Full wwPDB NMR Structure Validation Report (i)

Jun 20, 2024 – 04:37 pm BST

PDB ID	:	8RQ6
BMRB ID	:	34893
Title	:	Solution NMR structure of Amyloid beta precursor like protein 2 TMD
Authors	:	Muhle-Goll, C.; Moser, C.
Deposited on	:	2024-01-17

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 (i) 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 (i)) were used in the production of this report:

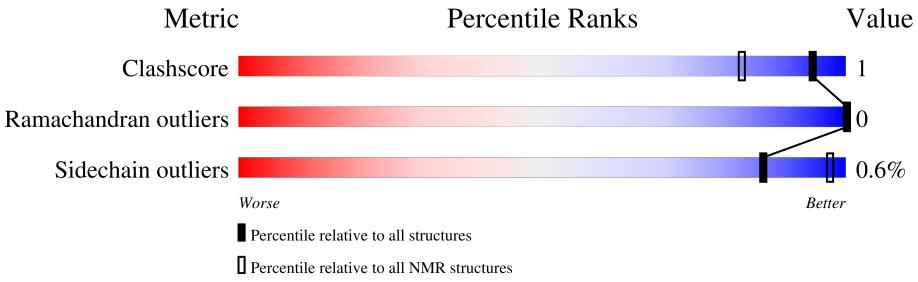
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 77%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	31	52% 48%

2 Ensemble composition and analysis (i)

This entry contains 40 models. Model 32 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:697-A:712 (16)	0.53	32

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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 495 atoms, of which 271 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Amyloid beta precursor like protein 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	31	495	147	271	38	38	1	0

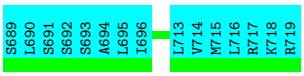
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Amyloid beta precursor like protein 2

Chain A: 



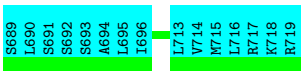
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Amyloid beta precursor like protein 2

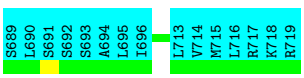
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: Amyloid beta precursor like protein 2

Chain A: 



4.2.3 Score per residue for model 3

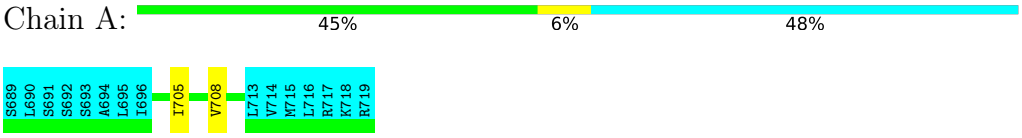
• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.4 Score per residue for model 4

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.6 Score per residue for model 6

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.7 Score per residue for model 7

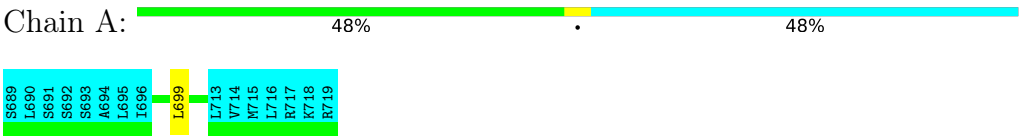
• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.8 Score per residue for model 8

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.10 Score per residue for model 10

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.11 Score per residue for model 11

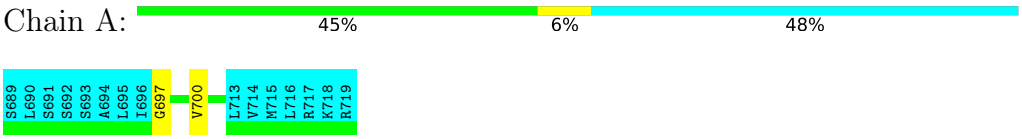
• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.12 Score per residue for model 12

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.14 Score per residue for model 14

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.15 Score per residue for model 15

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.16 Score per residue for model 16

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.17 Score per residue for model 17

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.18 Score per residue for model 18

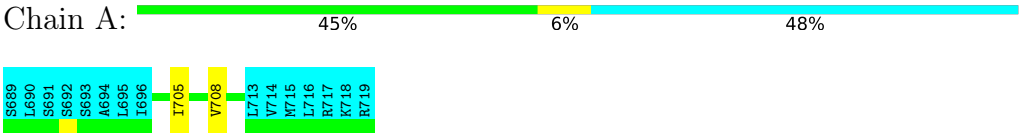
• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.19 Score per residue for model 19

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:



4.2.20 Score per residue for model 20

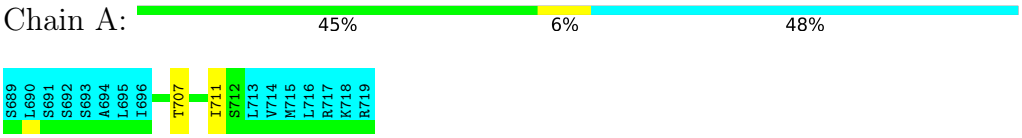
• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.21 Score per residue for model 21

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.23 Score per residue for model 23

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.24 Score per residue for model 24

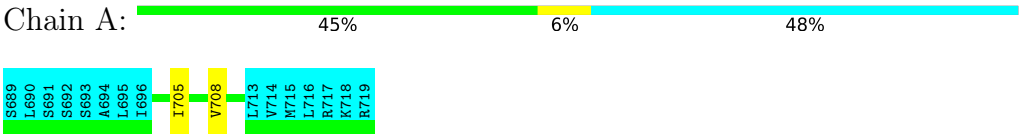
• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.25 Score per residue for model 25

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:



4.2.26 Score per residue for model 26

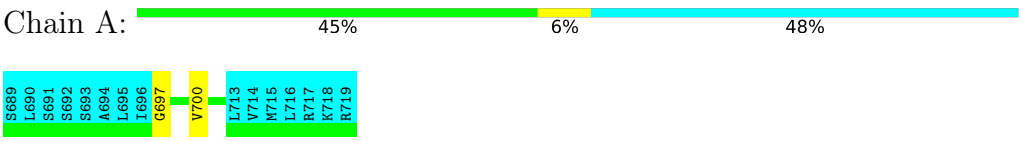
• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.27 Score per residue for model 27

• Molecule 1: Amyloid beta precursor like protein 2

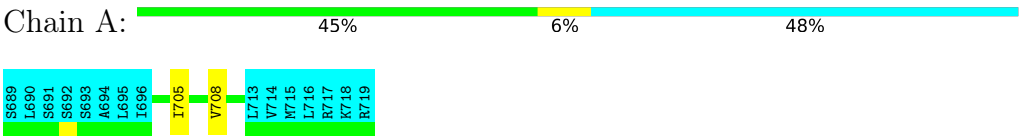
Chain A:



4.2.28 Score per residue for model 28

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:



4.2.29 Score per residue for model 29

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.30 Score per residue for model 30

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.31 Score per residue for model 31

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.32 Score per residue for model 32 (medoid)

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.33 Score per residue for model 33

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.34 Score per residue for model 34

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.35 Score per residue for model 35

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.36 Score per residue for model 36

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.37 Score per residue for model 37

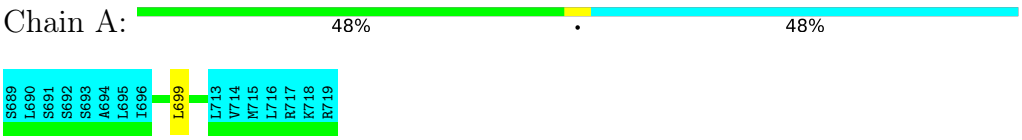
• Molecule 1: Amyloid beta precursor like protein 2

Chain A:

4.2.38 Score per residue for model 38

• Molecule 1: Amyloid beta precursor like protein 2

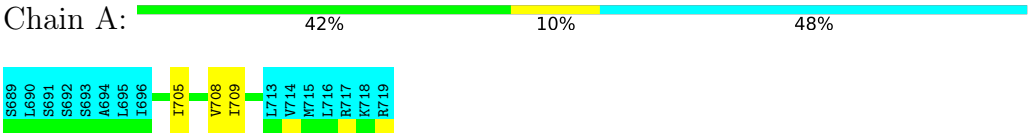
Chain A:



4.2.39 Score per residue for model 39

• Molecule 1: Amyloid beta precursor like protein 2

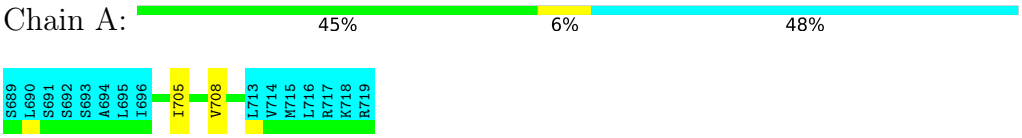
Chain A:



4.2.40 Score per residue for model 40

• Molecule 1: Amyloid beta precursor like protein 2

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 40 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	2.3.2
ARIA	refinement	2.3.2

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	295
Number of shifts mapped to atoms	295
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	108	132	132	0±0
All	All	4320	5280	5280	11

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:705:ILE:O	1:A:708:VAL:HG12	0.56	2.01	39	6
1:A:705:ILE:N	1:A:705:ILE:HD12	0.42	2.28	35	1
1:A:705:ILE:O	1:A:709:ILE:HG13	0.41	2.14	39	1
1:A:697:GLY:O	1:A:700:VAL:HG12	0.41	2.16	27	2
1:A:707:THR:O	1:A:711:ILE:HG12	0.40	2.16	21	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	16/31 (52%)	16±0 (100±1%)	0±0 (0±1%)	0±0 (0±0%)	100	100
All	All	640/1240 (52%)	639 (100%)	1 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	12/26 (46%)	12±0 (99±2%)	0±0 (1±2%)	86	97
All	All	480/1040 (46%)	477 (99%)	3 (1%)	86	97

All 1 unique residues with a non-rotameric sidechain are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	699	LEU	3

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 66% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping

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

Total number of shifts	295
Number of shifts mapped to atoms	295
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	27	-0.03 ± 0.28	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	26	0.94 ± 0.08	Should be checked
$^{13}C'$	0	—	None (insufficient data)
^{15}N	0	—	None (insufficient 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 77%, i.e. 169 atoms were assigned a chemical shift out of a possible 220. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	49/81 (60%)	33/33 (100%)	16/32 (50%)	0/16 (0%)
Sidechain	120/139 (86%)	86/97 (89%)	34/42 (81%)	0/0 (—%)

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	Total	^{1}H	^{13}C	^{15}N
Overall	169/220 (77%)	119/130 (92%)	50/74 (68%)	0/16 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 66%, i.e. 294 atoms were assigned a chemical shift out of a possible 445. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	82/156 (53%)	55/63 (87%)	27/62 (44%)	0/31 (0%)
Sidechain	212/289 (73%)	152/197 (77%)	60/85 (71%)	0/7 (0%)
Overall	294/445 (66%)	207/260 (80%)	87/147 (59%)	0/38 (0%)

7.1.4 Statistically unusual chemical shifts (i)

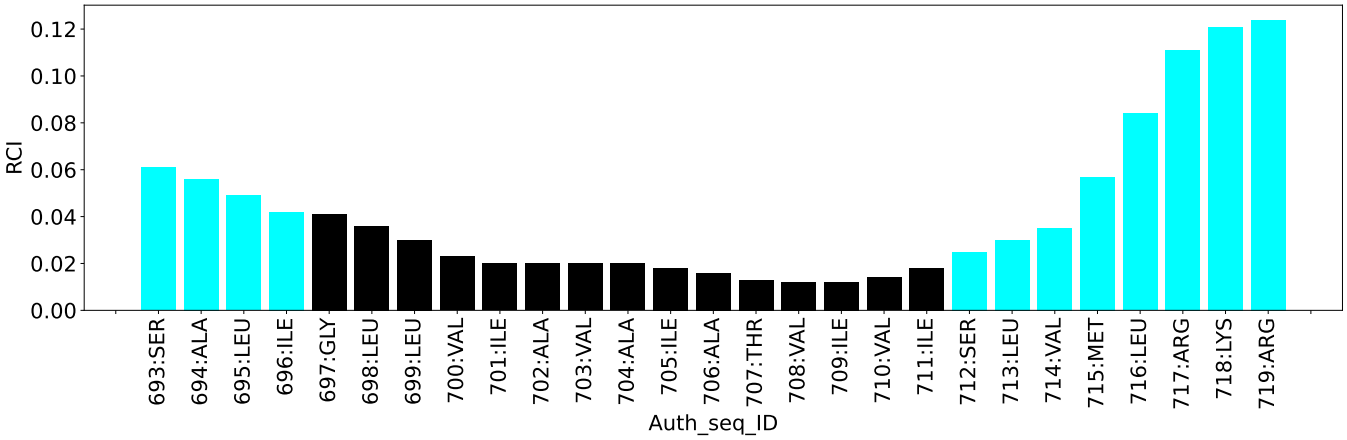
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	707	THR	HG1	5.54	0.08 – 2.19	20.9

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:


RCI
0.12
0.10
0.08
0.06
0.04
0.02
0.00
693:SER
694:ALA
695:LEU
696:ILE
697:GLY
698:LEU
699:LEU
700:VAL
701:ILE
702:ALA
703:VAL
704:ALA
705:ILE
706:ALA
707:THR
708:VAL
709:ILE
710:VAL
711:ILE
712:SER
713:LEU
714:VAL
715:MET
716:LEU
717:ARG
718:LYS
719:ARG
Auth_seq_ID

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	380
Intra-residue (|i-j|=0)	141
Sequential (|i-j|=1)	111
Medium range (|i-j|>1 and |i-j|<5)	127
Long range (|i-j|≥5)	1
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	12.3
Number of long range restraints per residue[1]	0.0

[1]Long 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)	3.5	0.2
0.2-0.5 (Medium)	4.2	0.5
>0.5 (Large)	9.6	4.28

8.2.2 Average number of dihedral-angle violations per model ⓘ

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

9 Distance violation analysis (i)

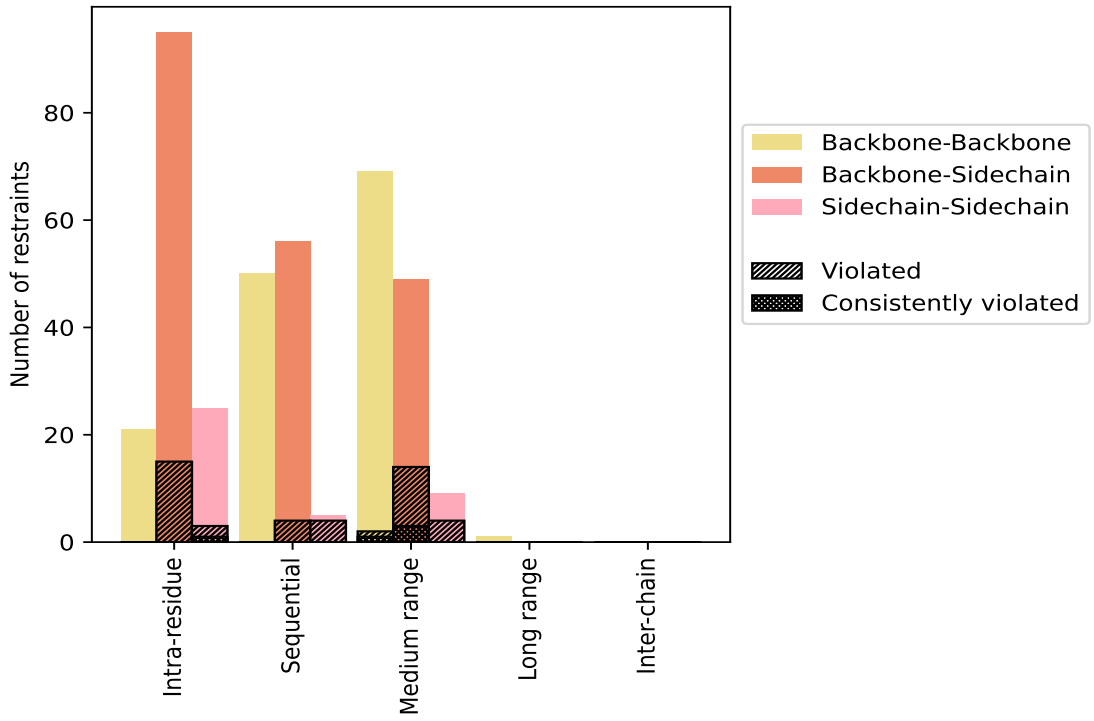
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	141	37.1	18	12.8	4.7	1	0.7	0.3
Backbone-Backbone	21	5.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	95	25.0	15	15.8	3.9	0	0.0	0.0
Sidechain-Sidechain	25	6.6	3	12.0	0.8	1	4.0	0.3
Sequential (|i-j|=1)	111	29.2	8	7.2	2.1	0	0.0	0.0
Backbone-Backbone	50	13.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	56	14.7	4	7.1	1.1	0	0.0	0.0
Sidechain-Sidechain	5	1.3	4	80.0	1.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	127	33.4	20	15.7	5.3	4	3.1	1.1
Backbone-Backbone	69	18.2	2	2.9	0.5	1	1.4	0.3
Backbone-Sidechain	49	12.9	14	28.6	3.7	3	6.1	0.8
Sidechain-Sidechain	9	2.4	4	44.4	1.1	0	0.0	0.0
Long range (|i-j|≥5)	1	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	1	0.3	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
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	380	100.0	46	12.1	12.1	5	1.3	1.3
Backbone-Backbone	141	37.1	2	1.4	0.5	1	0.7	0.3
Backbone-Sidechain	200	52.6	33	16.5	8.7	3	1.5	0.8
Sidechain-Sidechain	39	10.3	11	28.2	2.9	1	2.6	0.3

[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



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

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	7	2	8	0	0	17	1.08	3.82	0.94	0.94
2	4	2	8	0	0	14	0.72	1.74	0.59	0.45
3	4	3	9	0	0	16	0.73	1.81	0.55	0.5
4	4	3	8	0	0	15	0.88	3.4	0.85	0.49
5	6	2	7	0	0	15	1.16	4.2	1.22	0.49
6	7	2	10	0	0	19	0.9	2.25	0.66	0.87
7	7	2	9	0	0	18	1.19	4.09	1.13	0.8
8	5	2	10	0	0	17	0.94	3.26	0.9	0.51
9	6	2	9	0	0	17	0.95	4.16	0.94	0.59
10	4	3	9	0	0	16	0.91	2.94	0.78	0.52

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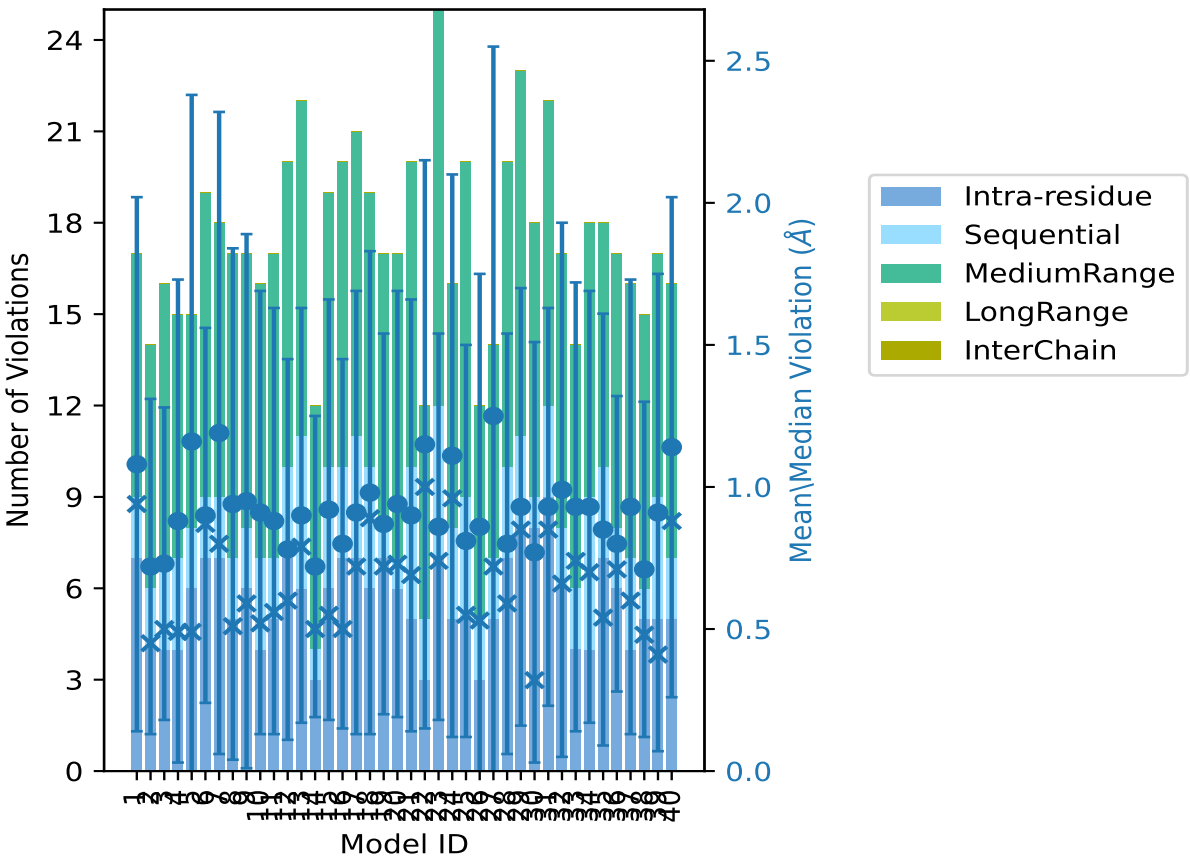
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	5	2	10	0	0	17	0.88	3.12	0.75	0.56
12	7	3	10	0	0	20	0.78	2.26	0.67	0.6
13	6	5	11	0	0	22	0.9	3.24	0.73	0.79
14	3	1	8	0	0	12	0.72	1.59	0.53	0.5
15	6	4	9	0	0	19	0.92	2.75	0.74	0.55
16	7	3	10	0	0	20	0.8	2.1	0.65	0.5
17	7	4	10	0	0	21	0.91	3.09	0.78	0.72
18	6	4	9	0	0	19	0.98	3.42	0.85	0.89
19	7	1	9	0	0	17	0.87	2.6	0.67	0.72
20	6	1	10	0	0	17	0.94	2.78	0.75	0.73
21	5	5	10	0	0	20	0.9	3.22	0.76	0.69
22	3	2	7	0	0	12	1.15	3.96	1.0	1.0
23	7	5	13	0	0	25	0.86	2.75	0.68	0.74
24	5	3	8	0	0	16	1.11	3.48	0.99	0.96
25	5	4	11	0	0	20	0.81	2.69	0.69	0.55
26	3	2	7	0	0	12	0.86	3.4	0.89	0.53
27	5	2	7	0	0	14	1.25	4.28	1.3	0.72
28	7	3	10	0	0	20	0.8	3.37	0.74	0.59
29	8	3	12	0	0	23	0.93	2.87	0.77	0.85
30	8	1	9	0	0	18	0.77	2.68	0.74	0.32
31	9	3	10	0	0	22	0.93	2.78	0.7	0.85
32	6	2	9	0	0	17	0.99	3.64	0.94	0.66
33	4	2	8	0	0	14	0.93	3.24	0.79	0.74
34	4	5	9	0	0	18	0.93	3.2	0.76	0.7
35	7	3	8	0	0	18	0.85	2.66	0.76	0.54
36	6	2	9	0	0	17	0.8	2.09	0.52	0.71
37	4	3	9	0	0	16	0.93	3.06	0.8	0.6
38	5	1	9	0	0	15	0.71	2.16	0.59	0.48
39	5	4	8	0	0	17	0.91	3.03	0.84	0.41
40	5	2	9	0	0	16	1.14	3.21	0.88	0.88

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard 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, 334(IR:123, SQ:103, MR:107, LR:1, 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]	%
2	1	1	0	0	4	1	2.5
2	0	1	0	0	3	2	5.0
4	0	3	0	0	7	3	7.5
2	0	0	0	0	2	4	10.0
0	0	1	0	0	1	5	12.5
1	0	1	0	0	2	6	15.0

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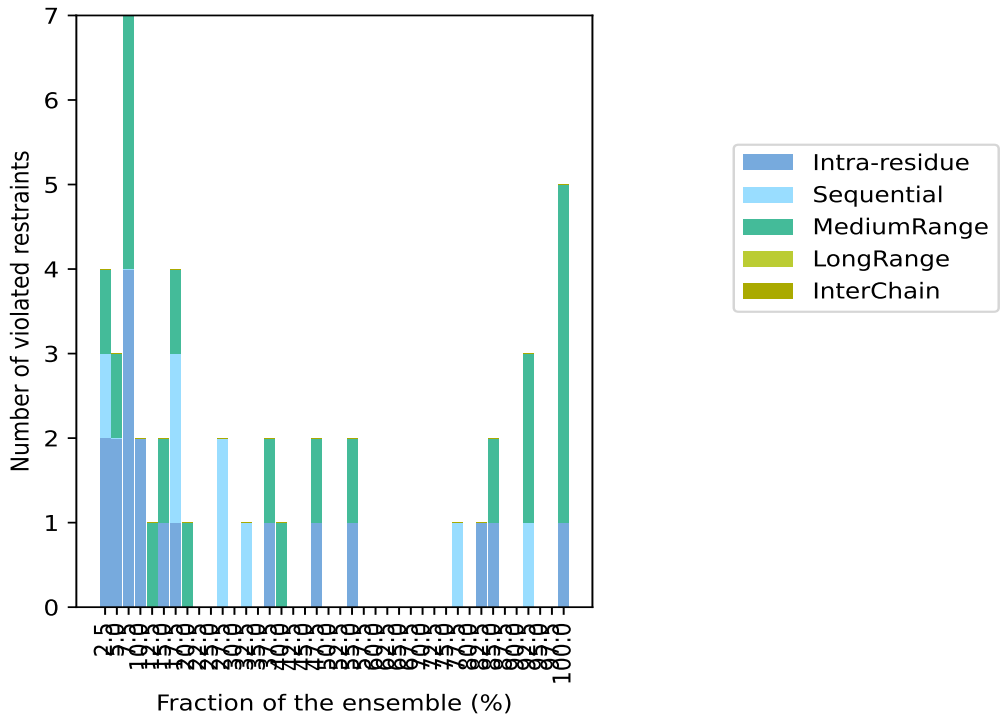
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
1	2	1	0	0	4	7	17.5
0	0	1	0	0	1	8	20.0
0	0	0	0	0	0	9	22.5
0	0	0	0	0	0	10	25.0
0	2	0	0	0	2	11	27.5
0	0	0	0	0	0	12	30.0
0	1	0	0	0	1	13	32.5
0	0	0	0	0	0	14	35.0
1	0	1	0	0	2	15	37.5
0	0	1	0	0	1	16	40.0
0	0	0	0	0	0	17	42.5
0	0	0	0	0	0	18	45.0
1	0	1	0	0	2	19	47.5
0	0	0	0	0	0	20	50.0
0	0	0	0	0	0	21	52.5
1	0	1	0	0	2	22	55.0
0	0	0	0	0	0	23	57.5
0	0	0	0	0	0	24	60.0
0	0	0	0	0	0	25	62.5
0	0	0	0	0	0	26	65.0
0	0	0	0	0	0	27	67.5
0	0	0	0	0	0	28	70.0
0	0	0	0	0	0	29	72.5
0	0	0	0	0	0	30	75.0
0	1	0	0	0	1	31	77.5
0	0	0	0	0	0	32	80.0
1	0	0	0	0	1	33	82.5
1	0	1	0	0	2	34	85.0
0	0	0	0	0	0	35	87.5
0	0	0	0	0	0	36	90.0
0	1	2	0	0	3	37	92.5
0	0	0	0	0	0	38	95.0
0	0	0	0	0	0	39	97.5
1	0	4	0	0	5	40	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

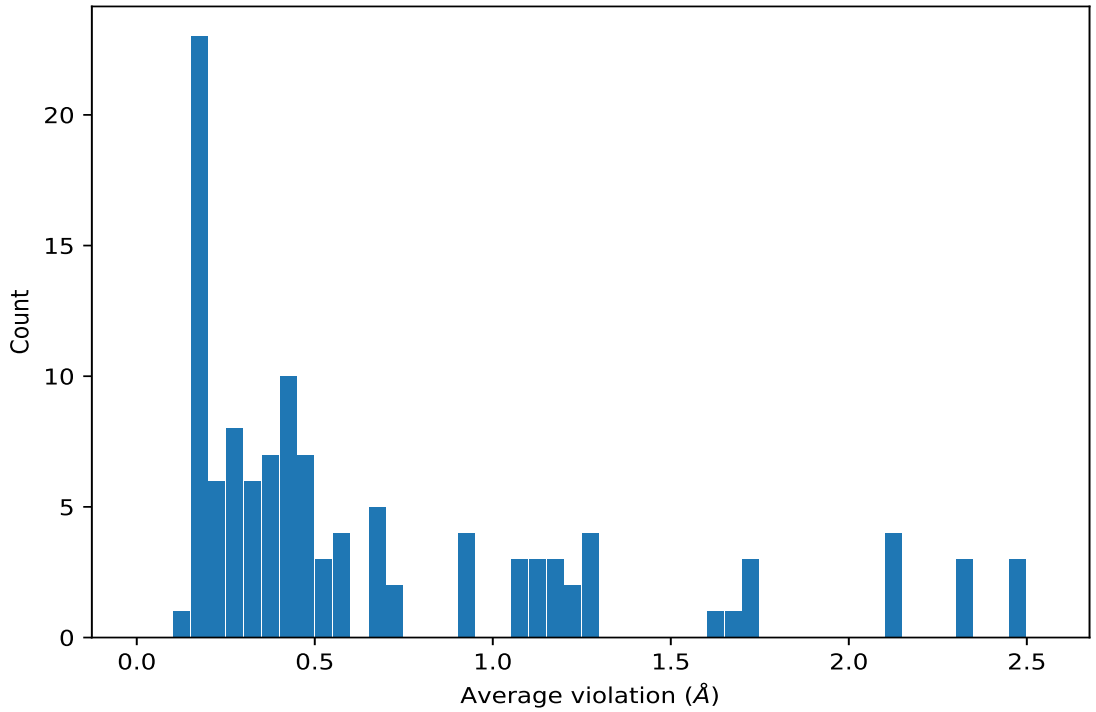
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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

The following table provides the mean and the standard deviation of theviolation 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)
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	40	2.33	0.94	2.06
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	40	2.33	0.94	2.06
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	40	2.33	0.94	2.06
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	40	1.65	0.04	1.66
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	40	1.61	0.5	1.56
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	40	0.68	0.35	0.53
(1,316)	1:711:A:ILE:HG23	1:711:A:ILE:HD13	40	0.19	0.03	0.2
(1,316)	1:709:A:ILE:HG23	1:709:A:ILE:HD12	40	0.19	0.03	0.2
(1,316)	1:711:A:ILE:HG23	1:711:A:ILE:HD11	40	0.19	0.03	0.2
(1,316)	1:711:A:ILE:HG21	1:711:A:ILE:HD12	40	0.19	0.03	0.2
(1,316)	1:711:A:ILE:HG22	1:711:A:ILE:HD13	40	0.19	0.03	0.2
(1,316)	1:711:A:ILE:HG22	1:711:A:ILE:HD11	40	0.19	0.03	0.2
(1,316)	1:709:A:ILE:HG21	1:709:A:ILE:HD11	40	0.19	0.03	0.2
(1,316)	1:709:A:ILE:HG21	1:709:A:ILE:HD13	40	0.19	0.03	0.2
(1,316)	1:709:A:ILE:HG21	1:709:A:ILE:HD12	40	0.19	0.03	0.2
(1,316)	1:709:A:ILE:HG23	1:709:A:ILE:HD13	40	0.19	0.03	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,316)	1:711:A:ILE:HG22	1:711:A:ILE:HD12	40	0.19	0.03	0.2
(1,316)	1:711:A:ILE:HG23	1:711:A:ILE:HD12	40	0.19	0.03	0.2
(1,316)	1:711:A:ILE:HG21	1:711:A:ILE:HD11	40	0.19	0.03	0.2
(1,316)	1:709:A:ILE:HG22	1:709:A:ILE:HD13	40	0.19	0.03	0.2
(1,316)	1:711:A:ILE:HG21	1:711:A:ILE:HD13	40	0.19	0.03	0.2
(1,316)	1:709:A:ILE:HG22	1:709:A:ILE:HD11	40	0.19	0.03	0.2
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	37	1.16	0.36	1.16
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	37	1.16	0.36	1.16
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	37	1.16	0.36	1.16
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG21	37	0.4	0.12	0.4
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG23	37	0.4	0.12	0.4
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG22	37	0.4	0.12	0.4
(1,295)	1:702:A:ALA:HA	1:699:A:LEU:HD12	37	0.4	0.12	0.4
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	37	0.39	0.18	0.41
(1,328)	1:707:A:THR:HG22	1:705:A:ILE:HA	37	0.39	0.18	0.41
(1,328)	1:707:A:THR:HG21	1:705:A:ILE:HA	37	0.39	0.18	0.41
(1,328)	1:707:A:THR:HG21	1:703:A:VAL:HA	37	0.39	0.18	0.41
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	34	0.9	0.09	0.9
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	34	0.16	0.02	0.16
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	33	0.2	0.0	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	33	0.2	0.0	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	33	0.2	0.0	0.2
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	31	2.14	1.35	2.87
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG11	22	1.25	0.25	1.26
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG12	22	1.25	0.25	1.26
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG13	22	1.25	0.25	1.26
(1,293)	1:707:A:THR:HG1	1:703:A:VAL:HG12	22	1.25	0.25	1.26
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	22	0.49	0.0	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	22	0.49	0.0	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	22	0.49	0.0	0.49
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	19	1.08	0.0	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	19	1.08	0.0	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	19	1.08	0.0	1.08
(1,329)	1:703:A:VAL:HA	1:703:A:VAL:HG22	19	0.26	0.11	0.33
(1,329)	1:705:A:ILE:HA	1:708:A:VAL:HG11	19	0.26	0.11	0.33
(1,329)	1:703:A:VAL:HA	1:703:A:VAL:HG21	19	0.26	0.11	0.33
(1,329)	1:705:A:ILE:HA	1:708:A:VAL:HG12	19	0.26	0.11	0.33
(1,329)	1:705:A:ILE:HA	1:708:A:VAL:HG13	19	0.26	0.11	0.33
(1,329)	1:703:A:VAL:HA	1:703:A:VAL:HG23	19	0.26	0.11	0.33
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	16	0.52	0.2	0.52
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	16	0.52	0.2	0.52
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	16	0.52	0.2	0.52

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG11	15	2.14	0.1	2.14
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG12	15	2.14	0.1	2.14
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG13	15	2.14	0.1	2.14
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG11	15	0.94	0.01	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG12	15	0.94	0.01	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG13	15	0.94	0.01	0.94
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG11	13	0.57	0.34	0.38
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG12	13	0.57	0.34	0.38
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG13	13	0.57	0.34	0.38
(1,311)	1:709:A:ILE:HG13	1:709:A:ILE:HG22	11	0.21	0.01	0.21
(1,311)	1:709:A:ILE:HG13	1:709:A:ILE:HG21	11	0.21	0.01	0.21
(1,311)	1:709:A:ILE:HG13	1:709:A:ILE:HG23	11	0.21	0.01	0.21
(1,233)	1:710:A:VAL:H	1:709:A:ILE:HG13	11	0.16	0.07	0.12
(1,233)	1:704:A:ALA:H	1:703:A:VAL:HG21	11	0.16	0.07	0.12
(1,233)	1:704:A:ALA:H	1:703:A:VAL:HG23	11	0.16	0.07	0.12
(1,220)	1:719:A:ARG:H	1:717:A:ARG:HA	8	0.27	0.1	0.24
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG11	7	1.73	0.25	1.72
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG12	7	1.73	0.25	1.72
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG13	7	1.73	0.25	1.72
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG11	7	1.13	0.01	1.13
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG12	7	1.13	0.01	1.13
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG13	7	1.13	0.01	1.13
(1,269)	1:700:A:VAL:HG11	1:699:A:LEU:HA	7	0.4	0.03	0.41
(1,269)	1:700:A:VAL:HG12	1:699:A:LEU:HA	7	0.4	0.03	0.41
(1,269)	1:700:A:VAL:HG13	1:699:A:LEU:HA	7	0.4	0.03	0.41
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG11	7	0.32	0.14	0.35
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG12	7	0.32	0.14	0.35
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG13	7	0.32	0.14	0.35
(1,256)	1:713:A:LEU:HD11	1:716:A:LEU:HB2	6	2.49	0.52	2.72
(1,256)	1:713:A:LEU:HD12	1:716:A:LEU:HB2	6	2.49	0.52	2.72
(1,256)	1:713:A:LEU:HD13	1:716:A:LEU:HB2	6	2.49	0.52	2.72
(1,270)	1:713:A:LEU:HD11	1:713:A:LEU:HA	6	0.66	0.2	0.74
(1,270)	1:713:A:LEU:HD12	1:713:A:LEU:HA	6	0.66	0.2	0.74
(1,270)	1:713:A:LEU:HD13	1:713:A:LEU:HA	6	0.66	0.2	0.74
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG11	5	0.32	0.12	0.29
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG12	5	0.32	0.12	0.29
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG13	5	0.32	0.12	0.29
(1,336)	1:718:A:LYS:H	1:718:A:LYS:HD3	4	0.59	0.34	0.56
(1,309)	1:699:A:LEU:HB3	1:699:A:LEU:HD21	4	0.48	0.0	0.48
(1,309)	1:699:A:LEU:HB3	1:699:A:LEU:HD22	4	0.48	0.0	0.48
(1,309)	1:699:A:LEU:HB3	1:699:A:LEU:HD23	4	0.48	0.0	0.48
(2,37)	1:707:A:THR:HG1	1:709:A:ILE:HG13	3	1.21	0.04	1.21

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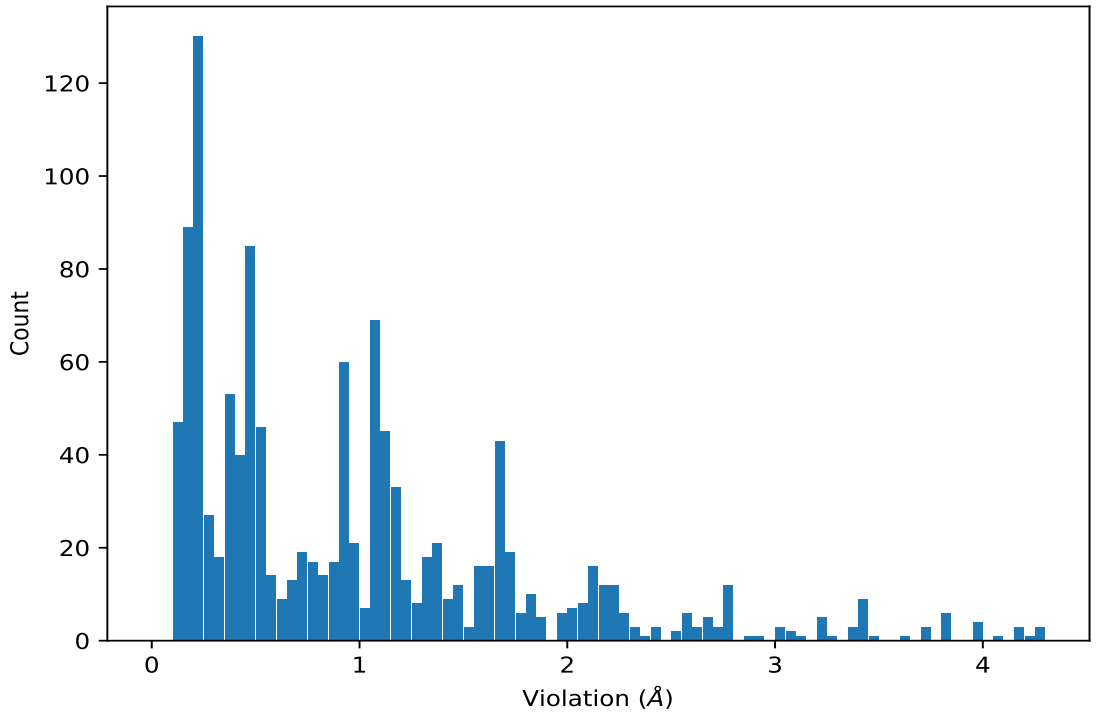
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,232)	1:711:A:ILE:H	1:709:A:ILE:HG13	3	1.2	0.01	1.21
(1,299)	1:709:A:ILE:HA	1:709:A:ILE:HG13	3	0.66	0.02	0.67
(1,228)	1:698:A:LEU:H	1:698:A:LEU:HB2	3	0.46	0.01	0.46
(1,113)	1:709:A:ILE:H	1:709:A:ILE:HG13	3	0.26	0.03	0.26
(1,235)	1:699:A:LEU:H	1:696:A:ILE:HG23	3	0.18	0.02	0.18
(1,235)	1:699:A:LEU:H	1:698:A:LEU:HD11	3	0.18	0.02	0.18
(1,235)	1:699:A:LEU:H	1:696:A:ILE:HG21	3	0.18	0.02	0.18
(1,110)	1:696:A:ILE:H	1:696:A:ILE:HG12	3	0.1	0.0	0.1
(1,297)	1:716:A:LEU:HA	1:716:A:LEU:HD23	2	0.71	0.11	0.71
(1,297)	1:695:A:LEU:HA	1:695:A:LEU:HD11	2	0.71	0.11	0.71
(1,310)	1:716:A:LEU:HB3	1:716:A:LEU:HD21	2	0.42	0.0	0.42
(1,310)	1:716:A:LEU:HB3	1:716:A:LEU:HD22	2	0.42	0.0	0.42
(1,310)	1:716:A:LEU:HB3	1:716:A:LEU:HD23	2	0.42	0.0	0.42
(1,236)	1:697:A:GLY:H	1:700:A:VAL:HG11	2	0.38	0.18	0.38
(1,236)	1:697:A:GLY:H	1:700:A:VAL:HG12	2	0.38	0.18	0.38
(1,236)	1:697:A:GLY:H	1:700:A:VAL:HG13	2	0.38	0.18	0.38

[1]Number of violated models, [2]Standard 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)
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	27	4.28
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	27	4.28
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	27	4.28
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	5	4.2
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	9	4.16
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	9	4.16
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	9	4.16
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	7	4.09
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	22	3.96
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	22	3.96
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	22	3.96
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	27	3.96
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	1	3.82
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	1	3.82
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	1	3.82
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	5	3.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	5	3.81
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	5	3.81
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	7	3.73
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	7	3.73
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	7	3.73
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	32	3.64
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	24	3.48
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	18	3.42
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	18	3.42
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	18	3.42
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	4	3.4
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	4	3.4
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	4	3.4
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	26	3.4
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	26	3.4
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	26	3.4
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	28	3.37
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	28	3.37
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	28	3.37
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	8	3.26
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	13	3.24
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	33	3.24
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	21	3.22
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	40	3.21
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	34	3.2
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	11	3.12
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	17	3.09
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	37	3.06
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	39	3.03
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	39	3.03
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	39	3.03
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	10	2.94
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	29	2.87
(1,256)	1:713:A:LEU:HD11	1:716:A:LEU:HB2	20	2.78
(1,256)	1:713:A:LEU:HD12	1:716:A:LEU:HB2	20	2.78
(1,256)	1:713:A:LEU:HD13	1:716:A:LEU:HB2	20	2.78
(1,256)	1:713:A:LEU:HD11	1:716:A:LEU:HB2	31	2.78
(1,256)	1:713:A:LEU:HD12	1:716:A:LEU:HB2	31	2.78
(1,256)	1:713:A:LEU:HD13	1:716:A:LEU:HB2	31	2.78
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	15	2.75
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	15	2.75
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	15	2.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:713:A:LEU:HD11	1:716:A:LEU:HB2	23	2.75
(1,256)	1:713:A:LEU:HD12	1:716:A:LEU:HB2	23	2.75
(1,256)	1:713:A:LEU:HD13	1:716:A:LEU:HB2	23	2.75
(1,256)	1:713:A:LEU:HD11	1:716:A:LEU:HB2	40	2.7
(1,256)	1:713:A:LEU:HD12	1:716:A:LEU:HB2	40	2.7
(1,256)	1:713:A:LEU:HD13	1:716:A:LEU:HB2	40	2.7
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	25	2.69
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	30	2.68
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	35	2.66
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	35	2.66
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	35	2.66
(1,256)	1:713:A:LEU:HD11	1:716:A:LEU:HB2	19	2.6
(1,256)	1:713:A:LEU:HD12	1:716:A:LEU:HB2	19	2.6
(1,256)	1:713:A:LEU:HD13	1:716:A:LEU:HB2	19	2.6
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	24	2.57
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	24	2.57
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	24	2.57
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	32	2.57
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	32	2.57
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	32	2.57
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	8	2.53
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	15	2.5
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	29	2.42
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	29	2.42
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	29	2.42
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	39	2.38
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG11	31	2.3
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG12	31	2.3
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG13	31	2.3
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG11	12	2.26
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG12	12	2.26
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG13	12	2.26
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG11	6	2.25
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG12	6	2.25
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG13	6	2.25
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG11	18	2.24
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG12	18	2.24
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG13	18	2.24
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG11	25	2.23
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG12	25	2.23
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG13	25	2.23
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG11	17	2.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG12	17	2.2
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG13	17	2.2
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG11	27	2.2
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG12	27	2.2
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG13	27	2.2
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	12	2.19
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	12	2.19
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	12	2.19
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	6	2.18
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	6	2.18
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	6	2.18
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG11	7	2.18
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG12	7	2.18
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG13	7	2.18
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	38	2.16
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	38	2.16
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	38	2.16
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG11	29	2.14
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG12	29	2.14
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG13	29	2.14
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG11	8	2.12
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG12	8	2.12
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG13	8	2.12
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG11	30	2.12
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG12	30	2.12
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG13	30	2.12
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	17	2.11
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	17	2.11
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	17	2.11
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	16	2.1
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG11	35	2.1
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG12	35	2.1
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG13	35	2.1
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	36	2.09
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	40	2.06
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG11	20	2.05
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG12	20	2.05
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG13	20	2.05
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG11	24	2.05
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG12	24	2.05
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG13	24	2.05
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	24	2.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	37	2.01
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	37	2.01
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	37	2.01
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	11	2.0
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	11	2.0
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	11	2.0
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG11	16	1.98
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG12	16	1.98
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG13	16	1.98
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG11	1	1.95
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG12	1	1.95
(1,112)	1:705:A:ILE:H	1:708:A:VAL:HG13	1	1.95
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	12	1.87
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	12	1.87
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	12	1.87
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	1	1.86
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	22	1.86
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	10	1.83
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	10	1.83
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	10	1.83
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	1	1.81
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	3	1.81
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	3	1.81
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	3	1.81
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG11	39	1.81
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG12	39	1.81
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG13	39	1.81
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG11	23	1.79
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG12	23	1.79
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG13	23	1.79
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	13	1.78
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	23	1.78
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	10	1.76
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	2	1.74
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	2	1.74
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	2	1.74
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	21	1.73
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	21	1.73
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	21	1.73
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	18	1.72
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	35	1.72
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	23	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	23	1.72
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	23	1.72
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG11	15	1.72
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG12	15	1.72
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG13	15	1.72
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	20	1.71
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	20	1.71
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	20	1.71
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	25	1.71
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	1	1.7
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	7	1.69
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	16	1.69
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	16	1.69
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	16	1.69
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	18	1.69
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	18	1.69
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	18	1.69
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	10	1.69
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	16	1.69
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	19	1.69
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	23	1.69
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	31	1.69
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	5	1.68
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	19	1.68
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	19	1.68
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	19	1.68
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG11	13	1.68
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG12	13	1.68
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG13	13	1.68
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	5	1.68
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	7	1.68
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	9	1.68
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	30	1.68
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	39	1.68
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	40	1.68
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	11	1.67
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	13	1.67
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	15	1.67
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	26	1.67
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	32	1.67
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	35	1.67
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG11	1	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	3	1.66
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	4	1.66
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	6	1.66
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	8	1.66
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	33	1.66
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	34	1.66
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	37	1.65
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	37	1.65
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	37	1.65
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	2	1.65
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	36	1.65
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	6	1.64
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	6	1.64
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	6	1.64
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	23	1.64
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	17	1.64
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	18	1.64
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	20	1.64
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	28	1.64
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	21	1.63
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	34	1.63
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	22	1.63
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	12	1.62
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG11	4	1.61
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG11	29	1.61
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG13	31	1.61
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	21	1.61
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	14	1.59
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	24	1.59
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	37	1.59
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	2	1.58
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	38	1.58
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	17	1.57
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	17	1.57
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	17	1.57
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	27	1.57
(1,215)	1:715:A:MET:HB3	1:713:A:LEU:HA	29	1.57
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	32	1.56
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	32	1.56
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	32	1.56
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	24	1.55
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	24	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	24	1.55
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	34	1.54
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	3	1.53
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	20	1.53
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG11	21	1.49
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG12	21	1.49
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG13	21	1.49
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG11	7	1.49
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	40	1.48
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	40	1.48
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	40	1.48
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG11	16	1.47
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	36	1.46
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	36	1.46
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	36	1.46
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	9	1.45
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	19	1.43
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	33	1.43
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	33	1.43
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	33	1.43
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	14	1.42
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	14	1.42
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	14	1.42
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	14	1.42
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	6	1.41
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	38	1.39
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG11	34	1.39
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG12	34	1.39
(1,302)	1:697:A:GLY:HA2	1:700:A:VAL:HG13	34	1.39
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	9	1.38
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	18	1.38
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	40	1.37
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	40	1.37
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	40	1.37
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	22	1.37
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	22	1.37
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	22	1.37
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG11	9	1.37
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	35	1.36
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	28	1.35
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	33	1.35
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	33	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	33	1.35
(1,256)	1:713:A:LEU:HD11	1:716:A:LEU:HB2	37	1.35
(1,256)	1:713:A:LEU:HD12	1:716:A:LEU:HB2	37	1.35
(1,256)	1:713:A:LEU:HD13	1:716:A:LEU:HB2	37	1.35
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	13	1.34
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	13	1.34
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	13	1.34
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	34	1.33
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	34	1.33
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	34	1.33
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG12	32	1.33
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	31	1.32
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	25	1.32
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	25	1.32
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	25	1.32
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	31	1.32
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	31	1.32
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	31	1.32
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	27	1.31
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	27	1.31
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	27	1.31
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	4	1.3
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	32	1.28
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG13	6	1.28
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG12	10	1.28
(2,37)	1:707:A:THR:HG1	1:709:A:ILE:HG13	31	1.27
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	17	1.26
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG13	22	1.26
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG11	25	1.26
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG13	5	1.25
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	22	1.23
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	21	1.23
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG12	13	1.22
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	29	1.21
(2,37)	1:707:A:THR:HG1	1:709:A:ILE:HG13	29	1.21
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	30	1.21
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	30	1.21
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	30	1.21
(1,232)	1:711:A:ILE:H	1:709:A:ILE:HG13	28	1.21
(1,232)	1:711:A:ILE:H	1:709:A:ILE:HG13	31	1.21
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	14	1.2
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	14	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	14	1.2
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	35	1.19
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	35	1.19
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	35	1.19
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	4	1.18
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	4	1.18
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	4	1.18
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	11	1.18
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	11	1.18
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	11	1.18
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	28	1.18
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	28	1.18
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	28	1.18
(1,232)	1:711:A:ILE:H	1:709:A:ILE:HG13	29	1.18
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	7	1.17
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	7	1.17
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	7	1.17
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	15	1.17
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	37	1.16
(2,37)	1:707:A:THR:HG1	1:709:A:ILE:HG13	28	1.16
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	3	1.16
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	3	1.16
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	3	1.16
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	19	1.16
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	19	1.16
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	19	1.16
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	20	1.16
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	20	1.16
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	20	1.16
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	26	1.15
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG12	23	1.15
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG11	39	1.15
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG12	39	1.15
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG13	39	1.15
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG11	13	1.14
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG12	13	1.14
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG13	13	1.14
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG13	19	1.14
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	31	1.13
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	31	1.13
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	31	1.13
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG11	15	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG12	15	1.13
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG13	15	1.13
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG11	21	1.13
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG12	21	1.13
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG13	21	1.13
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG11	23	1.13
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG12	23	1.13
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG13	23	1.13
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG11	25	1.13
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG12	25	1.13
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG13	25	1.13
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG11	34	1.13
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG12	34	1.13
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG13	34	1.13
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	1	1.12
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	1	1.12
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	1	1.12
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	9	1.12
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	9	1.12
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	9	1.12
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	10	1.12
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	10	1.12
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	10	1.12
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	29	1.12
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	29	1.12
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	29	1.12
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG11	13	1.12
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG12	13	1.12
(1,119)	1:700:A:VAL:H	1:700:A:VAL:HG13	13	1.12
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	2	1.11
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	2	1.11
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	2	1.11
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG12	3	1.11
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	26	1.1
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	26	1.1
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	26	1.1
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	6	1.1
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	5	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	5	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	5	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	9	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	9	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	9	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	13	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	13	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	13	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	16	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	16	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	16	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	18	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	18	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	18	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	21	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	21	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	21	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	32	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	32	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	32	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	36	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	36	1.09
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	36	1.09
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	18	1.09
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	24	1.09
(1,336)	1:718:A:LYS:H	1:718:A:LYS:HD3	29	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	1	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	1	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	1	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	2	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	2	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	2	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	6	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	6	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	6	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	7	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	7	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	7	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	15	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	15	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	15	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	19	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	19	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	19	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	23	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	23	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	23	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	30	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	30	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	30	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	38	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	38	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	38	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	39	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	39	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	39	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG11	40	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG12	40	1.08
(1,118)	1:714:A:VAL:H	1:714:A:VAL:HG13	40	1.08
(1,342)	1:695:A:LEU:HD21	1:698:A:LEU:HA	8	1.06
(1,342)	1:695:A:LEU:HD22	1:698:A:LEU:HA	8	1.06
(1,342)	1:695:A:LEU:HD23	1:698:A:LEU:HA	8	1.06
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	16	1.06
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	16	1.06
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	16	1.06
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	5	1.05
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	5	1.05
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	5	1.05
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG13	11	1.03
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	28	1.03
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	30	1.02
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	30	1.02
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	30	1.02
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	39	1.02
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	33	1.0
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	15	0.98
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	24	0.97
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG13	12	0.96
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	35	0.96
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	40	0.96
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	39	0.95
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG11	23	0.95
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG12	23	0.95
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG13	23	0.95
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG11	18	0.95
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG12	18	0.95
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG13	18	0.95
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG11	30	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG12	30	0.95
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG13	30	0.95
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG11	31	0.95
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG12	31	0.95
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG13	31	0.95
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG11	35	0.95
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG12	35	0.95
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG13	35	0.95
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	11	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG11	1	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG12	1	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG13	1	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG11	8	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG12	8	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG13	8	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG11	20	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG12	20	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG13	20	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG11	24	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG12	24	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG13	24	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG11	27	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG12	27	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG13	27	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG11	29	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG12	29	0.94
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG13	29	0.94
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	21	0.94
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	30	0.94
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	31	0.94
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	38	0.93
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	38	0.93
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	38	0.93
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG13	36	0.93
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG11	6	0.93
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG12	6	0.93
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG13	6	0.93
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG11	7	0.93
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG12	7	0.93
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG13	7	0.93
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG11	12	0.93
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG12	12	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG13	12	0.93
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG11	16	0.93
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG12	16	0.93
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG13	16	0.93
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG11	17	0.93
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG12	17	0.93
(1,115)	1:708:A:VAL:H	1:708:A:VAL:HG13	17	0.93
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	34	0.93
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	13	0.92
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	33	0.92
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG11	15	0.92
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG12	15	0.92
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG13	15	0.92
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	4	0.92
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	17	0.91
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG11	21	0.91
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG12	21	0.91
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG13	21	0.91
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	3	0.91
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	23	0.91
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	36	0.91
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	36	0.9
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	36	0.9
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	36	0.9
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	8	0.9
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	12	0.9
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	33	0.89
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	18	0.89
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	36	0.89
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG11	34	0.89
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG12	34	0.89
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG13	34	0.89
(1,293)	1:707:A:THR:HG1	1:710:A:VAL:HG13	17	0.89
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	32	0.88
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	14	0.88
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	2	0.87
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	6	0.87
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	16	0.87
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	38	0.87
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	11	0.86
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	25	0.85
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	26	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	29	0.85
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	19	0.84
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	20	0.84
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	4	0.83
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	10	0.83
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	28	0.82
(1,297)	1:716:A:LEU:HA	1:716:A:LEU:HD23	17	0.82
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	37	0.82
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	8	0.81
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	8	0.81
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	8	0.81
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	23	0.8
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	40	0.8
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	40	0.8
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	40	0.8
(1,328)	1:707:A:THR:HG21	1:703:A:VAL:HA	13	0.79
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	13	0.79
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	9	0.78
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	9	0.78
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	9	0.78
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	22	0.76
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	27	0.76
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	37	0.76
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	40	0.76
(1,328)	1:707:A:THR:HG22	1:705:A:ILE:HA	11	0.76
(1,270)	1:713:A:LEU:HD11	1:713:A:LEU:HA	31	0.76
(1,270)	1:713:A:LEU:HD12	1:713:A:LEU:HA	31	0.76
(1,270)	1:713:A:LEU:HD13	1:713:A:LEU:HA	31	0.76
(1,270)	1:713:A:LEU:HD11	1:713:A:LEU:HA	40	0.76
(1,270)	1:713:A:LEU:HD12	1:713:A:LEU:HA	40	0.76
(1,270)	1:713:A:LEU:HD13	1:713:A:LEU:HA	40	0.76
(1,212)	1:713:A:LEU:HB3	1:710:A:VAL:HA	18	0.75
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	12	0.74
(1,270)	1:713:A:LEU:HD11	1:713:A:LEU:HA	23	0.74
(1,270)	1:713:A:LEU:HD12	1:713:A:LEU:HA	23	0.74
(1,270)	1:713:A:LEU:HD13	1:713:A:LEU:HA	23	0.74
(1,270)	1:713:A:LEU:HD11	1:713:A:LEU:HA	20	0.73
(1,270)	1:713:A:LEU:HD12	1:713:A:LEU:HA	20	0.73
(1,270)	1:713:A:LEU:HD13	1:713:A:LEU:HA	20	0.73
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	12	0.72
(1,270)	1:713:A:LEU:HD11	1:713:A:LEU:HA	19	0.72
(1,270)	1:713:A:LEU:HD12	1:713:A:LEU:HA	19	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:713:A:LEU:HD13	1:713:A:LEU:HA	19	0.72
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	17	0.72
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	36	0.71
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	36	0.71
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	36	0.71
(1,293)	1:707:A:THR:HG1	1:703:A:VAL:HG12	28	0.7
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	20	0.7
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	20	0.7
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	20	0.7
(1,299)	1:709:A:ILE:HA	1:709:A:ILE:HG13	28	0.69
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	27	0.68
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	27	0.68
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	27	0.68
(1,328)	1:707:A:THR:HG21	1:705:A:ILE:HA	36	0.67
(1,299)	1:709:A:ILE:HA	1:709:A:ILE:HG13	31	0.67
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	7	0.66
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	7	0.66
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	7	0.66
(1,95)	1:699:A:LEU:H	1:695:A:LEU:HB2	32	0.66
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG11	12	0.65
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG12	12	0.65
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG13	12	0.65
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG21	17	0.64
(1,299)	1:709:A:ILE:HA	1:709:A:ILE:HG13	29	0.63
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	3	0.62
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	13	0.62
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	13	0.62
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	13	0.62
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	25	0.6
(1,328)	1:707:A:THR:HG21	1:705:A:ILE:HA	33	0.6
(1,297)	1:695:A:LEU:HA	1:695:A:LEU:HD11	27	0.6
(1,328)	1:707:A:THR:HG21	1:705:A:ILE:HA	9	0.59
(1,336)	1:718:A:LYS:H	1:718:A:LYS:HD3	35	0.58
(1,328)	1:707:A:THR:HG22	1:705:A:ILE:HA	2	0.56
(1,328)	1:707:A:THR:HG21	1:705:A:ILE:HA	26	0.56
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG23	36	0.56
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	11	0.56
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	11	0.56
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	11	0.56
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	25	0.55
(1,336)	1:718:A:LYS:H	1:718:A:LYS:HD3	15	0.55
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG22	38	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,236)	1:697:A:GLY:H	1:700:A:VAL:HG11	25	0.55
(1,236)	1:697:A:GLY:H	1:700:A:VAL:HG12	25	0.55
(1,236)	1:697:A:GLY:H	1:700:A:VAL:HG13	25	0.55
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	11	0.54
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	20	0.54
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG22	12	0.54
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG21	15	0.54
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG11	25	0.54
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG12	25	0.54
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG13	25	0.54
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG23	23	0.53
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	10	0.53
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	10	0.53
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	10	0.53
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	14	0.52
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	16	0.52
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG22	13	0.52
(1,328)	1:707:A:THR:HG21	1:705:A:ILE:HA	15	0.51
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG21	11	0.51
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG22	34	0.51
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	8	0.51
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	8	0.51
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	8	0.51
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG11	25	0.51
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG12	25	0.51
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG13	25	0.51
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	3	0.5
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	7	0.5
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	19	0.5
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	35	0.5
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	10	0.5
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	22	0.5
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG23	7	0.5
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG21	26	0.5
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	7	0.5
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	7	0.5
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	7	0.5
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	13	0.5
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	13	0.5
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	13	0.5
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	17	0.5
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	17	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	17	0.5
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	25	0.5
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	25	0.5
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	25	0.5
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	31	0.5
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	31	0.5
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	31	0.5
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	10	0.49
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	14	0.49
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	33	0.49
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	33	0.49
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	33	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	3	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	3	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	3	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	4	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	4	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	4	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	5	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	5	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	5	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	6	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	6	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	6	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	9	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	9	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	9	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	10	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	10	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	10	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	11	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	11	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	11	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	12	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	12	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	12	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	16	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	16	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	16	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	19	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	19	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	19	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	22	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	22	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	22	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	23	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	23	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	23	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	28	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	28	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	28	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	29	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	29	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	29	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	32	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	32	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	32	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	36	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	36	0.49
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	36	0.49
(2,38)	1:696:A:ILE:H	1:700:A:VAL:HA	27	0.48
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	28	0.48
(1,309)	1:699:A:LEU:HB3	1:699:A:LEU:HD21	8	0.48
(1,309)	1:699:A:LEU:HB3	1:699:A:LEU:HD22	8	0.48
(1,309)	1:699:A:LEU:HB3	1:699:A:LEU:HD23	8	0.48
(1,309)	1:699:A:LEU:HB3	1:699:A:LEU:HD21	34	0.48
(1,309)	1:699:A:LEU:HB3	1:699:A:LEU:HD22	34	0.48
(1,309)	1:699:A:LEU:HB3	1:699:A:LEU:HD23	34	0.48
(1,309)	1:699:A:LEU:HB3	1:699:A:LEU:HD21	36	0.48
(1,309)	1:699:A:LEU:HB3	1:699:A:LEU:HD22	36	0.48
(1,309)	1:699:A:LEU:HB3	1:699:A:LEU:HD23	36	0.48
(1,309)	1:699:A:LEU:HB3	1:699:A:LEU:HD21	38	0.48
(1,309)	1:699:A:LEU:HB3	1:699:A:LEU:HD22	38	0.48
(1,309)	1:699:A:LEU:HB3	1:699:A:LEU:HD23	38	0.48
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG11	1	0.48
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG12	1	0.48
(1,125)	1:710:A:VAL:H	1:710:A:VAL:HG13	1	0.48
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	16	0.47
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG22	40	0.47
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	21	0.47
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	21	0.47
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	21	0.47
(1,228)	1:698:A:LEU:H	1:698:A:LEU:HB2	9	0.47
(1,295)	1:702:A:ALA:HA	1:699:A:LEU:HD12	14	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG23	33	0.46
(1,228)	1:698:A:LEU:H	1:698:A:LEU:HB2	28	0.46
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	21	0.45
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG23	8	0.45
(1,269)	1:700:A:VAL:HG11	1:699:A:LEU:HA	25	0.45
(1,269)	1:700:A:VAL:HG12	1:699:A:LEU:HA	25	0.45
(1,269)	1:700:A:VAL:HG13	1:699:A:LEU:HA	25	0.45
(1,228)	1:698:A:LEU:H	1:698:A:LEU:HB2	11	0.45
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	9	0.44
(1,328)	1:707:A:THR:HG21	1:705:A:ILE:HA	37	0.44
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	3	0.44
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	3	0.44
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	3	0.44
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	1	0.43
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	5	0.43
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG21	32	0.43
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG22	37	0.43
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	31	0.42
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	4	0.42
(1,310)	1:716:A:LEU:HB3	1:716:A:LEU:HD21	5	0.42
(1,310)	1:716:A:LEU:HB3	1:716:A:LEU:HD22	5	0.42
(1,310)	1:716:A:LEU:HB3	1:716:A:LEU:HD23	5	0.42
(1,310)	1:716:A:LEU:HB3	1:716:A:LEU:HD21	33	0.42
(1,310)	1:716:A:LEU:HB3	1:716:A:LEU:HD22	33	0.42
(1,310)	1:716:A:LEU:HB3	1:716:A:LEU:HD23	33	0.42
(1,269)	1:700:A:VAL:HG11	1:699:A:LEU:HA	15	0.42
(1,269)	1:700:A:VAL:HG12	1:699:A:LEU:HA	15	0.42
(1,269)	1:700:A:VAL:HG13	1:699:A:LEU:HA	15	0.42
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	4	0.41
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	5	0.41
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	26	0.41
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	3	0.41
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	23	0.41
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	38	0.41
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG23	6	0.41
(1,269)	1:700:A:VAL:HG11	1:699:A:LEU:HA	23	0.41
(1,269)	1:700:A:VAL:HG12	1:699:A:LEU:HA	23	0.41
(1,269)	1:700:A:VAL:HG13	1:699:A:LEU:HA	23	0.41
(1,269)	1:700:A:VAL:HG11	1:699:A:LEU:HA	39	0.41
(1,269)	1:700:A:VAL:HG12	1:699:A:LEU:HA	39	0.41
(1,269)	1:700:A:VAL:HG13	1:699:A:LEU:HA	39	0.41
(1,220)	1:719:A:ARG:H	1:717:A:ARG:HA	17	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	29	0.4
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG21	9	0.4
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG11	39	0.4
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG12	39	0.4
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG13	39	0.4
(1,220)	1:719:A:ARG:H	1:717:A:ARG:HA	37	0.4
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG22	22	0.39
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	34	0.39
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	34	0.39
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	34	0.39
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG11	21	0.39
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG12	21	0.39
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG13	21	0.39
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	34	0.38
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	34	0.38
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	34	0.38
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG11	39	0.38
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG12	39	0.38
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG13	39	0.38
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG21	25	0.38
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG11	15	0.38
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG12	15	0.38
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG13	15	0.38
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	15	0.37
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	21	0.37
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	21	0.37
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	21	0.37
(1,329)	1:703:A:VAL:HA	1:703:A:VAL:HG21	31	0.37
(1,328)	1:707:A:THR:HG22	1:705:A:ILE:HA	6	0.37
(1,328)	1:707:A:THR:HG22	1:705:A:ILE:HA	40	0.37
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG21	1	0.37
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG21	10	0.37
(1,269)	1:700:A:VAL:HG11	1:699:A:LEU:HA	13	0.37
(1,269)	1:700:A:VAL:HG12	1:699:A:LEU:HA	13	0.37
(1,269)	1:700:A:VAL:HG13	1:699:A:LEU:HA	13	0.37
(1,269)	1:700:A:VAL:HG11	1:699:A:LEU:HA	34	0.37
(1,269)	1:700:A:VAL:HG12	1:699:A:LEU:HA	34	0.37
(1,269)	1:700:A:VAL:HG13	1:699:A:LEU:HA	34	0.37
(1,329)	1:703:A:VAL:HA	1:703:A:VAL:HG22	1	0.36
(1,329)	1:703:A:VAL:HA	1:703:A:VAL:HG21	24	0.36
(1,329)	1:703:A:VAL:HA	1:703:A:VAL:HG23	35	0.36
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG11	37	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG12	37	0.36
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG13	37	0.36
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG23	3	0.36
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG23	19	0.36
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG23	20	0.36
(1,269)	1:700:A:VAL:HG11	1:699:A:LEU:HA	21	0.36
(1,269)	1:700:A:VAL:HG12	1:699:A:LEU:HA	21	0.36
(1,269)	1:700:A:VAL:HG13	1:699:A:LEU:HA	21	0.36
(1,329)	1:703:A:VAL:HA	1:703:A:VAL:HG21	12	0.35
(1,329)	1:703:A:VAL:HA	1:703:A:VAL:HG23	30	0.35
(1,328)	1:707:A:THR:HG22	1:705:A:ILE:HA	19	0.35
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG11	25	0.35
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG12	25	0.35
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG13	25	0.35
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG11	23	0.35
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG12	23	0.35
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG13	23	0.35
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	2	0.34
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	38	0.34
(1,329)	1:703:A:VAL:HA	1:703:A:VAL:HG21	6	0.34
(1,329)	1:703:A:VAL:HA	1:703:A:VAL:HG21	20	0.34
(1,328)	1:707:A:THR:HG21	1:705:A:ILE:HA	32	0.34
(1,328)	1:707:A:THR:HG22	1:705:A:ILE:HA	34	0.34
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG22	4	0.34
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG23	5	0.34
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG21	21	0.34
(1,329)	1:703:A:VAL:HA	1:703:A:VAL:HG21	7	0.33
(1,329)	1:703:A:VAL:HA	1:703:A:VAL:HG22	16	0.33
(1,220)	1:719:A:ARG:H	1:717:A:ARG:HA	8	0.33
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG23	2	0.32
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG23	18	0.32
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	28	0.31
(1,329)	1:703:A:VAL:HA	1:703:A:VAL:HG22	17	0.3
(1,233)	1:704:A:ALA:H	1:703:A:VAL:HG21	29	0.3
(1,113)	1:709:A:ILE:H	1:709:A:ILE:HG13	29	0.3
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	30	0.29
(1,329)	1:703:A:VAL:HA	1:703:A:VAL:HG22	18	0.29
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG21	24	0.29
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG11	15	0.29
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG12	15	0.29
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG13	15	0.29
(1,233)	1:704:A:ALA:H	1:703:A:VAL:HG21	28	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG11	39	0.29
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG12	39	0.29
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG13	39	0.29
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG23	16	0.28
(1,328)	1:707:A:THR:HG22	1:705:A:ILE:HA	17	0.27
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG11	6	0.27
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG12	6	0.27
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG13	6	0.27
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG11	18	0.27
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG12	18	0.27
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG13	18	0.27
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG22	35	0.27
(1,220)	1:719:A:ARG:H	1:717:A:ARG:HA	6	0.27
(1,113)	1:709:A:ILE:H	1:709:A:ILE:HG13	31	0.26
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	27	0.25
(1,316)	1:709:A:ILE:HG23	1:709:A:ILE:HD12	16	0.25
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	12	0.25
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	12	0.25
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	12	0.25
(1,233)	1:704:A:ALA:H	1:703:A:VAL:HG23	31	0.25
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	36	0.24
(1,316)	1:709:A:ILE:HG23	1:709:A:ILE:HD12	7	0.24
(1,316)	1:709:A:ILE:HG21	1:709:A:ILE:HD11	17	0.24
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG11	13	0.24
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG12	13	0.24
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG13	13	0.24
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	18	0.23
(1,316)	1:711:A:ILE:HG23	1:711:A:ILE:HD13	1	0.23
(1,316)	1:711:A:ILE:HG22	1:711:A:ILE:HD13	12	0.23
(1,113)	1:709:A:ILE:H	1:709:A:ILE:HG13	28	0.23
(1,316)	1:709:A:ILE:HG21	1:709:A:ILE:HD11	10	0.22
(1,316)	1:709:A:ILE:HG23	1:709:A:ILE:HD13	18	0.22
(1,316)	1:711:A:ILE:HG23	1:711:A:ILE:HD12	30	0.22
(1,316)	1:711:A:ILE:HG21	1:711:A:ILE:HD13	37	0.22
(1,311)	1:709:A:ILE:HG13	1:709:A:ILE:HG22	15	0.22
(1,311)	1:709:A:ILE:HG13	1:709:A:ILE:HG21	23	0.22
(1,311)	1:709:A:ILE:HG13	1:709:A:ILE:HG23	30	0.22
(1,311)	1:709:A:ILE:HG13	1:709:A:ILE:HG23	39	0.22
(1,270)	1:713:A:LEU:HD11	1:713:A:LEU:HA	37	0.22
(1,270)	1:713:A:LEU:HD12	1:713:A:LEU:HA	37	0.22
(1,270)	1:713:A:LEU:HD13	1:713:A:LEU:HA	37	0.22
(1,220)	1:719:A:ARG:H	1:717:A:ARG:HA	23	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG21	23	0.21
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG22	23	0.21
(1,340)	1:699:A:LEU:HB3	1:700:A:VAL:HG23	23	0.21
(1,328)	1:707:A:THR:HG21	1:705:A:ILE:HA	24	0.21
(1,316)	1:709:A:ILE:HG21	1:709:A:ILE:HD12	15	0.21
(1,316)	1:709:A:ILE:HG21	1:709:A:ILE:HD13	26	0.21
(1,316)	1:711:A:ILE:HG21	1:711:A:ILE:HD11	31	0.21
(1,316)	1:709:A:ILE:HG22	1:709:A:ILE:HD11	38	0.21
(1,311)	1:709:A:ILE:HG13	1:709:A:ILE:HG22	1	0.21
(1,311)	1:709:A:ILE:HG13	1:709:A:ILE:HG21	5	0.21
(1,311)	1:709:A:ILE:HG13	1:709:A:ILE:HG23	13	0.21
(1,235)	1:699:A:LEU:H	1:696:A:ILE:HG21	30	0.21
(1,220)	1:719:A:ARG:H	1:717:A:ARG:HA	32	0.21
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	1	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	1	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	1	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	2	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	2	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	2	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	3	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	3	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	3	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	4	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	4	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	4	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	5	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	5	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	5	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	6	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	6	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	6	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	7	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	7	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	7	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	8	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	8	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	8	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	9	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	9	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	9	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	10	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	10	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	11	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	11	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	11	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	14	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	14	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	14	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	16	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	16	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	16	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	17	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	17	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	17	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	18	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	18	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	18	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	19	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	19	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	19	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	20	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	20	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	20	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	22	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	22	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	22	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	24	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	24	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	24	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	26	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	26	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	26	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	28	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	28	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	28	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	29	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	29	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	29	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	30	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	30	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	30	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	33	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	33	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	33	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	35	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	35	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	35	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	36	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	36	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	36	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	38	0.2
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	38	0.2
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	38	0.2
(1,316)	1:711:A:ILE:HG21	1:711:A:ILE:HD12	5	0.2
(1,316)	1:709:A:ILE:HG23	1:709:A:ILE:HD12	6	0.2
(1,316)	1:709:A:ILE:HG21	1:709:A:ILE:HD13	11	0.2
(1,316)	1:709:A:ILE:HG21	1:709:A:ILE:HD11	14	0.2
(1,316)	1:711:A:ILE:HG22	1:711:A:ILE:HD13	22	0.2
(1,316)	1:709:A:ILE:HG23	1:709:A:ILE:HD12	33	0.2
(1,316)	1:709:A:ILE:HG22	1:709:A:ILE:HD13	34	0.2
(1,316)	1:709:A:ILE:HG23	1:709:A:ILE:HD12	36	0.2
(1,311)	1:709:A:ILE:HG13	1:709:A:ILE:HG21	7	0.2
(1,311)	1:709:A:ILE:HG13	1:709:A:ILE:HG23	12	0.2
(1,311)	1:709:A:ILE:HG13	1:709:A:ILE:HG21	19	0.2
(1,236)	1:697:A:GLY:H	1:700:A:VAL:HG11	39	0.2
(1,236)	1:697:A:GLY:H	1:700:A:VAL:HG12	39	0.2
(1,236)	1:697:A:GLY:H	1:700:A:VAL:HG13	39	0.2
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	12	0.19
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	12	0.19
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	12	0.19
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	27	0.19
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	27	0.19
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	27	0.19
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	31	0.19
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	31	0.19
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	31	0.19
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	32	0.19
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	32	0.19
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	32	0.19
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	37	0.19
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	37	0.19
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	37	0.19
(1,338)	1:700:A:VAL:HG11	1:700:A:VAL:HA	40	0.19
(1,338)	1:700:A:VAL:HG12	1:700:A:VAL:HA	40	0.19
(1,338)	1:700:A:VAL:HG13	1:700:A:VAL:HA	40	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,316)	1:709:A:ILE:HG23	1:709:A:ILE:HD12	2	0.19
(1,316)	1:711:A:ILE:HG22	1:711:A:ILE:HD11	9	0.19
(1,316)	1:711:A:ILE:HG22	1:711:A:ILE:HD11	13	0.19
(1,316)	1:711:A:ILE:HG22	1:711:A:ILE:HD13	20	0.19
(1,316)	1:709:A:ILE:HG21	1:709:A:ILE:HD11	21	0.19
(1,316)	1:709:A:ILE:HG21	1:709:A:ILE:HD13	24	0.19
(1,316)	1:711:A:ILE:HG22	1:711:A:ILE:HD12	40	0.19
(1,311)	1:709:A:ILE:HG13	1:709:A:ILE:HG22	25	0.19
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	38	0.19
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	38	0.19
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	38	0.19
(1,220)	1:719:A:ARG:H	1:717:A:ARG:HA	11	0.19
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	2	0.19
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	11	0.19
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	19	0.19
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	29	0.19
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	37	0.19
(1,339)	1:701:A:ILE:H	1:699:A:LEU:HB3	8	0.18
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	1	0.18
(1,328)	1:707:A:THR:HG21	1:705:A:ILE:HA	30	0.18
(1,316)	1:711:A:ILE:HG22	1:711:A:ILE:HD11	25	0.18
(1,316)	1:711:A:ILE:HG22	1:711:A:ILE:HD12	27	0.18
(1,316)	1:711:A:ILE:HG22	1:711:A:ILE:HD12	28	0.18
(1,316)	1:711:A:ILE:HG23	1:711:A:ILE:HD12	32	0.18
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG11	17	0.18
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG12	17	0.18
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG13	17	0.18
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG22	30	0.18
(1,235)	1:699:A:LEU:H	1:698:A:LEU:HD11	35	0.18
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	13	0.18
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	14	0.18
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	17	0.18
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	21	0.18
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	25	0.18
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	31	0.18
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	33	0.18
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	34	0.18
(1,84)	1:696:A:ILE:H	1:696:A:ILE:HB	35	0.18
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	7	0.17
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	29	0.17
(1,316)	1:711:A:ILE:HG22	1:711:A:ILE:HD13	8	0.17
(1,316)	1:711:A:ILE:HG22	1:711:A:ILE:HD12	29	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG11	23	0.17
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG12	23	0.17
(1,237)	1:698:A:LEU:H	1:700:A:VAL:HG13	23	0.17
(1,124)	1:701:A:ILE:H	1:700:A:VAL:HG22	12	0.17
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	6	0.17
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	12	0.17
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	38	0.17
(1,316)	1:711:A:ILE:HG23	1:711:A:ILE:HD11	3	0.16
(1,316)	1:711:A:ILE:HG21	1:711:A:ILE:HD12	23	0.16
(1,316)	1:711:A:ILE:HG22	1:711:A:ILE:HD11	39	0.16
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	3	0.16
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	10	0.16
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	16	0.16
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	20	0.16
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	30	0.16
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	36	0.16
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	40	0.16
(1,329)	1:705:A:ILE:HA	1:708:A:VAL:HG12	13	0.15
(1,316)	1:711:A:ILE:HG23	1:711:A:ILE:HD11	4	0.15
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG22	29	0.15
(1,235)	1:699:A:LEU:H	1:696:A:ILE:HG23	8	0.15
(1,233)	1:710:A:VAL:H	1:709:A:ILE:HG13	16	0.15
(1,131)	1:698:A:LEU:H	1:698:A:LEU:HD11	30	0.15
(1,131)	1:698:A:LEU:H	1:698:A:LEU:HD12	30	0.15
(1,131)	1:698:A:LEU:H	1:698:A:LEU:HD13	30	0.15
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	4	0.15
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	8	0.15
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	23	0.15
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	26	0.15
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	31	0.14
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	39	0.14
(1,328)	1:707:A:THR:HG22	1:705:A:ILE:HA	12	0.14
(1,316)	1:711:A:ILE:HG23	1:711:A:ILE:HD12	35	0.14
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG11	13	0.14
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG12	13	0.14
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG13	13	0.14
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	15	0.14
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	18	0.14
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	28	0.14
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	35	0.14
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	39	0.14
(1,336)	1:718:A:LYS:H	1:718:A:LYS:HD3	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:705:A:ILE:HA	1:708:A:VAL:HG12	9	0.13
(1,329)	1:705:A:ILE:HA	1:708:A:VAL:HG13	14	0.13
(1,329)	1:705:A:ILE:HA	1:708:A:VAL:HG11	23	0.13
(1,328)	1:707:A:THR:HG23	1:705:A:ILE:HA	16	0.13
(1,328)	1:707:A:THR:HG21	1:705:A:ILE:HA	20	0.13
(1,295)	1:706:A:ALA:HA	1:709:A:ILE:HG21	28	0.13
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	32	0.13
(1,329)	1:705:A:ILE:HA	1:708:A:VAL:HG13	38	0.12
(1,316)	1:711:A:ILE:HG22	1:711:A:ILE:HD11	19	0.12
(1,233)	1:710:A:VAL:H	1:709:A:ILE:HG13	18	0.12
(1,233)	1:710:A:VAL:H	1:709:A:ILE:HG13	25	0.12
(1,220)	1:719:A:ARG:H	1:717:A:ARG:HA	16	0.12
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG11	34	0.12
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG12	34	0.12
(1,120)	1:699:A:LEU:H	1:700:A:VAL:HG13	34	0.12
(1,341)	1:695:A:LEU:HB2	1:696:A:ILE:HG12	26	0.11
(1,329)	1:705:A:ILE:HA	1:708:A:VAL:HG11	2	0.11
(1,328)	1:707:A:THR:HG22	1:705:A:ILE:HA	35	0.11
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG11	24	0.11
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG12	24	0.11
(1,308)	1:699:A:LEU:HB3	1:700:A:VAL:HG13	24	0.11
(1,248)	1:711:A:ILE:HG21	1:715:A:MET:HG3	29	0.11
(1,248)	1:711:A:ILE:HG22	1:715:A:MET:HG3	29	0.11
(1,248)	1:711:A:ILE:HG23	1:715:A:MET:HG3	29	0.11
(1,233)	1:710:A:VAL:H	1:709:A:ILE:HG13	2	0.11
(1,233)	1:710:A:VAL:H	1:709:A:ILE:HG13	3	0.11
(1,233)	1:710:A:VAL:H	1:709:A:ILE:HG13	10	0.11
(1,233)	1:710:A:VAL:H	1:709:A:ILE:HG13	17	0.11
(1,329)	1:705:A:ILE:HA	1:708:A:VAL:HG11	21	0.1
(1,233)	1:710:A:VAL:H	1:709:A:ILE:HG13	4	0.1
(1,110)	1:696:A:ILE:H	1:696:A:ILE:HG12	21	0.1
(1,110)	1:696:A:ILE:H	1:696:A:ILE:HG12	27	0.1
(1,110)	1:696:A:ILE:H	1:696:A:ILE:HG12	32	0.1
(1,87)	1:695:A:LEU:H	1:695:A:LEU:HB3	24	0.1

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found