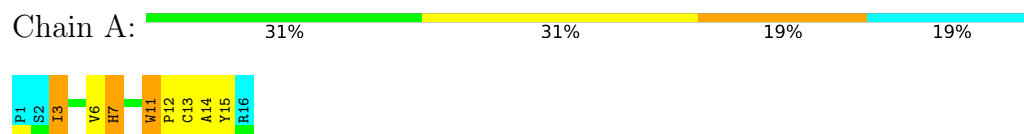
4.2.18 Score per residue for model 18

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



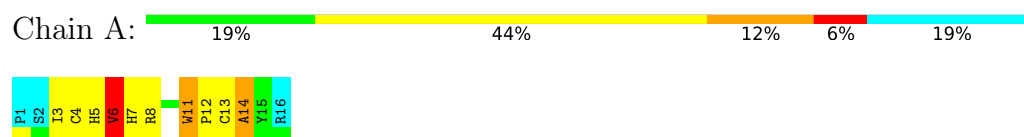
4.2.19 Score per residue for model 19

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



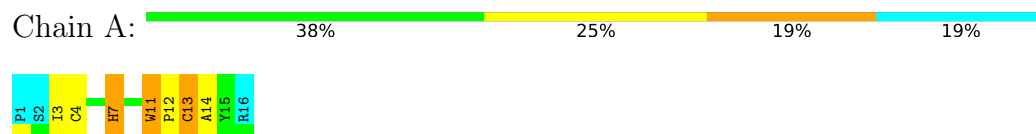
4.2.20 Score per residue for model 20

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



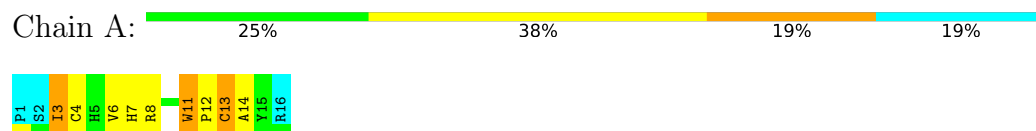
4.2.21 Score per residue for model 21

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



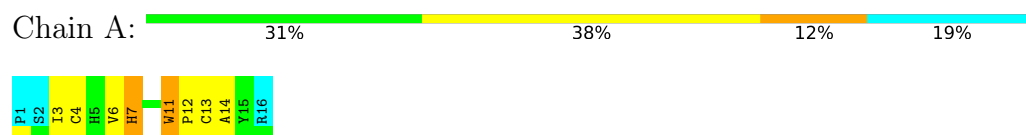
4.2.22 Score per residue for model 22

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



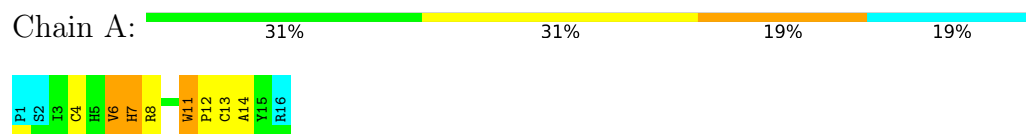
4.2.23 Score per residue for model 23

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



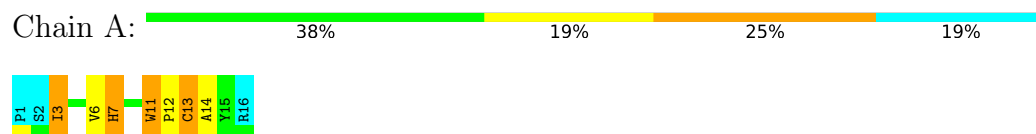
4.2.24 Score per residue for model 24

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



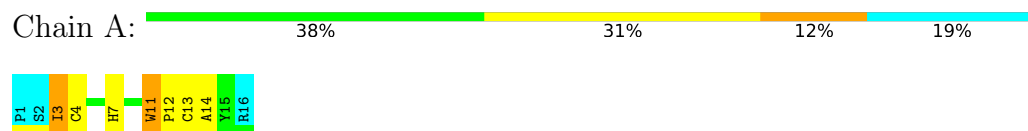
4.2.25 Score per residue for model 25

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



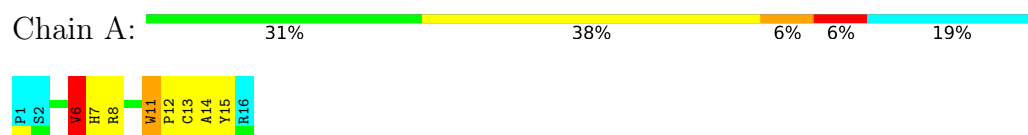
4.2.26 Score per residue for model 26

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



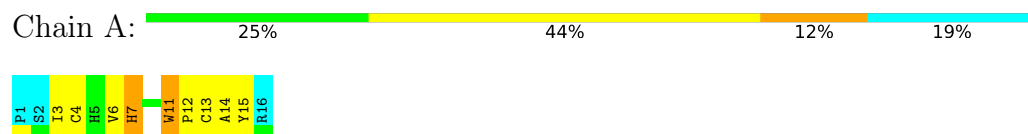
4.2.27 Score per residue for model 27

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



4.2.28 Score per residue for model 28

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



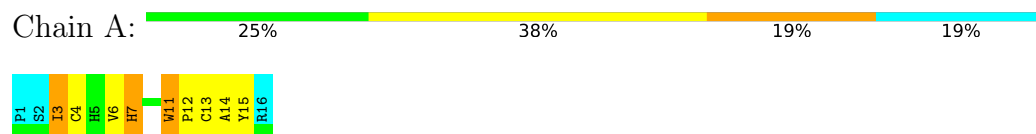
4.2.29 Score per residue for model 29

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



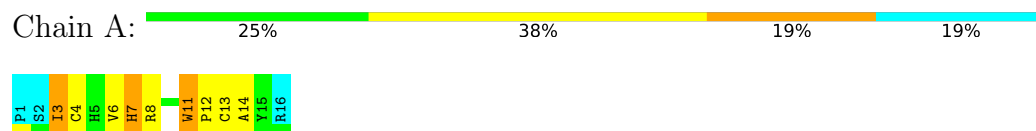
4.2.30 Score per residue for model 30

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



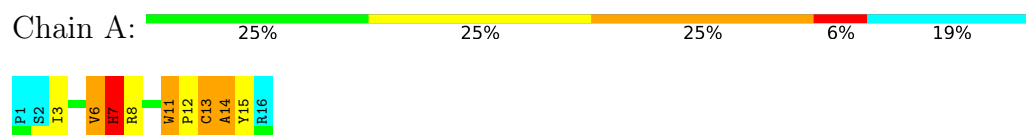
4.2.31 Score per residue for model 31

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



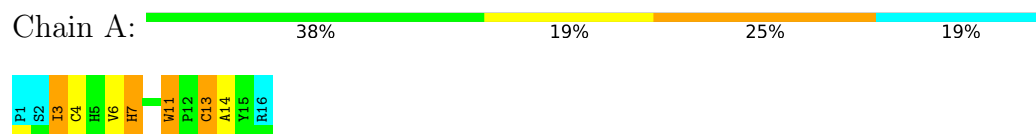
4.2.32 Score per residue for model 32

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



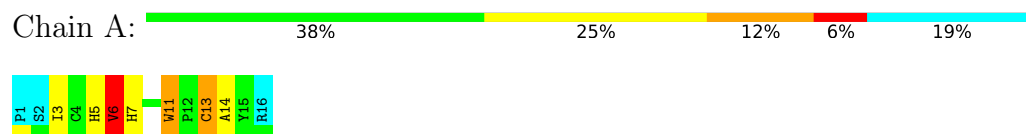
4.2.33 Score per residue for model 33

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



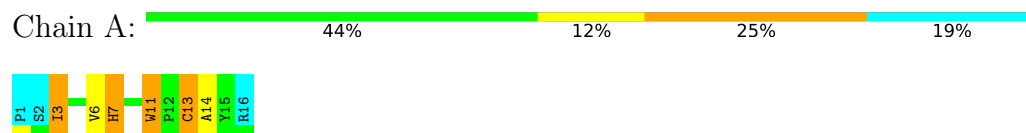
4.2.34 Score per residue for model 34

- Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



4.2.35 Score per residue for model 35

• Molecule 1: PRO-SER-ILE-CYS-HIS-VAL-HIS-ARG-PRO-ASP-TRP-PRO-CYS-ALA-TYR-ARG



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 35 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure calculation	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	97
Number of shifts mapped to atoms	97
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	46%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.44±0.03	0±0/118 (0.0± 0.0%)	0.88±0.06	0±0/164 (0.0± 0.1%)
All	All	0.44	0/4130 (0.0%)	0.88	1/5740 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	11	TRP	CB-CA-C	5.10	115.75	108.76	13	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	111	99	97	4±1
All	All	3885	3465	3395	151

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:ILE:HG23	1:A:13:CYS:SG	0.73	2.22	5	25

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:ARG:HB2	1:A:11:TRP:CD1	0.58	2.33	11	9
1:A:13:CYS:HB3	1:A:15:TYR:CE2	0.56	2.35	14	6
1:A:3:ILE:HG23	1:A:4:CYS:SG	0.54	2.42	15	5
1:A:8:ARG:HD3	1:A:11:TRP:CD2	0.52	2.40	11	8
1:A:4:CYS:C	1:A:13:CYS:SG	0.51	2.94	7	3
1:A:11:TRP:CD1	1:A:11:TRP:C	0.50	2.89	19	35
1:A:5:HIS:O	1:A:6:VAL:HB	0.48	2.08	2	3
1:A:8:ARG:HD2	1:A:11:TRP:CD2	0.47	2.44	22	2
1:A:4:CYS:N	1:A:13:CYS:SG	0.47	2.88	5	9
1:A:11:TRP:CZ2	1:A:14:ALA:HA	0.46	2.46	29	1
1:A:13:CYS:HB3	1:A:15:TYR:CZ	0.45	2.47	12	4
1:A:6:VAL:O	1:A:7:HIS:CD2	0.45	2.69	6	2
1:A:7:HIS:CD2	1:A:7:HIS:N	0.45	2.85	18	25
1:A:13:CYS:HB3	1:A:15:TYR:CE1	0.45	2.47	10	3
1:A:5:HIS:O	1:A:6:VAL:HG12	0.43	2.13	20	2
1:A:6:VAL:HG23	1:A:12:PRO:O	0.43	2.14	27	1
1:A:7:HIS:CD2	1:A:11:TRP:HE1	0.42	2.33	12	2
1:A:8:ARG:HB2	1:A:11:TRP:CG	0.42	2.50	17	1
1:A:3:ILE:HG21	1:A:14:ALA:HB3	0.42	1.90	16	2
1:A:13:CYS:O	1:A:14:ALA:HB2	0.41	2.15	32	1
1:A:8:ARG:HD3	1:A:11:TRP:CG	0.41	2.51	16	1
1:A:6:VAL:HG22	1:A:12:PRO:O	0.40	2.15	18	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	13/16 (81%)	7±1 (51±10%)	3±1 (24±11%)	3±1 (25±8%)	0 1
All	All	455/560 (81%)	232 (51%)	108 (24%)	115 (25%)	0 1

All 8 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	14	ALA	34
1	A	12	PRO	26
1	A	13	CYS	19
1	A	6	VAL	17
1	A	3	ILE	12
1	A	7	HIS	4
1	A	4	CYS	2
1	A	9	PRO	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	12/15 (80%)	9±1 (78±6%)	3±1 (22±6%)	2	29
All	All	420/525 (80%)	326 (78%)	94 (22%)	2	29

All 6 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	35
1	A	11	TRP	35
1	A	6	VAL	13
1	A	3	ILE	5
1	A	15	TYR	4
1	A	13	CYS	2

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 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

The completeness of assignment taking into account all chemical shift lists is 46% for the well-defined parts and 43% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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	97
Number of shifts mapped to atoms	97
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

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

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 46%, i.e. 84 atoms were assigned a chemical shift out of a possible 183. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	24/61 (39%)	24/24 (100%)	0/26 (0%)	0/11 (0%)
Sidechain	47/85 (55%)	47/56 (84%)	0/26 (0%)	0/3 (0%)
Aromatic	13/37 (35%)	13/18 (72%)	0/14 (0%)	0/5 (0%)
Overall	84/183 (46%)	84/98 (86%)	0/66 (0%)	0/19 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 43%, i.e. 97 atoms were assigned a chemical shift out of a possible 226. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	28/74 (38%)	28/29 (97%)	0/32 (0%)	0/13 (0%)
Sidechain	56/115 (49%)	56/75 (75%)	0/34 (0%)	0/6 (0%)
Aromatic	13/37 (35%)	13/18 (72%)	0/14 (0%)	0/5 (0%)
Overall	97/226 (43%)	97/122 (80%)	0/80 (0%)	0/24 (0%)

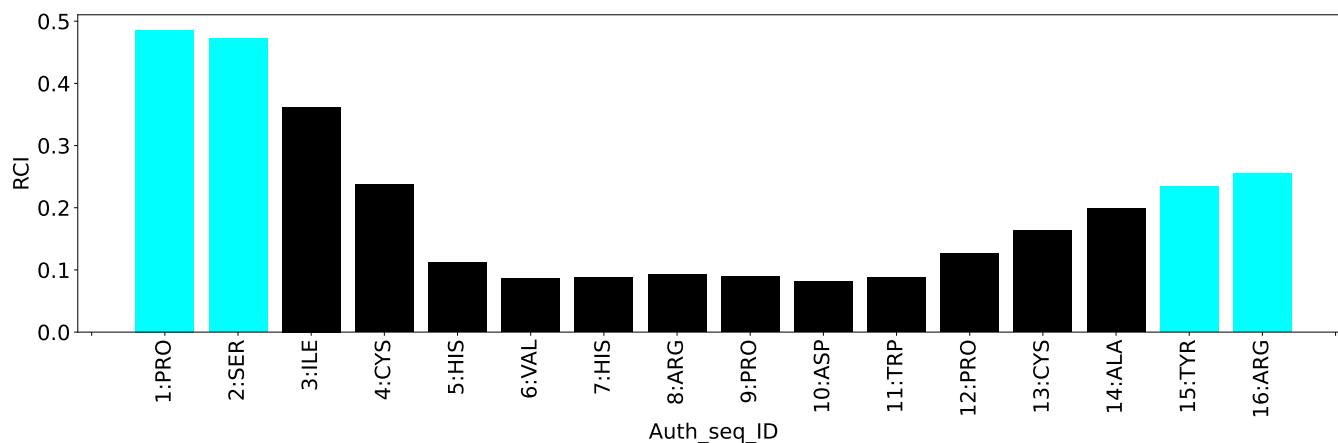
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	353
Intra-residue ($ i-j =0$)	139
Sequential ($ i-j =1$)	115
Medium range ($ i-j >1$ and $ i-j <5$)	68
Long range ($ i-j \geq 5$)	31
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	22.1
Number of long range restraints per residue ¹	1.9

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	4.8	0.2
0.2-0.5 (Medium)	5.3	0.5
>0.5 (Large)	9.8	2.06

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

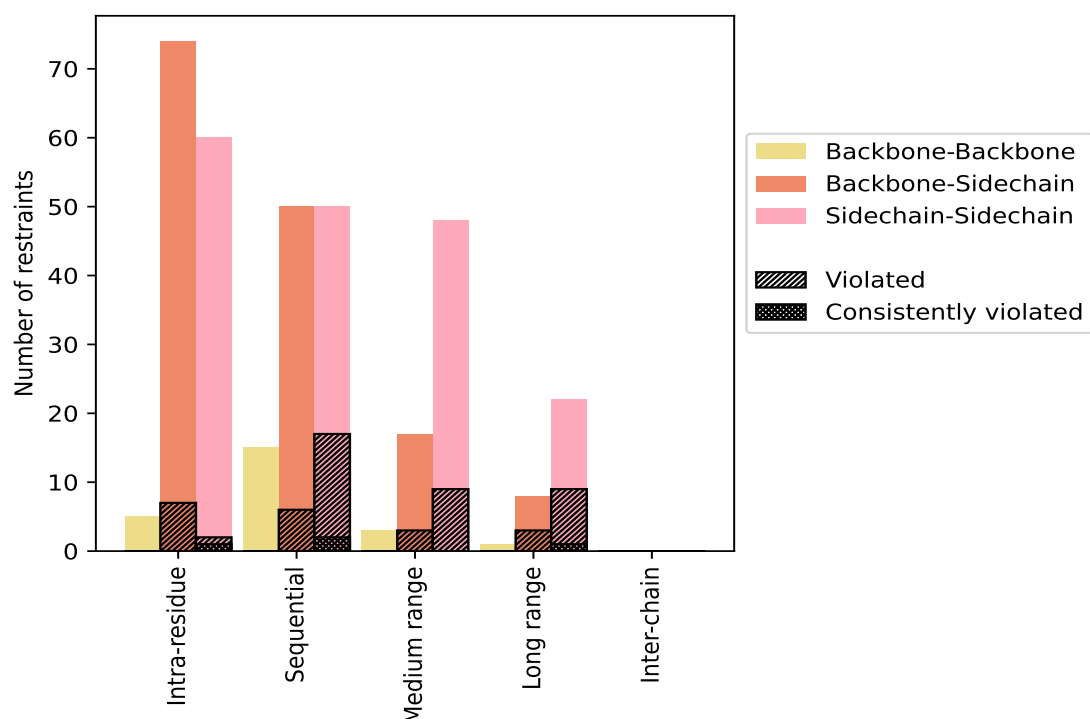
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	139	39.4	9	6.5	2.5	1	0.7	0.3
Backbone-Backbone	5	1.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	74	21.0	7	9.5	2.0	0	0.0	0.0
Sidechain-Sidechain	60	17.0	2	3.3	0.6	1	1.7	0.3
Sequential ($i-j =1$)	115	32.6	23	20.0	6.5	2	1.7	0.6
Backbone-Backbone	15	4.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	50	14.2	6	12.0	1.7	0	0.0	0.0
Sidechain-Sidechain	50	14.2	17	34.0	4.8	2	4.0	0.6
Medium range ($i-j >1$ & $i-j <5$)	68	19.3	12	17.6	3.4	0	0.0	0.0
Backbone-Backbone	3	0.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	17	4.8	3	17.6	0.8	0	0.0	0.0
Sidechain-Sidechain	48	13.6	9	18.8	2.5	0	0.0	0.0
Long range ($i-j \geq 5$)	31	8.8	12	38.7	3.4	1	3.2	0.3
Backbone-Backbone	1	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	8	2.3	3	37.5	0.8	0	0.0	0.0
Sidechain-Sidechain	22	6.2	9	40.9	2.5	1	4.5	0.3
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	353	100.0	56	15.9	15.9	4	1.1	1.1
Backbone-Backbone	24	6.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	149	42.2	19	12.8	5.4	0	0.0	0.0
Sidechain-Sidechain	180	51.0	37	20.6	10.5	4	2.2	1.1

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	2	7	4	6	0	19	0.63	1.86	0.45	0.52
2	3	11	5	5	0	24	0.53	1.38	0.41	0.43
3	1	7	1	7	0	16	0.76	1.86	0.49	0.64
4	3	6	3	7	0	19	0.69	1.52	0.45	0.69
5	3	11	6	6	0	26	0.5	1.47	0.43	0.32
6	3	6	4	6	0	19	0.67	1.44	0.43	0.69
7	2	8	4	7	0	21	0.57	1.36	0.38	0.58
8	2	8	6	7	0	23	0.62	1.73	0.42	0.49
9	3	7	4	4	0	18	0.53	1.34	0.43	0.36
10	4	7	4	5	0	20	0.57	1.63	0.47	0.44

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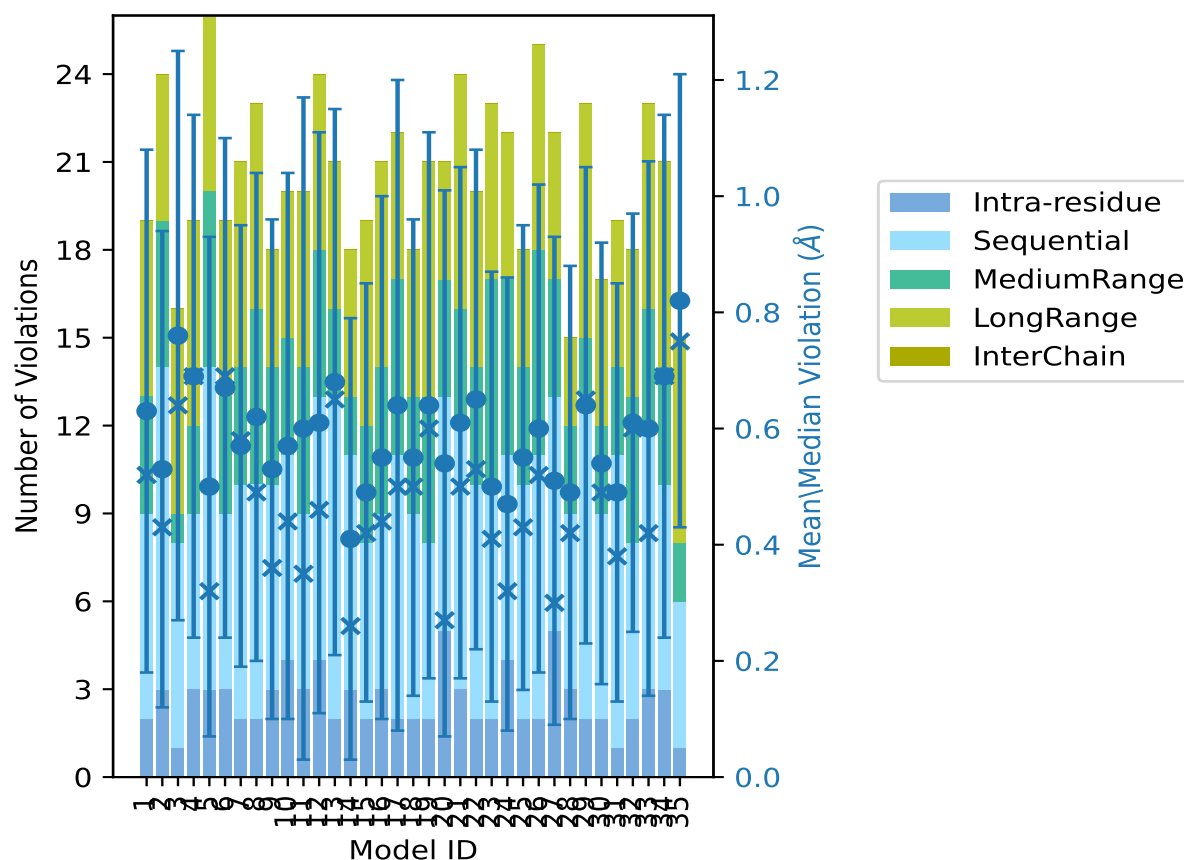
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	3	6	5	6	0	20	0.6	2.01	0.57	0.35
12	4	9	5	6	0	24	0.61	1.9	0.5	0.46
13	2	11	3	5	0	21	0.68	1.63	0.47	0.65
14	3	8	2	5	0	18	0.41	1.37	0.38	0.26
15	2	6	4	7	0	19	0.49	1.27	0.36	0.42
16	3	6	5	7	0	21	0.55	1.9	0.45	0.44
17	2	9	6	5	0	22	0.64	2.06	0.56	0.5
18	2	7	4	5	0	18	0.55	1.49	0.41	0.5
19	2	6	5	8	0	21	0.64	1.94	0.47	0.6
20	5	8	4	4	0	21	0.54	1.55	0.47	0.27
21	3	9	4	8	0	24	0.61	1.54	0.44	0.5
22	2	8	4	6	0	20	0.65	1.51	0.43	0.53
23	2	8	7	6	0	23	0.5	1.26	0.37	0.41
24	4	7	6	5	0	22	0.47	1.34	0.39	0.32
25	2	8	4	4	0	18	0.55	1.29	0.4	0.43
26	2	9	7	7	0	25	0.6	1.45	0.42	0.52
27	5	8	4	5	0	22	0.51	1.37	0.42	0.3
28	3	6	3	3	0	15	0.49	1.36	0.39	0.42
29	2	11	2	8	0	23	0.64	1.4	0.41	0.65
30	2	7	3	5	0	17	0.54	1.41	0.38	0.49
31	1	10	3	5	0	19	0.49	1.24	0.36	0.38
32	2	6	5	5	0	18	0.61	1.27	0.36	0.6
33	3	9	4	7	0	23	0.6	1.56	0.46	0.42
34	3	7	4	7	0	21	0.69	1.66	0.45	0.69
35	1	5	2	7	0	15	0.82	1.54	0.39	0.75

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 297(IR:130, SQ:92, MR:56, LR:19, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	5	2	0	0	8	1	2.9
3	2	0	1	0	6	2	5.7
0	1	0	1	0	2	3	8.6
1	1	2	1	0	5	4	11.4
0	0	2	0	0	2	5	14.3
0	1	0	0	0	1	6	17.1

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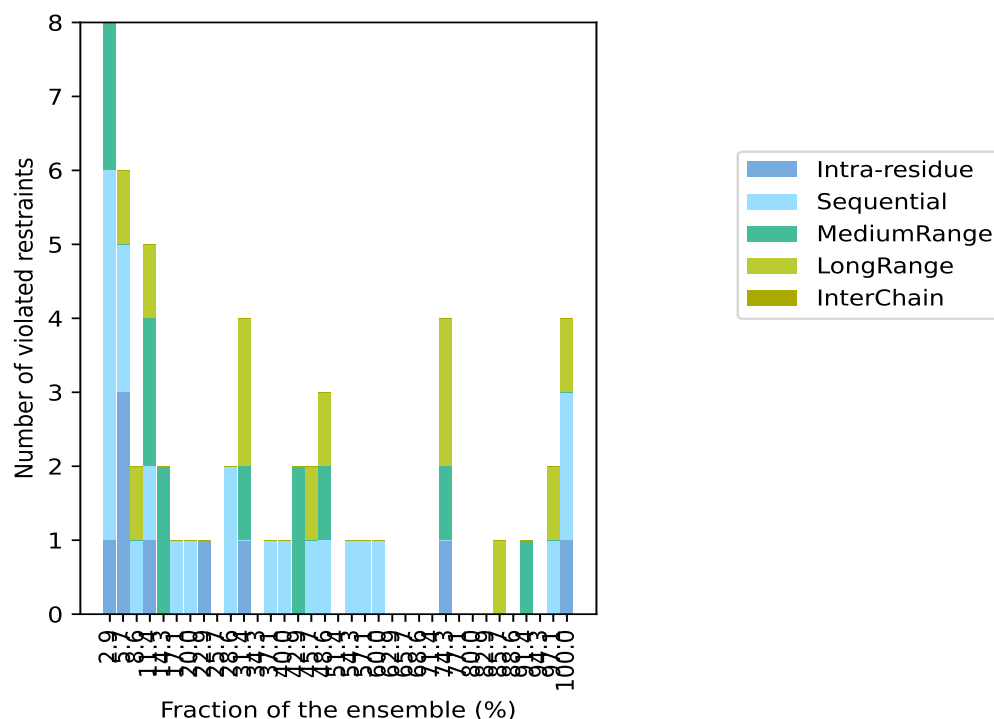
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	1	0	0	0	1	7	20.0
1	0	0	0	0	1	8	22.9
0	0	0	0	0	0	9	25.7
0	2	0	0	0	2	10	28.6
1	0	1	2	0	4	11	31.4
0	0	0	0	0	0	12	34.3
0	1	0	0	0	1	13	37.1
0	1	0	0	0	1	14	40.0
0	0	2	0	0	2	15	42.9
0	1	0	1	0	2	16	45.7
0	1	1	1	0	3	17	48.6
0	0	0	0	0	0	18	51.4
0	1	0	0	0	1	19	54.3
0	1	0	0	0	1	20	57.1
0	1	0	0	0	1	21	60.0
0	0	0	0	0	0	22	62.9
0	0	0	0	0	0	23	65.7
0	0	0	0	0	0	24	68.6
0	0	0	0	0	0	25	71.4
1	0	1	2	0	4	26	74.3
0	0	0	0	0	0	27	77.1
0	0	0	0	0	0	28	80.0
0	0	0	0	0	0	29	82.9
0	0	0	1	0	1	30	85.7
0	0	0	0	0	0	31	88.6
0	0	1	0	0	1	32	91.4
0	0	0	0	0	0	33	94.3
0	1	0	1	0	2	34	97.1
1	2	0	1	0	4	35	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

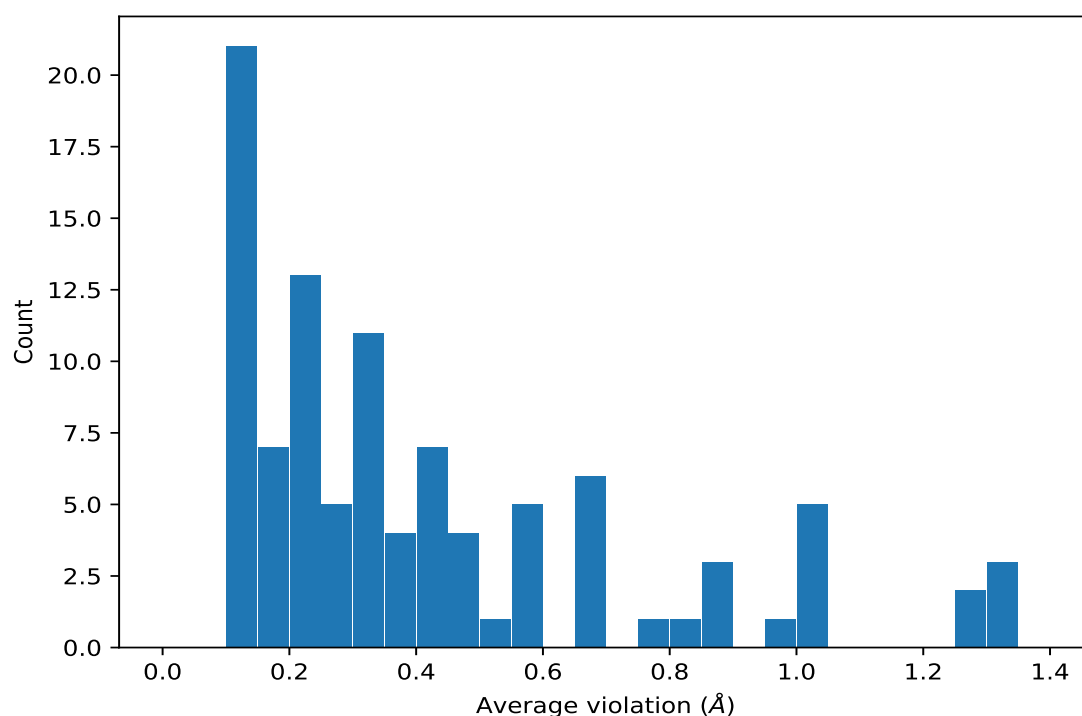
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	35	1.28	0.09	1.28
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	35	1.26	0.04	1.25
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	35	0.69	0.12	0.73
(1,347)	1:11:A:TRP:HH2	1:8:A:ARG:HB2	35	0.69	0.12	0.73
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	35	0.69	0.01	0.69
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	34	0.41	0.13	0.42
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	34	0.41	0.13	0.42
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	34	0.41	0.13	0.42
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	34	0.18	0.04	0.18
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	34	0.18	0.04	0.18
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	34	0.18	0.04	0.18
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	32	0.77	0.21	0.79
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	30	0.48	0.15	0.46
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	30	0.48	0.15	0.46
(1,335)	1:15:A:TYR:HE1	1:4:A:CYS:HA	30	0.48	0.15	0.46
(1,335)	1:15:A:TYR:HE2	1:4:A:CYS:HA	30	0.48	0.15	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	26	1.33	0.51	1.46
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	26	1.33	0.51	1.46
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	26	1.33	0.51	1.46
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	26	1.04	0.53	1.12
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	26	1.04	0.53	1.12
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	26	1.04	0.53	1.12
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	26	0.34	0.1	0.32
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	26	0.34	0.1	0.32
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	26	0.34	0.1	0.32
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG21	26	0.34	0.1	0.32
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG22	26	0.34	0.1	0.32
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG23	26	0.34	0.1	0.32
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	26	0.21	0.03	0.22
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	21	0.65	0.04	0.65
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	21	0.65	0.04	0.65
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	21	0.65	0.04	0.65
(1,343)	1:10:A:ASP:HB3	1:9:A:PRO:HD3	20	0.58	0.36	0.5
(1,343)	1:8:A:ARG:HD2	1:9:A:PRO:HD3	20	0.58	0.36	0.5
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	19	1.0	0.26	1.03
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	19	1.0	0.26	1.03
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	17	0.97	0.5	0.81
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	17	0.35	0.09	0.37
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	17	0.13	0.02	0.13
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	16	0.8	0.39	0.82
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	16	0.52	0.41	0.48
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG11	15	0.41	0.26	0.32
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG12	15	0.41	0.26	0.32
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG13	15	0.41	0.26	0.32
(1,299)	1:15:A:TYR:HB3	1:12:A:PRO:HG2	15	0.38	0.28	0.21
(1,340)	1:6:A:VAL:HG21	1:7:A:HIS:HB2	14	0.57	0.15	0.62
(1,340)	1:6:A:VAL:HG22	1:7:A:HIS:HB2	14	0.57	0.15	0.62
(1,340)	1:6:A:VAL:HG23	1:7:A:HIS:HB2	14	0.57	0.15	0.62
(1,243)	1:7:A:HIS:HD2	1:8:A:ARG:HD2	13	0.27	0.08	0.23
(1,189)	1:14:A:ALA:HB1	1:2:A:SER:HB3	11	0.85	0.48	0.82
(1,189)	1:14:A:ALA:HB2	1:2:A:SER:HB3	11	0.85	0.48	0.82
(1,189)	1:14:A:ALA:HB3	1:2:A:SER:HB3	11	0.85	0.48	0.82
(1,338)	1:7:A:HIS:HD2	1:14:A:ALA:HA	11	0.28	0.17	0.23
(1,316)	1:11:A:TRP:HZ2	1:8:A:ARG:HG2	11	0.12	0.02	0.12
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG21	11	0.1	0.0	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG22	11	0.1	0.0	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG23	11	0.1	0.0	0.1
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG21	10	0.26	0.06	0.27

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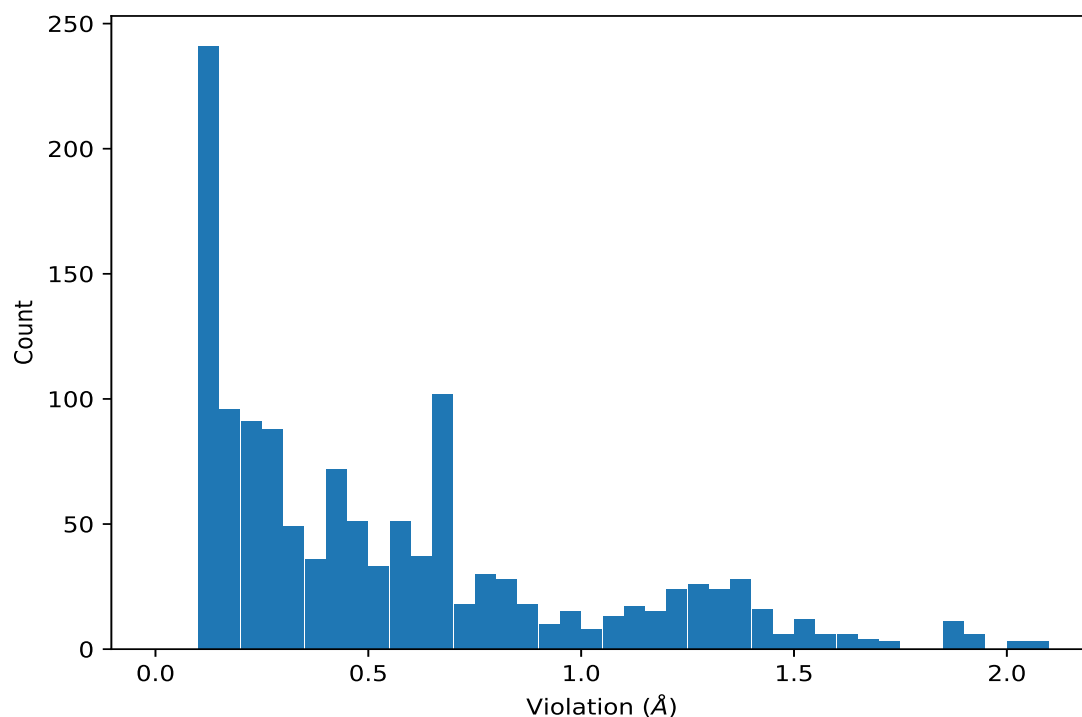
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG22	10	0.26	0.06	0.27
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG23	10	0.26	0.06	0.27
(1,332)	1:3:A:ILE:HG21	1:4:A:CYS:HA	10	0.22	0.14	0.15
(1,332)	1:3:A:ILE:HG22	1:4:A:CYS:HA	10	0.22	0.14	0.15
(1,332)	1:3:A:ILE:HG23	1:4:A:CYS:HA	10	0.22	0.14	0.15
(1,332)	1:6:A:VAL:HG11	1:5:A:HIS:HA	10	0.22	0.14	0.15
(1,332)	1:6:A:VAL:HG12	1:5:A:HIS:HA	10	0.22	0.14	0.15
(1,332)	1:6:A:VAL:HG13	1:5:A:HIS:HA	10	0.22	0.14	0.15
(1,332)	1:6:A:VAL:HG11	1:8:A:ARG:HA	10	0.22	0.14	0.15
(1,332)	1:6:A:VAL:HG12	1:8:A:ARG:HA	10	0.22	0.14	0.15
(1,332)	1:6:A:VAL:HG13	1:8:A:ARG:HA	10	0.22	0.14	0.15
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG21	8	0.12	0.02	0.12
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG22	8	0.12	0.02	0.12
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG23	8	0.12	0.02	0.12
(1,121)	1:7:A:HIS:HD2	1:8:A:ARG:HG2	7	0.11	0.01	0.11
(1,34)	1:13:A:CYS:HB2	1:12:A:PRO:HG2	6	0.18	0.04	0.2
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG21	5	0.14	0.02	0.13
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG22	5	0.14	0.02	0.13
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG23	5	0.14	0.02	0.13
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB1	5	0.11	0.0	0.11
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB2	5	0.11	0.0	0.11
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB3	5	0.11	0.0	0.11
(1,20)	1:15:A:TYR:HD1	1:2:A:SER:HB3	4	0.37	0.22	0.33
(1,20)	1:15:A:TYR:HD2	1:2:A:SER:HB3	4	0.37	0.22	0.33
(1,11)	1:15:A:TYR:HE1	1:12:A:PRO:HD3	4	0.32	0.2	0.29
(1,11)	1:15:A:TYR:HE2	1:12:A:PRO:HD3	4	0.32	0.2	0.29
(1,162)	1:11:A:TRP:H	1:9:A:PRO:HG3	4	0.18	0.06	0.2
(1,213)	1:11:A:TRP:HE3	1:11:A:TRP:HA	4	0.13	0.02	0.13
(1,97)	1:7:A:HIS:HE1	1:8:A:ARG:HG3	4	0.11	0.01	0.11
(1,339)	1:13:A:CYS:HB2	1:3:A:ILE:HG21	3	0.22	0.08	0.27
(1,339)	1:13:A:CYS:HB2	1:3:A:ILE:HG22	3	0.22	0.08	0.27
(1,339)	1:13:A:CYS:HB2	1:3:A:ILE:HG23	3	0.22	0.08	0.27
(1,6)	1:7:A:HIS:HD2	1:6:A:VAL:HB	3	0.12	0.01	0.12
(1,289)	1:16:A:ARG:HA	1:16:A:ARG:HD2	2	0.43	0.01	0.43
(1,256)	1:15:A:TYR:HE1	1:15:A:TYR:HA	2	0.3	0.2	0.3
(1,256)	1:15:A:TYR:HE2	1:15:A:TYR:HA	2	0.3	0.2	0.3
(1,345)	1:14:A:ALA:HA	1:13:A:CYS:HB2	2	0.3	0.19	0.3
(1,227)	1:7:A:HIS:HD2	1:8:A:ARG:HD3	2	0.18	0.03	0.18
(1,276)	1:9:A:PRO:HD3	1:9:A:PRO:HB2	2	0.16	0.02	0.16
(1,38)	1:15:A:TYR:HB3	1:3:A:ILE:HG21	2	0.1	0.0	0.1
(1,38)	1:15:A:TYR:HB3	1:3:A:ILE:HG22	2	0.1	0.0	0.1
(1,38)	1:15:A:TYR:HB3	1:3:A:ILE:HG23	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	17	2.06
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	17	2.06
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	17	2.06
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	11	2.01
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	11	2.01
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	11	2.01
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	19	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	19	1.94
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	19	1.94
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	11	1.93
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	11	1.93
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	11	1.93
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	16	1.9
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	16	1.9
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	16	1.9
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	12	1.9
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	17	1.88
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	17	1.88
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	17	1.88
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	1	1.86
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	1	1.86
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	1	1.86
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	3	1.86
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	8	1.73
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	8	1.73
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	8	1.73
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	12	1.68
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	12	1.68
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	12	1.68
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	34	1.66
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	10	1.63
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	10	1.63
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	10	1.63
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	13	1.63
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	13	1.63
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	13	1.63
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	33	1.56
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	33	1.56
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	33	1.56
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	20	1.55
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	20	1.55
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	20	1.55
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	13	1.54
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	21	1.54
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	35	1.54
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	4	1.52
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	4	1.52
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	4	1.52
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	4	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	4	1.52
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	4	1.52
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	22	1.51
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	22	1.51
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	22	1.51
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	18	1.49
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	33	1.49
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	20	1.48
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	20	1.48
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	20	1.48
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	5	1.47
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	26	1.45
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	26	1.45
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	26	1.45
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	6	1.44
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	6	1.44
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	6	1.44
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	13	1.44
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	13	1.44
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	13	1.44
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	35	1.43
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	35	1.43
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	35	1.43
(1,189)	1:14:A:ALA:HB1	1:2:A:SER:HB3	21	1.42
(1,189)	1:14:A:ALA:HB2	1:2:A:SER:HB3	21	1.42
(1,189)	1:14:A:ALA:HB3	1:2:A:SER:HB3	21	1.42
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	30	1.41
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	29	1.4
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	29	1.4
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	29	1.4
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	3	1.4
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	29	1.4
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	4	1.39
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	10	1.39
(1,189)	1:14:A:ALA:HB1	1:2:A:SER:HB3	34	1.39
(1,189)	1:14:A:ALA:HB2	1:2:A:SER:HB3	34	1.39
(1,189)	1:14:A:ALA:HB3	1:2:A:SER:HB3	34	1.39
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	6	1.39
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	6	1.39
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	6	1.39
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	26	1.39
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	26	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	26	1.39
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	2	1.38
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	12	1.38
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	27	1.37
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	27	1.37
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	27	1.37
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	22	1.37
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	22	1.37
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	22	1.37
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	14	1.37
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	7	1.36
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	28	1.36
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	14	1.35
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	19	1.34
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	9	1.34
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	9	1.34
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	24	1.34
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	24	1.34
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	21	1.33
(1,189)	1:14:A:ALA:HB1	1:2:A:SER:HB3	5	1.33
(1,189)	1:14:A:ALA:HB2	1:2:A:SER:HB3	5	1.33
(1,189)	1:14:A:ALA:HB3	1:2:A:SER:HB3	5	1.33
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	2	1.33
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	5	1.33
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	9	1.33
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	9	1.32
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	3	1.31
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	3	1.31
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	3	1.31
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	22	1.31
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	3	1.31
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	7	1.31
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	34	1.3
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	1	1.3
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	1	1.3
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	1	1.3
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	28	1.3
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	25	1.29
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	18	1.29
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	18	1.29
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	18	1.29
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	30	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	5	1.28
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	8	1.28
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	25	1.28
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	2	1.27
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	2	1.27
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	15	1.27
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	32	1.27
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	15	1.26
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	21	1.26
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	22	1.26
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	23	1.26
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	27	1.26
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	1	1.25
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	23	1.25
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	26	1.25
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	29	1.25
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	21	1.25
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	21	1.25
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	4	1.25
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	12	1.25
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	29	1.25
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	8	1.24
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	19	1.24
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	24	1.24
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	26	1.24
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	31	1.24
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	35	1.23
(1,189)	1:14:A:ALA:HB1	1:2:A:SER:HB3	33	1.23
(1,189)	1:14:A:ALA:HB2	1:2:A:SER:HB3	33	1.23
(1,189)	1:14:A:ALA:HB3	1:2:A:SER:HB3	33	1.23
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	10	1.23
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	17	1.23
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	20	1.23
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	24	1.22
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	19	1.22
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	19	1.22
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	19	1.22
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	6	1.22
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	13	1.22
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	20	1.21
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	31	1.21
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	32	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	33	1.21
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	11	1.21
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	34	1.21
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	13	1.2
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	16	1.2
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	7	1.2
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	23	1.2
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	23	1.2
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	3	1.2
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	3	1.2
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	3	1.2
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	1	1.2
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	16	1.2
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	35	1.2
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	17	1.18
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	25	1.18
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	25	1.18
(1,29)	1:8:A:ARG:HB3	1:7:A:HIS:HB3	33	1.17
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	12	1.15
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	12	1.15
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	12	1.15
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	10	1.14
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	10	1.14
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	10	1.14
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	6	1.13
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	11	1.13
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	27	1.13
(1,343)	1:8:A:ARG:HD2	1:9:A:PRO:HD3	10	1.12
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	2	1.12
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	8	1.11
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	8	1.11
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	8	1.11
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	32	1.1
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	32	1.1
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	32	1.1
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	31	1.09
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	31	1.09
(1,189)	1:14:A:ALA:HB1	1:2:A:SER:HB3	35	1.09
(1,189)	1:14:A:ALA:HB2	1:2:A:SER:HB3	35	1.09
(1,189)	1:14:A:ALA:HB3	1:2:A:SER:HB3	35	1.09
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	29	1.08
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	29	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,337)	1:8:A:ARG:HB2	1:7:A:HIS:HB3	27	1.07
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	19	1.07
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	17	1.07
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	27	1.05
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	27	1.05
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	27	1.05
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	16	1.04
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	16	1.04
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	16	1.04
(1,343)	1:8:A:ARG:HD2	1:9:A:PRO:HD3	26	1.03
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	6	1.03
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	17	1.03
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	17	1.03
(1,343)	1:8:A:ARG:HD2	1:9:A:PRO:HD3	6	1.02
(1,343)	1:8:A:ARG:HD2	1:9:A:PRO:HD3	2	0.99
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	34	0.99
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	20	0.98
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	26	0.98
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	26	0.98
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	34	0.98
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	34	0.98
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	34	0.98
(1,343)	1:8:A:ARG:HD2	1:9:A:PRO:HD3	32	0.97
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	34	0.96
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	34	0.96
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	34	0.96
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	22	0.96
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	34	0.96
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	34	0.96
(1,343)	1:8:A:ARG:HD2	1:9:A:PRO:HD3	25	0.95
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	4	0.95
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	7	0.93
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	33	0.93
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	33	0.93
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	33	0.93
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	8	0.92
(1,299)	1:15:A:TYR:HB3	1:12:A:PRO:HG2	12	0.91
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	26	0.91
(1,343)	1:8:A:ARG:HD2	1:9:A:PRO:HD3	15	0.9
(1,347)	1:11:A:TRP:HH2	1:8:A:ARG:HB2	9	0.89
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	22	0.89
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	22	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG11	33	0.89
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG12	33	0.89
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG13	33	0.89
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	8	0.88
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	24	0.88
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	17	0.87
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG11	35	0.87
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG12	35	0.87
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG13	35	0.87
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	29	0.87
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	29	0.87
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	29	0.87
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	4	0.86
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	9	0.86
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	13	0.86
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	4	0.85
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	23	0.85
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	32	0.85
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	31	0.84
(1,343)	1:8:A:ARG:HD2	1:9:A:PRO:HD3	17	0.84
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	6	0.83
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	11	0.83
(1,347)	1:11:A:TRP:HH2	1:8:A:ARG:HB2	25	0.82
(1,299)	1:15:A:TYR:HB3	1:12:A:PRO:HG2	23	0.82
(1,189)	1:14:A:ALA:HB1	1:2:A:SER:HB3	29	0.82
(1,189)	1:14:A:ALA:HB2	1:2:A:SER:HB3	29	0.82
(1,189)	1:14:A:ALA:HB3	1:2:A:SER:HB3	29	0.82
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	32	0.82
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	32	0.82
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	32	0.82
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	21	0.81
(1,347)	1:11:A:TRP:HH2	1:8:A:ARG:HB2	34	0.81
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	8	0.81
(1,347)	1:11:A:TRP:HH2	1:8:A:ARG:HB2	5	0.8
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	15	0.8
(1,347)	1:11:A:TRP:HH2	1:8:A:ARG:HB2	22	0.8
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	30	0.8
(1,299)	1:15:A:TYR:HB3	1:12:A:PRO:HG2	19	0.8
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	35	0.8
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	7	0.8
(1,189)	1:14:A:ALA:HB1	1:2:A:SER:HB3	13	0.8
(1,189)	1:14:A:ALA:HB2	1:2:A:SER:HB3	13	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,189)	1:14:A:ALA:HB3	1:2:A:SER:HB3	13	0.8
(1,340)	1:6:A:VAL:HG21	1:7:A:HIS:HB2	2	0.79
(1,340)	1:6:A:VAL:HG22	1:7:A:HIS:HB2	2	0.79
(1,340)	1:6:A:VAL:HG23	1:7:A:HIS:HB2	2	0.79
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	25	0.79
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	29	0.79
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	30	0.79
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	13	0.79
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	13	0.79
(1,347)	1:11:A:TRP:HH2	1:8:A:ARG:HB2	13	0.78
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	5	0.78
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	5	0.78
(1,189)	1:14:A:ALA:HB1	1:2:A:SER:HB3	7	0.78
(1,189)	1:14:A:ALA:HB2	1:2:A:SER:HB3	7	0.78
(1,189)	1:14:A:ALA:HB3	1:2:A:SER:HB3	7	0.78
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	24	0.78
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	28	0.77
(1,299)	1:15:A:TYR:HB3	1:12:A:PRO:HG2	26	0.77
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	8	0.77
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	8	0.77
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	15	0.76
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	7	0.75
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	33	0.75
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	27	0.75
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	27	0.75
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	12	0.75
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	31	0.75
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	3	0.75
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	35	0.75
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	35	0.75
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	35	0.75
(1,347)	1:11:A:TRP:HH2	1:8:A:ARG:HB2	24	0.74
(1,347)	1:11:A:TRP:HH2	1:8:A:ARG:HB2	26	0.74
(1,335)	1:15:A:TYR:HE1	1:4:A:CYS:HA	11	0.74
(1,335)	1:15:A:TYR:HE2	1:4:A:CYS:HA	11	0.74
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	8	0.73
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	23	0.73
(1,335)	1:15:A:TYR:HE1	1:4:A:CYS:HA	6	0.73
(1,335)	1:15:A:TYR:HE2	1:4:A:CYS:HA	6	0.73
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	27	0.73
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	27	0.73
(1,338)	1:7:A:HIS:HD2	1:14:A:ALA:HA	2	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	4	0.72
(1,347)	1:11:A:TRP:HH2	1:8:A:ARG:HB2	32	0.71
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	6	0.71
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	6	0.71
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	6	0.71
(1,20)	1:15:A:TYR:HD1	1:2:A:SER:HB3	21	0.71
(1,20)	1:15:A:TYR:HD2	1:2:A:SER:HB3	21	0.71
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	21	0.7
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	21	0.7
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	1	0.7
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	1	0.7
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	1	0.7
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	22	0.7
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	22	0.7
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	22	0.7
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	32	0.7
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	32	0.7
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	32	0.7
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	2	0.7
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	5	0.7
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	18	0.7
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	19	0.7
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	23	0.7
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	29	0.7
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	31	0.7
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	33	0.7
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	35	0.7
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	29	0.69
(1,343)	1:8:A:ARG:HD2	1:9:A:PRO:HD3	4	0.69
(1,340)	1:6:A:VAL:HG21	1:7:A:HIS:HB2	5	0.69
(1,340)	1:6:A:VAL:HG22	1:7:A:HIS:HB2	5	0.69
(1,340)	1:6:A:VAL:HG23	1:7:A:HIS:HB2	5	0.69
(1,340)	1:6:A:VAL:HG21	1:7:A:HIS:HB2	9	0.69
(1,340)	1:6:A:VAL:HG22	1:7:A:HIS:HB2	9	0.69
(1,340)	1:6:A:VAL:HG23	1:7:A:HIS:HB2	9	0.69
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	34	0.69
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	5	0.69
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	1	0.69
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	3	0.69
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	4	0.69
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	6	0.69
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	7	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	10	0.69
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	11	0.69
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	13	0.69
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	16	0.69
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	17	0.69
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	22	0.69
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	25	0.69
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	26	0.69
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	27	0.69
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	28	0.69
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	30	0.69
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	34	0.69
(1,340)	1:6:A:VAL:HG21	1:7:A:HIS:HB2	30	0.68
(1,340)	1:6:A:VAL:HG22	1:7:A:HIS:HB2	30	0.68
(1,340)	1:6:A:VAL:HG23	1:7:A:HIS:HB2	30	0.68
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	23	0.68
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	8	0.68
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	8	0.68
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	8	0.68
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	11	0.68
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	11	0.68
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	11	0.68
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	9	0.68
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	12	0.68
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	15	0.68
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	20	0.68
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	21	0.68
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	24	0.68
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	32	0.68
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	10	0.67
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	19	0.67
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	35	0.67
(1,340)	1:6:A:VAL:HG21	1:7:A:HIS:HB2	7	0.67
(1,340)	1:6:A:VAL:HG22	1:7:A:HIS:HB2	7	0.67
(1,340)	1:6:A:VAL:HG23	1:7:A:HIS:HB2	7	0.67
(1,340)	1:6:A:VAL:HG21	1:7:A:HIS:HB2	18	0.67
(1,340)	1:6:A:VAL:HG22	1:7:A:HIS:HB2	18	0.67
(1,340)	1:6:A:VAL:HG23	1:7:A:HIS:HB2	18	0.67
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	14	0.67
(1,347)	1:11:A:TRP:HH2	1:8:A:ARG:HB2	2	0.66
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	16	0.66
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	29	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	17	0.66
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	17	0.66
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	17	0.66
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	35	0.66
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	35	0.66
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	35	0.66
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG11	3	0.66
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG12	3	0.66
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG13	3	0.66
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	10	0.65
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	10	0.65
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	10	0.65
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	13	0.65
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	13	0.65
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	13	0.65
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	26	0.65
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	26	0.65
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	26	0.65
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	29	0.65
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	29	0.65
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	29	0.65
(1,105)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	8	0.65
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	26	0.65
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	26	0.65
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	26	0.65
(1,347)	1:11:A:TRP:HH2	1:8:A:ARG:HB2	11	0.64
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	19	0.64
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	16	0.64
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	16	0.64
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	16	0.64
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	33	0.64
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	33	0.64
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	33	0.64
(1,347)	1:11:A:TRP:HH2	1:8:A:ARG:HB2	20	0.63
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	3	0.63
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	3	0.63
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	3	0.63
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	7	0.63
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	7	0.63
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	7	0.63
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	1	0.62
(1,340)	1:6:A:VAL:HG21	1:7:A:HIS:HB2	21	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:6:A:VAL:HG22	1:7:A:HIS:HB2	21	0.62
(1,340)	1:6:A:VAL:HG23	1:7:A:HIS:HB2	21	0.62
(1,340)	1:6:A:VAL:HG21	1:7:A:HIS:HB2	25	0.62
(1,340)	1:6:A:VAL:HG22	1:7:A:HIS:HB2	25	0.62
(1,340)	1:6:A:VAL:HG23	1:7:A:HIS:HB2	25	0.62
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	19	0.62
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	19	0.62
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	19	0.62
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	12	0.61
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	20	0.61
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	20	0.61
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	30	0.61
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	30	0.61
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	18	0.61
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	4	0.61
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	4	0.61
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	4	0.61
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	12	0.61
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	12	0.61
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	12	0.61
(1,343)	1:8:A:ARG:HD2	1:9:A:PRO:HD3	30	0.6
(1,340)	1:6:A:VAL:HG21	1:7:A:HIS:HB2	15	0.6
(1,340)	1:6:A:VAL:HG22	1:7:A:HIS:HB2	15	0.6
(1,340)	1:6:A:VAL:HG23	1:7:A:HIS:HB2	15	0.6
(1,332)	1:6:A:VAL:HG11	1:5:A:HIS:HA	16	0.6
(1,332)	1:6:A:VAL:HG12	1:5:A:HIS:HA	16	0.6
(1,332)	1:6:A:VAL:HG13	1:5:A:HIS:HA	16	0.6
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	19	0.6
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	27	0.6
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	27	0.6
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	27	0.6
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG11	1	0.6
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG12	1	0.6
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG13	1	0.6
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG21	5	0.59
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG22	5	0.59
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG23	5	0.59
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	1	0.59
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG11	16	0.59
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG12	16	0.59
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG13	16	0.59
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	7	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	7	0.58
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	22	0.58
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	22	0.58
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	29	0.58
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	18	0.57
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	34	0.57
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	34	0.57
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	20	0.57
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	20	0.57
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	20	0.57
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG11	34	0.57
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG12	34	0.57
(1,155)	1:7:A:HIS:HD2	1:6:A:VAL:HG13	34	0.57
(1,48)	1:5:A:HIS:HB3	1:6:A:VAL:HA	20	0.57
(1,11)	1:15:A:TYR:HE1	1:12:A:PRO:HD3	14	0.57
(1,11)	1:15:A:TYR:HE2	1:12:A:PRO:HD3	14	0.57
(1,340)	1:6:A:VAL:HG21	1:7:A:HIS:HB2	28	0.56
(1,340)	1:6:A:VAL:HG22	1:7:A:HIS:HB2	28	0.56
(1,340)	1:6:A:VAL:HG23	1:7:A:HIS:HB2	28	0.56
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	13	0.56
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	13	0.56
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	17	0.56
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	17	0.56
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	33	0.56
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	33	0.56
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	28	0.56
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	23	0.56
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	23	0.56
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	23	0.56
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	2	0.54
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	2	0.54
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	21	0.54
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	21	0.54
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	21	0.54
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	18	0.53
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	18	0.53
(1,299)	1:15:A:TYR:HB3	1:12:A:PRO:HG2	32	0.53
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	35	0.53
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	13	0.53
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	3	0.53
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	3	0.53
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	3	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	5	0.53
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	5	0.53
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	5	0.53
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	25	0.53
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	25	0.53
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	25	0.53
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	14	0.52
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	1	0.52
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	1	0.52
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	26	0.52
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	6	0.52
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	1	0.52
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	1	0.52
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	1	0.52
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	12	0.51
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	12	0.51
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	18	0.51
(1,256)	1:15:A:TYR:HE1	1:15:A:TYR:HA	12	0.5
(1,256)	1:15:A:TYR:HE2	1:15:A:TYR:HA	12	0.5
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	10	0.5
(1,347)	1:11:A:TRP:HH2	1:8:A:ARG:HB2	6	0.49
(1,345)	1:14:A:ALA:HA	1:13:A:CYS:HB2	2	0.49
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	18	0.49
(1,231)	1:15:A:TYR:HE1	1:16:A:ARG:HG3	10	0.49
(1,231)	1:15:A:TYR:HE2	1:16:A:ARG:HG3	10	0.49
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	34	0.49
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	8	0.49
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	8	0.49
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	8	0.49
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	22	0.49
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	22	0.49
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	22	0.49
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	30	0.49
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	30	0.49
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	30	0.49
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	35	0.49
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	35	0.49
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	35	0.49
(1,347)	1:11:A:TRP:HH2	1:8:A:ARG:HB2	27	0.48
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	3	0.48
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	3	0.48
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	15	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	15	0.48
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	15	0.48
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG11	22	0.48
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG12	22	0.48
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG13	22	0.48
(1,340)	1:6:A:VAL:HG21	1:7:A:HIS:HB2	14	0.47
(1,340)	1:6:A:VAL:HG22	1:7:A:HIS:HB2	14	0.47
(1,340)	1:6:A:VAL:HG23	1:7:A:HIS:HB2	14	0.47
(1,338)	1:7:A:HIS:HD2	1:14:A:ALA:HA	21	0.47
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	2	0.47
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	14	0.46
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	14	0.46
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	14	0.46
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	1	0.46
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	1	0.46
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	1	0.46
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG21	4	0.46
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG22	4	0.46
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG23	4	0.46
(1,11)	1:15:A:TYR:HE1	1:12:A:PRO:HD3	8	0.46
(1,11)	1:15:A:TYR:HE2	1:12:A:PRO:HD3	8	0.46
(1,347)	1:11:A:TRP:HH2	1:8:A:ARG:HB2	17	0.45
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	19	0.45
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	19	0.45
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	32	0.45
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	32	0.45
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	29	0.45
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	29	0.45
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	29	0.45
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	7	0.44
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	7	0.44
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	7	0.44
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	19	0.44
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	19	0.44
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	19	0.44
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	8	0.44
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	8	0.44
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	15	0.44
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	15	0.44
(1,289)	1:16:A:ARG:HA	1:16:A:ARG:HD2	22	0.44
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	16	0.44
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	16	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	16	0.44
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	16	0.44
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	32	0.44
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	32	0.44
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	32	0.44
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	28	0.43
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	28	0.43
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	28	0.43
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	29	0.43
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	29	0.43
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	1	0.43
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	15	0.42
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	15	0.42
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	15	0.42
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	33	0.42
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	33	0.42
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	33	0.42
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	4	0.42
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	4	0.42
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	9	0.42
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	9	0.42
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	23	0.42
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	24	0.42
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	30	0.42
(1,298)	1:15:A:TYR:HB2	1:16:A:ARG:HG3	12	0.42
(1,289)	1:16:A:ARG:HA	1:16:A:ARG:HD2	23	0.42
(1,243)	1:7:A:HIS:HD2	1:8:A:ARG:HD2	16	0.42
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	33	0.42
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	4	0.42
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	4	0.42
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	4	0.42
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	28	0.42
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	28	0.42
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	28	0.42
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG11	29	0.42
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG12	29	0.42
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG13	29	0.42
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	31	0.41
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	31	0.41
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	31	0.41
(1,343)	1:10:A:ASP:HB3	1:9:A:PRO:HD3	33	0.41
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	21	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	21	0.41
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	21	0.41
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	14	0.41
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	22	0.41
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	23	0.41
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	6	0.41
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	6	0.41
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	6	0.41
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	8	0.4
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	8	0.4
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	8	0.4
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	10	0.4
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	10	0.4
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	10	0.4
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	26	0.4
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	26	0.4
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	15	0.4
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	21	0.39
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	21	0.39
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	21	0.39
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	31	0.39
(1,243)	1:7:A:HIS:HD2	1:8:A:ARG:HD2	31	0.39
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG21	2	0.39
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG22	2	0.39
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG23	2	0.39
(1,340)	1:6:A:VAL:HG21	1:7:A:HIS:HB2	23	0.38
(1,340)	1:6:A:VAL:HG22	1:7:A:HIS:HB2	23	0.38
(1,340)	1:6:A:VAL:HG23	1:7:A:HIS:HB2	23	0.38
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	24	0.38
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	24	0.38
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	24	0.38
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	31	0.38
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	31	0.38
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	31	0.38
(1,24)	1:15:A:TYR:H	1:13:A:CYS:HB2	26	0.38
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	23	0.37
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	23	0.37
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	23	0.37
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	24	0.37
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	24	0.37
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	24	0.37
(1,343)	1:10:A:ASP:HB3	1:9:A:PRO:HD3	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	7	0.37
(1,20)	1:15:A:TYR:HD1	1:2:A:SER:HB3	5	0.37
(1,20)	1:15:A:TYR:HD2	1:2:A:SER:HB3	5	0.37
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG11	18	0.36
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG12	18	0.36
(1,346)	1:11:A:TRP:HB3	1:6:A:VAL:HG13	18	0.36
(1,343)	1:8:A:ARG:HD2	1:9:A:PRO:HD3	3	0.36
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	11	0.36
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	9	0.36
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	9	0.36
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	9	0.36
(1,347)	1:11:A:TRP:HH2	1:3:A:ILE:HG12	3	0.35
(1,338)	1:7:A:HIS:HD2	1:14:A:ALA:HA	32	0.35
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	31	0.35
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	31	0.35
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	9	0.35
(1,243)	1:7:A:HIS:HD2	1:8:A:ARG:HD2	29	0.35
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	5	0.34
(1,243)	1:7:A:HIS:HD2	1:8:A:ARG:HD2	1	0.34
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	11	0.34
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	11	0.34
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	11	0.34
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	19	0.34
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	19	0.34
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	19	0.34
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	34	0.34
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	34	0.34
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	34	0.34
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	13	0.33
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	13	0.33
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	13	0.33
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	25	0.33
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	25	0.33
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	25	0.33
(1,332)	1:6:A:VAL:HG11	1:8:A:ARG:HA	24	0.33
(1,332)	1:6:A:VAL:HG12	1:8:A:ARG:HA	24	0.33
(1,332)	1:6:A:VAL:HG13	1:8:A:ARG:HA	24	0.33
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	16	0.33
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	8	0.33
(1,243)	1:7:A:HIS:HD2	1:8:A:ARG:HD2	8	0.32
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	10	0.32
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	10	0.32
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG11	34	0.32
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG12	34	0.32
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG13	34	0.32
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	9	0.31
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	9	0.31
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	9	0.31
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG21	26	0.31
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG22	26	0.31
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG23	26	0.31
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	31	0.31
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	31	0.31
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	31	0.31
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	28	0.31
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	27	0.31
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	18	0.31
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	18	0.31
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	18	0.31
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	16	0.3
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	16	0.3
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	16	0.3
(1,340)	1:6:A:VAL:HG21	1:7:A:HIS:HB2	24	0.3
(1,340)	1:6:A:VAL:HG22	1:7:A:HIS:HB2	24	0.3
(1,340)	1:6:A:VAL:HG23	1:7:A:HIS:HB2	24	0.3
(1,340)	1:6:A:VAL:HG21	1:7:A:HIS:HB2	31	0.3
(1,340)	1:6:A:VAL:HG22	1:7:A:HIS:HB2	31	0.3
(1,340)	1:6:A:VAL:HG23	1:7:A:HIS:HB2	31	0.3
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	24	0.3
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	24	0.3
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	31	0.3
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	12	0.29
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	12	0.29
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	12	0.29
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	23	0.29
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	23	0.29
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	23	0.29
(1,339)	1:13:A:CYS:HB2	1:3:A:ILE:HG21	27	0.29
(1,339)	1:13:A:CYS:HB2	1:3:A:ILE:HG22	27	0.29
(1,339)	1:13:A:CYS:HB2	1:3:A:ILE:HG23	27	0.29
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG21	5	0.29
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG22	5	0.29
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG23	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG21	9	0.29
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG22	9	0.29
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG23	9	0.29
(1,20)	1:15:A:TYR:HD1	1:2:A:SER:HB3	33	0.29
(1,20)	1:15:A:TYR:HD2	1:2:A:SER:HB3	33	0.29
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	3	0.29
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	3	0.29
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	3	0.29
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG21	6	0.28
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG22	6	0.28
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG23	6	0.28
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	30	0.28
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	30	0.28
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	30	0.28
(1,332)	1:3:A:ILE:HG21	1:4:A:CYS:HA	13	0.28
(1,332)	1:3:A:ILE:HG22	1:4:A:CYS:HA	13	0.28
(1,332)	1:3:A:ILE:HG23	1:4:A:CYS:HA	13	0.28
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG21	30	0.28
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG22	30	0.28
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG23	30	0.28
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	12	0.28
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	12	0.28
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	12	0.28
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	26	0.28
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	26	0.28
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	26	0.28
(1,339)	1:13:A:CYS:HB2	1:3:A:ILE:HG21	2	0.27
(1,339)	1:13:A:CYS:HB2	1:3:A:ILE:HG22	2	0.27
(1,339)	1:13:A:CYS:HB2	1:3:A:ILE:HG23	2	0.27
(1,338)	1:7:A:HIS:HD2	1:14:A:ALA:HA	12	0.27
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	16	0.27
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	16	0.27
(1,243)	1:7:A:HIS:HD2	1:8:A:ARG:HD2	12	0.27
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG21	7	0.27
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG22	7	0.27
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG23	7	0.27
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG21	18	0.27
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG22	18	0.27
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG23	18	0.27
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	20	0.27
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	20	0.27
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	20	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	32	0.27
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	32	0.27
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	32	0.27
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG21	3	0.26
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG22	3	0.26
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG23	3	0.26
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	14	0.26
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	14	0.26
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	14	0.26
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	25	0.26
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG11	19	0.26
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG12	19	0.26
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG13	19	0.26
(1,343)	1:10:A:ASP:HB3	1:9:A:PRO:HD3	11	0.25
(1,338)	1:7:A:HIS:HD2	1:14:A:ALA:HA	19	0.25
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	14	0.25
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	14	0.25
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	12	0.25
(1,162)	1:11:A:TRP:H	1:9:A:PRO:HG3	12	0.25
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	33	0.25
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	33	0.25
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	33	0.25
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	10	0.24
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	10	0.24
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	2	0.24
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	6	0.24
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	8	0.24
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	12	0.24
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	24	0.24
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	28	0.24
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	30	0.24
(1,343)	1:10:A:ASP:HB3	1:9:A:PRO:HD3	5	0.23
(1,338)	1:7:A:HIS:HD2	1:14:A:ALA:HA	23	0.23
(1,299)	1:15:A:TYR:HB3	1:12:A:PRO:HG2	20	0.23
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	2	0.23
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	19	0.23
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	20	0.23
(1,243)	1:7:A:HIS:HD2	1:8:A:ARG:HD2	13	0.23
(1,243)	1:7:A:HIS:HD2	1:8:A:ARG:HD2	20	0.23
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	25	0.23
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	13	0.23
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	13	0.23
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	17	0.22
(1,299)	1:15:A:TYR:HB3	1:12:A:PRO:HG2	24	0.22
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	1	0.22
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	5	0.22
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	10	0.22
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	15	0.22
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	17	0.22
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	29	0.22
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG21	21	0.22
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG22	21	0.22
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG23	21	0.22
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG21	25	0.22
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG22	25	0.22
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG23	25	0.22
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG11	11	0.22
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG12	11	0.22
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG13	11	0.22
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG11	26	0.22
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG12	26	0.22
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG13	26	0.22
(1,34)	1:13:A:CYS:HB2	1:12:A:PRO:HG2	26	0.22
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	2	0.22
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	2	0.22
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	2	0.22
(1,338)	1:7:A:HIS:HD2	1:14:A:ALA:HA	15	0.21
(1,299)	1:15:A:TYR:HB3	1:12:A:PRO:HG2	22	0.21
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	7	0.21
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	32	0.21
(1,260)	1:2:A:SER:HB3	1:13:A:CYS:HB2	1	0.21
(1,162)	1:11:A:TRP:H	1:9:A:PRO:HG3	32	0.21
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	21	0.21
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	22	0.21
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG11	4	0.21
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG12	4	0.21
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG13	4	0.21
(1,34)	1:13:A:CYS:HB2	1:12:A:PRO:HG2	2	0.21
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	18	0.21
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	18	0.21
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	18	0.21
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	34	0.21
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	34	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	34	0.21
(1,299)	1:15:A:TYR:HB3	1:12:A:PRO:HG2	2	0.2
(1,299)	1:15:A:TYR:HB3	1:12:A:PRO:HG2	21	0.2
(1,299)	1:15:A:TYR:HB3	1:12:A:PRO:HG2	27	0.2
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	13	0.2
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	21	0.2
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	25	0.2
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	26	0.2
(1,243)	1:7:A:HIS:HD2	1:8:A:ARG:HD2	19	0.2
(1,227)	1:7:A:HIS:HD2	1:8:A:ARG:HD3	22	0.2
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG21	15	0.2
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG22	15	0.2
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG23	15	0.2
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	17	0.2
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	17	0.2
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	17	0.2
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	25	0.2
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	25	0.2
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	25	0.2
(1,34)	1:13:A:CYS:HB2	1:12:A:PRO:HG2	5	0.2
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	8	0.2
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	8	0.2
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	8	0.2
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	19	0.2
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	19	0.2
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	19	0.2
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	22	0.2
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	22	0.2
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	22	0.2
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG21	35	0.19
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG22	35	0.19
(1,341)	1:11:A:TRP:HB2	1:6:A:VAL:HG23	35	0.19
(1,338)	1:7:A:HIS:HD2	1:14:A:ALA:HA	7	0.19
(1,299)	1:15:A:TYR:HB3	1:12:A:PRO:HG2	17	0.19
(1,243)	1:7:A:HIS:HD2	1:8:A:ARG:HD2	17	0.19
(1,243)	1:7:A:HIS:HD2	1:8:A:ARG:HD2	24	0.19
(1,34)	1:13:A:CYS:HB2	1:12:A:PRO:HG2	31	0.19
(1,23)	1:15:A:TYR:HD1	1:13:A:CYS:HB2	26	0.19
(1,23)	1:15:A:TYR:HD2	1:13:A:CYS:HB2	26	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	6	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	6	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	9	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	9	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	9	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	11	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	11	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	11	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	12	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	12	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	12	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	21	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	21	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	21	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	23	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	23	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	23	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	33	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	33	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	33	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	35	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	35	0.19
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	35	0.19
(1,343)	1:10:A:ASP:HB3	1:9:A:PRO:HD3	1	0.18
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	22	0.18
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	22	0.18
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	22	0.18
(1,276)	1:9:A:PRO:HD3	1:9:A:PRO:HB2	16	0.18
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	27	0.18
(1,162)	1:11:A:TRP:H	1:9:A:PRO:HG3	5	0.18
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	10	0.18
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	27	0.18
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	27	0.18
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	27	0.18
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	1	0.18
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	1	0.18
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	1	0.18
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	4	0.18
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	4	0.18
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	4	0.18
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	20	0.18
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	20	0.18
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	20	0.18
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	30	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	30	0.18
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	30	0.18
(1,343)	1:10:A:ASP:HB3	1:9:A:PRO:HD3	21	0.17
(1,243)	1:7:A:HIS:HD2	1:8:A:ARG:HD2	33	0.17
(1,189)	1:14:A:ALA:HB1	1:2:A:SER:HB3	8	0.17
(1,189)	1:14:A:ALA:HB2	1:2:A:SER:HB3	8	0.17
(1,189)	1:14:A:ALA:HB3	1:2:A:SER:HB3	8	0.17
(1,156)	1:7:A:HIS:HE1	1:6:A:VAL:HA	32	0.17
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	24	0.17
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	24	0.17
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	24	0.17
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG21	18	0.17
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG22	18	0.17
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG23	18	0.17
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	10	0.17
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	10	0.17
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	10	0.17
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	13	0.17
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	13	0.17
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	13	0.17
(1,343)	1:10:A:ASP:HB3	1:9:A:PRO:HD3	29	0.16
(1,338)	1:7:A:HIS:HD2	1:14:A:ALA:HA	16	0.16
(1,316)	1:11:A:TRP:HZ2	1:8:A:ARG:HG2	31	0.16
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG21	14	0.16
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG22	14	0.16
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG23	14	0.16
(1,299)	1:15:A:TYR:HB3	1:12:A:PRO:HG2	11	0.16
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	4	0.16
(1,243)	1:7:A:HIS:HD2	1:8:A:ARG:HD2	27	0.16
(1,213)	1:11:A:TRP:HE3	1:11:A:TRP:HA	27	0.16
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG21	28	0.16
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG22	28	0.16
(1,212)	1:7:A:HIS:HB2	1:6:A:VAL:HG23	28	0.16
(1,190)	1:2:A:SER:HB3	1:3:A:ILE:HG13	26	0.16
(1,111)	1:13:A:CYS:HB2	1:13:A:CYS:HA	24	0.16
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG21	2	0.16
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG22	2	0.16
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG23	2	0.16
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	7	0.16
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	7	0.16
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	7	0.16
(1,343)	1:10:A:ASP:HB3	1:9:A:PRO:HD3	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG21	17	0.15
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG22	17	0.15
(1,341)	1:4:A:CYS:HB2	1:6:A:VAL:HG23	17	0.15
(1,332)	1:3:A:ILE:HG21	1:4:A:CYS:HA	5	0.15
(1,332)	1:3:A:ILE:HG22	1:4:A:CYS:HA	5	0.15
(1,332)	1:3:A:ILE:HG23	1:4:A:CYS:HA	5	0.15
(1,332)	1:3:A:ILE:HG21	1:4:A:CYS:HA	33	0.15
(1,332)	1:3:A:ILE:HG22	1:4:A:CYS:HA	33	0.15
(1,332)	1:3:A:ILE:HG23	1:4:A:CYS:HA	33	0.15
(1,316)	1:11:A:TRP:HZ2	1:8:A:ARG:HG2	16	0.15
(1,276)	1:9:A:PRO:HD3	1:9:A:PRO:HB2	18	0.15
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	11	0.15
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	14	0.15
(1,227)	1:7:A:HIS:HD2	1:8:A:ARG:HD3	14	0.15
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	18	0.15
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	19	0.15
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	15	0.15
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	15	0.15
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	15	0.15
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	25	0.15
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	25	0.15
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	25	0.15
(1,338)	1:7:A:HIS:HD2	1:14:A:ALA:HA	26	0.14
(1,332)	1:3:A:ILE:HG21	1:4:A:CYS:HA	23	0.14
(1,332)	1:3:A:ILE:HG22	1:4:A:CYS:HA	23	0.14
(1,332)	1:3:A:ILE:HG23	1:4:A:CYS:HA	23	0.14
(1,332)	1:3:A:ILE:HG21	1:4:A:CYS:HA	26	0.14
(1,332)	1:3:A:ILE:HG22	1:4:A:CYS:HA	26	0.14
(1,332)	1:3:A:ILE:HG23	1:4:A:CYS:HA	26	0.14
(1,332)	1:3:A:ILE:HG21	1:4:A:CYS:HA	28	0.14
(1,332)	1:3:A:ILE:HG22	1:4:A:CYS:HA	28	0.14
(1,332)	1:3:A:ILE:HG23	1:4:A:CYS:HA	28	0.14
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG21	5	0.14
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG22	5	0.14
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG23	5	0.14
(1,189)	1:14:A:ALA:HB1	1:2:A:SER:HB3	15	0.14
(1,189)	1:14:A:ALA:HB2	1:2:A:SER:HB3	15	0.14
(1,189)	1:14:A:ALA:HB3	1:2:A:SER:HB3	15	0.14
(1,189)	1:14:A:ALA:HB1	1:2:A:SER:HB3	19	0.14
(1,189)	1:14:A:ALA:HB2	1:2:A:SER:HB3	19	0.14
(1,189)	1:14:A:ALA:HB3	1:2:A:SER:HB3	19	0.14
(1,121)	1:7:A:HIS:HD2	1:8:A:ARG:HG2	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	4	0.14
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	15	0.14
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	21	0.14
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	14	0.14
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	14	0.14
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	14	0.14
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	17	0.14
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	17	0.14
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	17	0.14
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	29	0.14
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	29	0.14
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	29	0.14
(1,343)	1:10:A:ASP:HB3	1:9:A:PRO:HD3	14	0.13
(1,338)	1:7:A:HIS:HD2	1:14:A:ALA:HA	22	0.13
(1,332)	1:3:A:ILE:HG21	1:4:A:CYS:HA	14	0.13
(1,332)	1:3:A:ILE:HG22	1:4:A:CYS:HA	14	0.13
(1,332)	1:3:A:ILE:HG23	1:4:A:CYS:HA	14	0.13
(1,316)	1:11:A:TRP:HZ2	1:8:A:ARG:HG2	24	0.13
(1,316)	1:11:A:TRP:HZ2	1:8:A:ARG:HG2	26	0.13
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG21	28	0.13
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG22	28	0.13
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG23	28	0.13
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG21	33	0.13
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG22	33	0.13
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG23	33	0.13
(1,299)	1:15:A:TYR:HB3	1:12:A:PRO:HG2	18	0.13
(1,267)	1:9:A:PRO:HA	1:9:A:PRO:HG3	33	0.13
(1,213)	1:11:A:TRP:HE3	1:11:A:TRP:HA	12	0.13
(1,213)	1:11:A:TRP:HE3	1:11:A:TRP:HA	20	0.13
(1,140)	1:15:A:TYR:HB3	1:16:A:ARG:HG3	5	0.13
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	5	0.13
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	7	0.13
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	20	0.13
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	23	0.13
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG11	17	0.13
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG12	17	0.13
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG13	17	0.13
(1,41)	1:16:A:ARG:H	1:15:A:TYR:HB3	23	0.13
(1,34)	1:13:A:CYS:HB2	1:12:A:PRO:HG2	14	0.13
(1,34)	1:13:A:CYS:HB2	1:12:A:PRO:HG2	30	0.13
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG21	5	0.13
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG22	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG23	5	0.13
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	28	0.13
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	28	0.13
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	28	0.13
(1,6)	1:7:A:HIS:HD2	1:6:A:VAL:HB	9	0.13
(1,332)	1:3:A:ILE:HG21	1:4:A:CYS:HA	31	0.12
(1,332)	1:3:A:ILE:HG22	1:4:A:CYS:HA	31	0.12
(1,332)	1:3:A:ILE:HG23	1:4:A:CYS:HA	31	0.12
(1,329)	1:11:A:TRP:HD1	1:6:A:VAL:HB	5	0.12
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB1	8	0.12
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB2	8	0.12
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB3	8	0.12
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB1	15	0.12
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB2	15	0.12
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB3	15	0.12
(1,316)	1:11:A:TRP:HZ2	1:8:A:ARG:HG2	1	0.12
(1,316)	1:11:A:TRP:HZ2	1:8:A:ARG:HG2	2	0.12
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG21	20	0.12
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG22	20	0.12
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG23	20	0.12
(1,299)	1:15:A:TYR:HB3	1:12:A:PRO:HG2	9	0.12
(1,121)	1:7:A:HIS:HD2	1:8:A:ARG:HG2	17	0.12
(1,121)	1:7:A:HIS:HD2	1:8:A:ARG:HG2	24	0.12
(1,97)	1:7:A:HIS:HE1	1:8:A:ARG:HG3	27	0.12
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	11	0.12
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	16	0.12
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	28	0.12
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	30	0.12
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	30	0.12
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	30	0.12
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	16	0.12
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	16	0.12
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	16	0.12
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	31	0.12
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	31	0.12
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	31	0.12
(1,11)	1:15:A:TYR:HE1	1:12:A:PRO:HD3	23	0.12
(1,11)	1:15:A:TYR:HE2	1:12:A:PRO:HD3	23	0.12
(1,6)	1:7:A:HIS:HD2	1:6:A:VAL:HB	7	0.12
(1,345)	1:14:A:ALA:HA	1:13:A:CYS:HB2	12	0.11
(1,339)	1:13:A:CYS:HB2	1:3:A:ILE:HG21	11	0.11
(1,339)	1:13:A:CYS:HB2	1:3:A:ILE:HG22	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:13:A:CYS:HB2	1:3:A:ILE:HG23	11	0.11
(1,335)	1:15:A:TYR:HE1	1:5:A:HIS:HA	25	0.11
(1,335)	1:15:A:TYR:HE2	1:5:A:HIS:HA	25	0.11
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB1	25	0.11
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB2	25	0.11
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB3	25	0.11
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB1	30	0.11
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB2	30	0.11
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB3	30	0.11
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB1	32	0.11
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB2	32	0.11
(1,320)	1:11:A:TRP:HE3	1:14:A:ALA:HB3	32	0.11
(1,316)	1:11:A:TRP:HZ2	1:8:A:ARG:HG2	5	0.11
(1,316)	1:11:A:TRP:HZ2	1:8:A:ARG:HG2	6	0.11
(1,316)	1:11:A:TRP:HZ2	1:8:A:ARG:HG2	23	0.11
(1,316)	1:11:A:TRP:HZ2	1:8:A:ARG:HG2	27	0.11
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG21	34	0.11
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG22	34	0.11
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG23	34	0.11
(1,283)	1:10:A:ASP:H	1:9:A:PRO:HG3	3	0.11
(1,256)	1:15:A:TYR:HE1	1:15:A:TYR:HA	27	0.11
(1,256)	1:15:A:TYR:HE2	1:15:A:TYR:HA	27	0.11
(1,237)	1:11:A:TRP:HD1	1:8:A:ARG:HD2	10	0.11
(1,213)	1:11:A:TRP:HE3	1:11:A:TRP:HA	6	0.11
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG21	2	0.11
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG22	2	0.11
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG23	2	0.11
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG21	9	0.11
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG22	9	0.11
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG23	9	0.11
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG21	16	0.11
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG22	16	0.11
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG23	16	0.11
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG21	20	0.11
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG22	20	0.11
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG23	20	0.11
(1,121)	1:7:A:HIS:HD2	1:8:A:ARG:HG2	29	0.11
(1,97)	1:7:A:HIS:HE1	1:8:A:ARG:HG3	20	0.11
(1,97)	1:7:A:HIS:HE1	1:8:A:ARG:HG3	29	0.11
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	12	0.11
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	17	0.11
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	33	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG21	14	0.11
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG22	14	0.11
(1,47)	1:11:A:TRP:HH2	1:3:A:ILE:HG23	14	0.11
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG11	8	0.11
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG12	8	0.11
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG13	8	0.11
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG11	9	0.11
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG12	9	0.11
(1,42)	1:12:A:PRO:HA	1:6:A:VAL:HG13	9	0.11
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG21	7	0.11
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG22	7	0.11
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG23	7	0.11
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG21	23	0.11
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG22	23	0.11
(1,26)	1:9:A:PRO:HA	1:6:A:VAL:HG23	23	0.11
(1,20)	1:15:A:TYR:HD1	1:2:A:SER:HB3	34	0.11
(1,20)	1:15:A:TYR:HD2	1:2:A:SER:HB3	34	0.11
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	5	0.11
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	5	0.11
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	5	0.11
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	15	0.11
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	15	0.11
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	15	0.11
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB1	27	0.11
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB2	27	0.11
(1,12)	1:13:A:CYS:HB2	1:14:A:ALA:HB3	27	0.11
(1,11)	1:15:A:TYR:HE1	1:12:A:PRO:HD3	34	0.11
(1,11)	1:15:A:TYR:HE2	1:12:A:PRO:HD3	34	0.11
(1,6)	1:7:A:HIS:HD2	1:6:A:VAL:HB	2	0.11
(1,316)	1:11:A:TRP:HZ2	1:8:A:ARG:HG2	8	0.1
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG21	9	0.1
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG22	9	0.1
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG23	9	0.1
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG21	10	0.1
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG22	10	0.1
(1,306)	1:3:A:ILE:H	1:3:A:ILE:HG23	10	0.1
(1,162)	1:11:A:TRP:H	1:9:A:PRO:HG3	24	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG21	4	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG22	4	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG23	4	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG21	10	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG22	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG23	10	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG21	11	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG22	11	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG23	11	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG21	21	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG22	21	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG23	21	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG21	24	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG22	24	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG23	24	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG21	27	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG22	27	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG23	27	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG21	34	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG22	34	0.1
(1,145)	1:3:A:ILE:HA	1:3:A:ILE:HG23	34	0.1
(1,121)	1:7:A:HIS:HD2	1:8:A:ARG:HG2	13	0.1
(1,121)	1:7:A:HIS:HD2	1:8:A:ARG:HG2	20	0.1
(1,121)	1:7:A:HIS:HD2	1:8:A:ARG:HG2	31	0.1
(1,97)	1:7:A:HIS:HE1	1:8:A:ARG:HG3	33	0.1
(1,77)	1:11:A:TRP:HE3	1:8:A:ARG:HG2	6	0.1
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG11	10	0.1
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG12	10	0.1
(1,43)	1:9:A:PRO:HB3	1:6:A:VAL:HG13	10	0.1
(1,38)	1:15:A:TYR:HB3	1:3:A:ILE:HG21	2	0.1
(1,38)	1:15:A:TYR:HB3	1:3:A:ILE:HG22	2	0.1
(1,38)	1:15:A:TYR:HB3	1:3:A:ILE:HG23	2	0.1
(1,38)	1:15:A:TYR:HB3	1:3:A:ILE:HG21	29	0.1
(1,38)	1:15:A:TYR:HB3	1:3:A:ILE:HG22	29	0.1
(1,38)	1:15:A:TYR:HB3	1:3:A:ILE:HG23	29	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found