Full wwPDB NMR Structure Validation Report

Jun 3, 2023 – 05:47 PM EDT

PDB ID	:	2MVD
BMRB ID	:	25261
Title	:	Solution structure of [GlnB22]-insulin mutant at pH 1.9
Authors	:	Hexnerova, R.; Krizkova, K.; Maletinska, L.; Jiracek, J.; Brzozowski, A.M.; Zakova, L.; Veverka, V.
Deposited on	:	2014-10-02

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

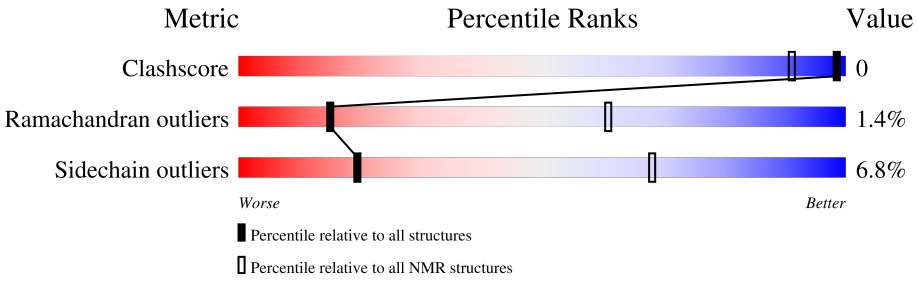
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 51%.

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	21	90% 10%
2	B	30	73% 7% 20%

2 Ensemble composition and analysis (i)

This entry contains 40 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:1-A:21, B:31-B:54 (45)	1.30	16

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 785 atoms, of which 382 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Insulin A chain.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	21	314	99	151	25	35	4	0

- Molecule 2 is a protein called Insulin B chain.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	30	471	157	231	38	43	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	52	GLN	ARG	engineered mutation	UNP P01308

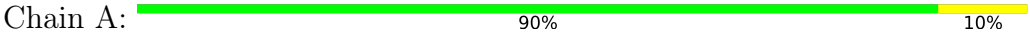
4 Residue-property plots

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: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

Chain B:

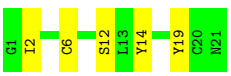
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Insulin A chain

Chain A:



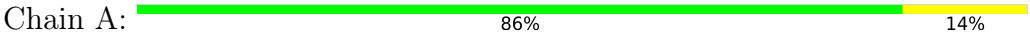
• Molecule 2: Insulin B chain

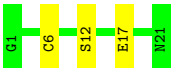
Chain B:

4.2.2 Score per residue for model 2

• Molecule 1: Insulin A chain

Chain A:





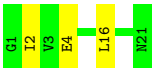
• Molecule 2: Insulin B chain

Chain B:

4.2.3 Score per residue for model 3

• Molecule 1: Insulin A chain

Chain A:



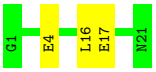
• Molecule 2: Insulin B chain

Chain B:

4.2.4 Score per residue for model 4

• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

Chain B:

4.2.5 Score per residue for model 5

• Molecule 1: Insulin A chain

Chain A:

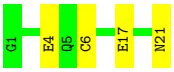
• Molecule 2: Insulin B chain

Chain B:

4.2.6 Score per residue for model 6

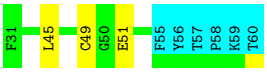
• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

Chain B:



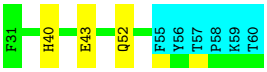
4.2.7 Score per residue for model 7

• Molecule 1: Insulin A chain

Chain A:

• Molecule 2: Insulin B chain

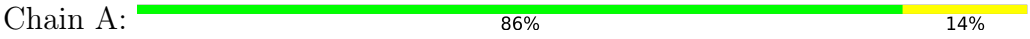
Chain B:

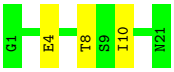


4.2.8 Score per residue for model 8

• Molecule 1: Insulin A chain

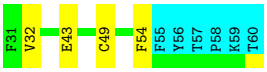
Chain A:





• Molecule 2: Insulin B chain

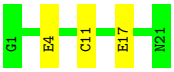
Chain B:



4.2.9 Score per residue for model 9

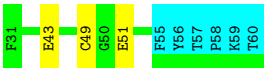
• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

Chain B:



4.2.10 Score per residue for model 10

• Molecule 1: Insulin A chain

Chain A:

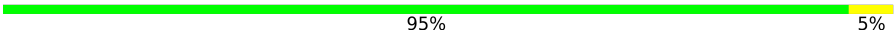
• Molecule 2: Insulin B chain

Chain B:

4.2.11 Score per residue for model 11

• Molecule 1: Insulin A chain

Chain A:



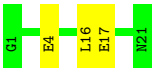
• Molecule 2: Insulin B chain

Chain B:

4.2.12 Score per residue for model 12

• Molecule 1: Insulin A chain

Chain A:



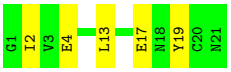
• Molecule 2: Insulin B chain

Chain B:

4.2.13 Score per residue for model 13

• Molecule 1: Insulin A chain

Chain A:



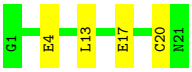
• Molecule 2: Insulin B chain

Chain B:

4.2.14 Score per residue for model 14

• Molecule 1: Insulin A chain

Chain A:



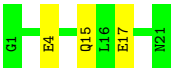
• Molecule 2: Insulin B chain

Chain B:

4.2.15 Score per residue for model 15

• Molecule 1: Insulin A chain

Chain A:



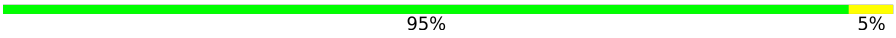
• Molecule 2: Insulin B chain

Chain B:

4.2.16 Score per residue for model 16 (medoid)

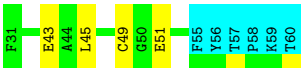
• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

Chain B:



4.2.17 Score per residue for model 17

• Molecule 1: Insulin A chain

Chain A:

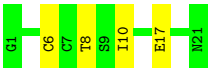
• Molecule 2: Insulin B chain

Chain B:

4.2.18 Score per residue for model 18

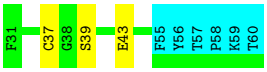
• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

Chain B:



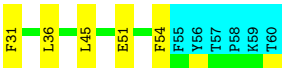
4.2.19 Score per residue for model 19

• Molecule 1: Insulin A chain

Chain A:

• Molecule 2: Insulin B chain

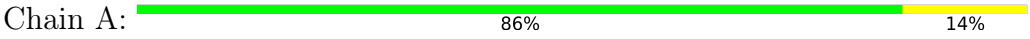
Chain B:

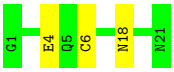


4.2.20 Score per residue for model 20

• Molecule 1: Insulin A chain

Chain A:





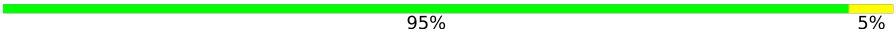
• Molecule 2: Insulin B chain

Chain B:

4.2.21 Score per residue for model 21

• Molecule 1: Insulin A chain

Chain A:



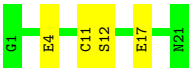
• Molecule 2: Insulin B chain

Chain B:

4.2.22 Score per residue for model 22

• Molecule 1: Insulin A chain

Chain A:



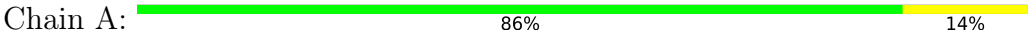
• Molecule 2: Insulin B chain

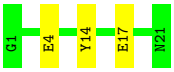
Chain B:

4.2.23 Score per residue for model 23

• Molecule 1: Insulin A chain

Chain A:





• Molecule 2: Insulin B chain

Chain B:

4.2.24 Score per residue for model 24

• Molecule 1: Insulin A chain

Chain A:

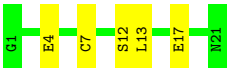
• Molecule 2: Insulin B chain

Chain B:

4.2.25 Score per residue for model 25

• Molecule 1: Insulin A chain

Chain A:



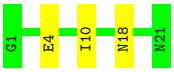
• Molecule 2: Insulin B chain

Chain B:

4.2.26 Score per residue for model 26

• Molecule 1: Insulin A chain

Chain A:



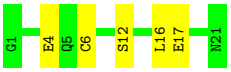
• Molecule 2: Insulin B chain

Chain B:

4.2.27 Score per residue for model 27

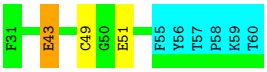
• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

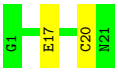
Chain B:



4.2.28 Score per residue for model 28

• Molecule 1: Insulin A chain

Chain A:



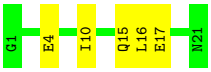
• Molecule 2: Insulin B chain

Chain B:

4.2.29 Score per residue for model 29

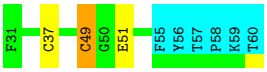
• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

Chain B:



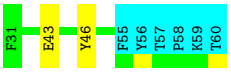
4.2.30 Score per residue for model 30

• Molecule 1: Insulin A chain

Chain A:

• Molecule 2: Insulin B chain

Chain B:



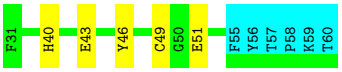
4.2.31 Score per residue for model 31

• Molecule 1: Insulin A chain

Chain A:

• Molecule 2: Insulin B chain

Chain B:



4.2.32 Score per residue for model 32

• Molecule 1: Insulin A chain

Chain A:

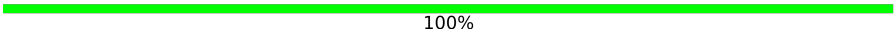
• Molecule 2: Insulin B chain

Chain B:

4.2.33 Score per residue for model 33

• Molecule 1: Insulin A chain

Chain A:



There are no outlier residues in this chain.

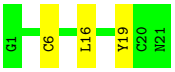
• Molecule 2: Insulin B chain

Chain B:

4.2.34 Score per residue for model 34

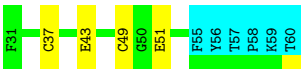
• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

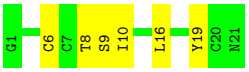
Chain B:



4.2.35 Score per residue for model 35

• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

Chain B:

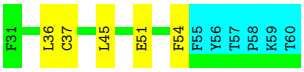
4.2.36 Score per residue for model 36

• Molecule 1: Insulin A chain

Chain A:

• Molecule 2: Insulin B chain

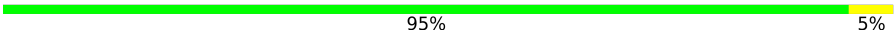
Chain B:



4.2.37 Score per residue for model 37

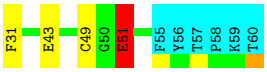
• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

Chain B:



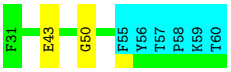
4.2.38 Score per residue for model 38

• Molecule 1: Insulin A chain

Chain A:

• Molecule 2: Insulin B chain

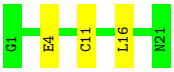
Chain B:



4.2.39 Score per residue for model 39

• Molecule 1: Insulin A chain

Chain A:



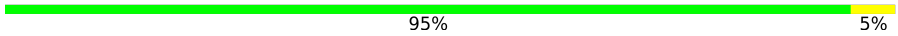
• Molecule 2: Insulin B chain

Chain B:

4.2.40 Score per residue for model 40

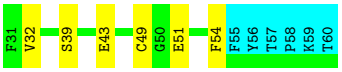
• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

Chain B:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 40 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	
YASARA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	344
Number of shifts mapped to atoms	344
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	51%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.31±0.13	2±1/164 (0.9± 0.5%)	0.87±0.10	0±0/220 (0.0± 0.0%)
2	B	1.19±0.12	1±1/191 (0.7± 0.4%)	0.90±0.09	0±0/259 (0.0± 0.1%)
All	All	1.25	117/14200 (0.8%)	0.89	3/19160 (0.0%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	4	GLU	CD-OE1	-8.83	1.16	1.25	14	24
1	A	17	GLU	CD-OE1	-8.44	1.16	1.25	19	23
2	B	51	GLU	CD-OE1	-7.45	1.17	1.25	37	19
1	A	4	GLU	CD-OE2	6.88	1.33	1.25	38	4
2	B	43	GLU	CD-OE1	-6.84	1.18	1.25	14	19
2	B	43	GLU	CD-OE2	6.79	1.33	1.25	38	9
1	A	21	ASN	C-OXT	6.45	1.35	1.23	6	2
1	A	19	TYR	CD1-CE1	6.42	1.49	1.39	16	2
2	B	51	GLU	CD-OE2	6.29	1.32	1.25	16	7
1	A	1	GLY	N-CA	6.27	1.55	1.46	32	1
1	A	17	GLU	CD-OE2	6.00	1.32	1.25	36	1
2	B	46	TYR	CE2-CZ	5.95	1.46	1.38	30	2
1	A	14	TYR	CD1-CE1	5.58	1.47	1.39	1	1
1	A	19	TYR	CE2-CZ	5.40	1.45	1.38	35	1
1	A	19	TYR	CD2-CE2	5.07	1.47	1.39	19	1
1	A	14	TYR	CB-CG	5.03	1.59	1.51	23	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	31	PHE	CB-CG-CD1	-5.78	116.75	120.80	10	1
2	B	31	PHE	CB-CG-CD2	-5.20	117.16	120.80	26	2

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	163	151	149	0±0
2	B	186	178	172	0±0
All	All	13960	13160	12840	4

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:ILE:HD12	1:A:19:TYR:CD2	0.52	2.39	1	2
1:A:2:ILE:HD12	1:A:19:TYR:CD1	0.43	2.48	10	1
1:A:13:LEU:HD21	2:B:31:PHE:CZ	0.42	2.50	19	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	19/21 (90%)	18±1 (94±6%)	1±1 (5±5%)	0±0 (1±2%)	21	69
2	B	23/30 (77%)	20±2 (88±8%)	2±2 (10±7%)	0±1 (2±3%)	12	54
All	All	1680/2040 (82%)	1526 (91%)	130 (8%)	24 (1%)	15	61

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	54	PHE	6
1	A	10	ILE	6
2	B	38	GLY	3
2	B	36	LEU	2
2	B	49	CYS	2
2	B	52	GLN	1
1	A	11	CYS	1
2	B	39	SER	1
2	B	51	GLU	1
2	B	50	GLY	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	20/20 (100%)	19±1 (94±5%)	1±1 (6±5%)	23	72
2	B	20/26 (77%)	18±1 (92±5%)	2±1 (8±5%)	16	64
All	All	1600/1840 (87%)	1491 (93%)	109 (7%)	19	68

All 25 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	49	CYS	12
1	A	6	CYS	11
2	B	51	GLU	9
1	A	16	LEU	8
2	B	45	LEU	8
2	B	40	HIS	8
2	B	37	CYS	7
1	A	12	SER	6
2	B	54	PHE	4
1	A	13	LEU	4
2	B	39	SER	3
2	B	32	VAL	3
1	A	8	THR	3
2	B	36	LEU	3
1	A	11	CYS	3

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Mol	Chain	Res	Type	Models (Total)
2	B	43	GLU	3
1	A	2	ILE	2
1	A	7	CYS	2
1	A	20	CYS	2
1	A	15	GLN	2
1	A	18	ASN	2
1	A	21	ASN	1
2	B	34	GLN	1
1	A	9	SER	1
2	B	42	VAL	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 51% for the well-defined parts and 51% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	344
Number of shifts mapped to atoms	344
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

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

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 51%, i.e. 298 atoms were assigned a chemical shift out of a possible 583. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	89/229 (39%)	89/94 (95%)	0/90 (0%)	0/45 (0%)
Sidechain	184/291 (63%)	184/191 (96%)	0/93 (0%)	0/7 (0%)
Aromatic	25/63 (40%)	25/30 (83%)	0/29 (0%)	0/4 (0%)
Overall	298/583 (51%)	298/315 (95%)	0/212 (0%)	0/56 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 51%, i.e. 344 atoms were assigned a chemical shift out of a possible 670. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	100/257 (39%)	100/105 (95%)	0/102 (0%)	0/50 (0%)
Sidechain	210/331 (63%)	210/217 (97%)	0/106 (0%)	0/8 (0%)
Aromatic	34/82 (41%)	34/39 (87%)	0/39 (0%)	0/4 (0%)
Overall	344/670 (51%)	344/361 (95%)	0/247 (0%)	0/62 (0%)

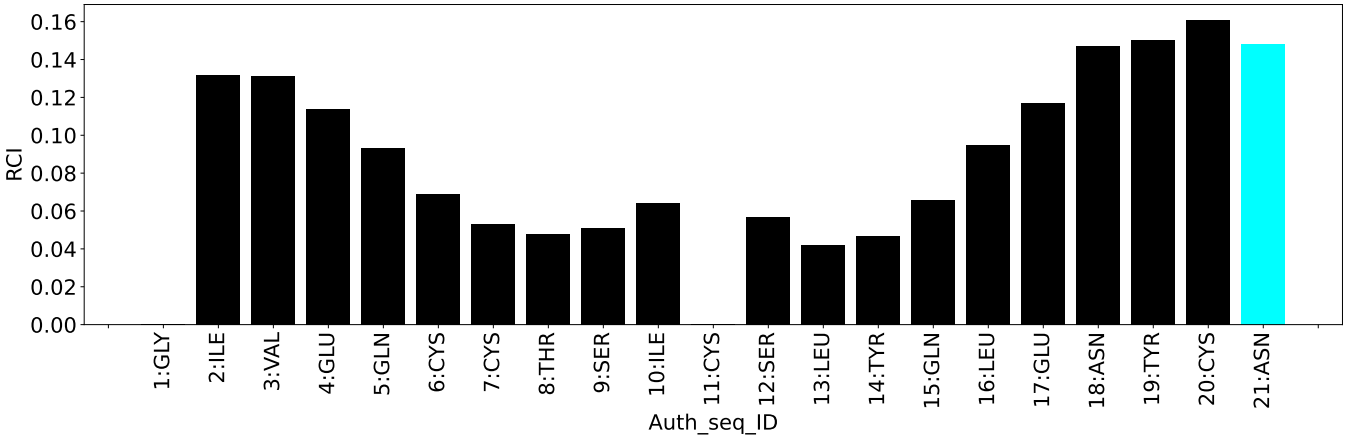
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

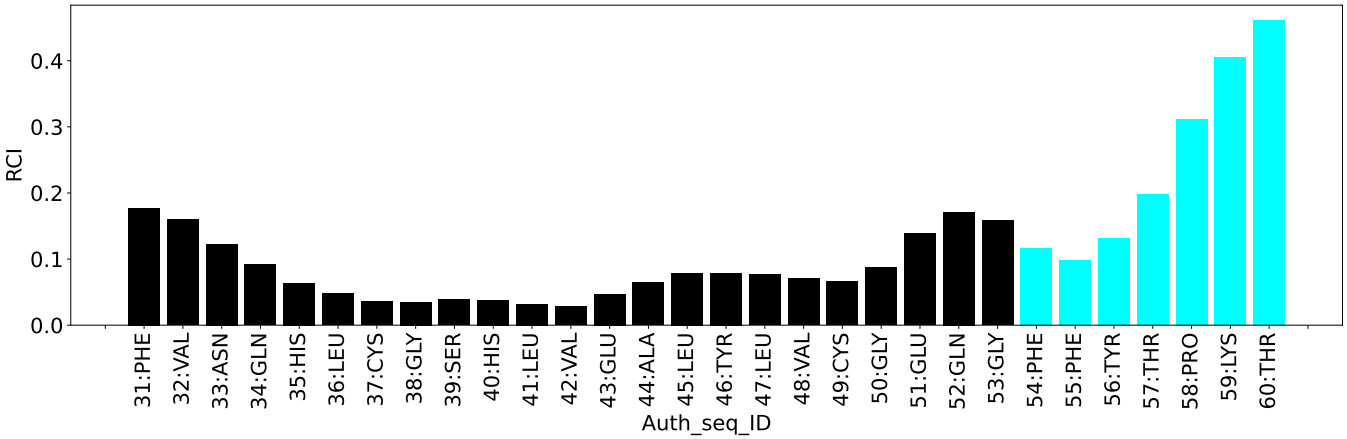
7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:


RCI
0.0
0.1
0.2
0.3
0.4
31:PHE
32:VAL
33:ASN
34:GLN
35:HIS
36:LEU
37:CYS
38:GLY
39:SER
40:HIS
41:LEU
42:VAL
43:GLU
44:ALA
45:LEU
46:TYR
47:LEU
48:VAL
49:CYS
50:GLY
51:GLU
52:GLN
53:GLY
54:PHE
55:PHE
56:TYR
57:THR
58:PRO
59:LYS
60:THR
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	646
Intra-residue (|i-j|=0)	178
Sequential (|i-j|=1)	156
Medium range (|i-j|>1 and |i-j|<5)	113
Long range (|i-j|≥5)	51
Inter-chain	66
Hydrogen bond restraints	64
Disulfide bond restraints	18
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	12.7
Number of long range restraints per residue[1]	1.1

[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)	8.8	0.2
0.2-0.5 (Medium)	4.7	0.5
>0.5 (Large)	None	None

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

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

9 Distance violation analysis (i)

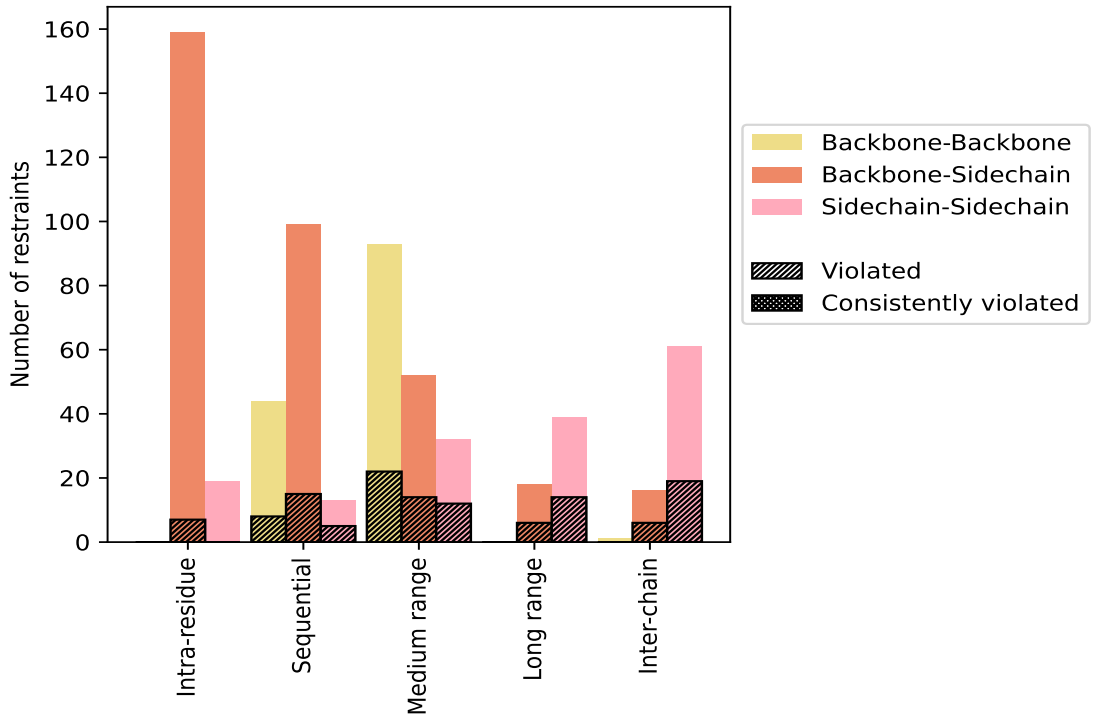
9.1 Summary of distance violations (i)

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)	178	27.6	7	3.9	1.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	159	24.6	7	4.4	1.1	0	0.0	0.0
Sidechain-Sidechain	19	2.9	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	156	24.1	28	17.9	4.3	0	0.0	0.0
Backbone-Backbone	44	6.8	8	18.2	1.2	0	0.0	0.0
Backbone-Sidechain	99	15.3	15	15.2	2.3	0	0.0	0.0
Sidechain-Sidechain	13	2.0	5	38.5	0.8	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	113	17.5	27	23.9	4.2	0	0.0	0.0
Backbone-Backbone	29	4.5	1	3.4	0.2	0	0.0	0.0
Backbone-Sidechain	52	8.0	14	26.9	2.2	0	0.0	0.0
Sidechain-Sidechain	32	5.0	12	37.5	1.9	0	0.0	0.0
Long range (|i-j|≥5)	51	7.9	20	39.2	3.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	18	2.8	6	33.3	0.9	0	0.0	0.0
Sidechain-Sidechain	33	5.1	14	42.4	2.2	0	0.0	0.0
Inter-chain	66	10.2	25	37.9	3.9	0	0.0	0.0
Backbone-Backbone	1	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	16	2.5	6	37.5	0.9	0	0.0	0.0
Sidechain-Sidechain	49	7.6	19	38.8	2.9	0	0.0	0.0
Hydrogen bond	64	9.9	21	32.8	3.3	0	0.0	0.0
Disulfide bond	18	2.8	0	0.0	0.0	0	0.0	0.0
Total	646	100.0	128	19.8	19.8	0	0.0	0.0
Backbone-Backbone	138	21.4	30	21.7	4.6	0	0.0	0.0
Backbone-Sidechain	344	53.3	48	14.0	7.4	0	0.0	0.0
Sidechain-Sidechain	164	25.4	50	30.5	7.7	0	0.0	0.0

[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	0	2	4	1	2	9	0.16	0.27	0.05	0.14
2	0	2	1	2	2	7	0.22	0.49	0.12	0.14
3	0	1	1	1	2	5	0.3	0.49	0.11	0.23
4	0	1	2	1	2	6	0.25	0.44	0.1	0.23
5	0	3	3	2	2	10	0.21	0.5	0.13	0.18
6	1	2	9	2	3	17	0.14	0.27	0.04	0.12
7	0	2	2	3	4	11	0.2	0.49	0.1	0.18
8	1	4	4	1	3	13	0.2	0.46	0.11	0.15
9	0	0	7	2	2	11	0.2	0.37	0.08	0.19
10	0	2	6	5	0	13	0.17	0.32	0.07	0.14
11	0	1	11	2	3	17	0.17	0.3	0.05	0.18

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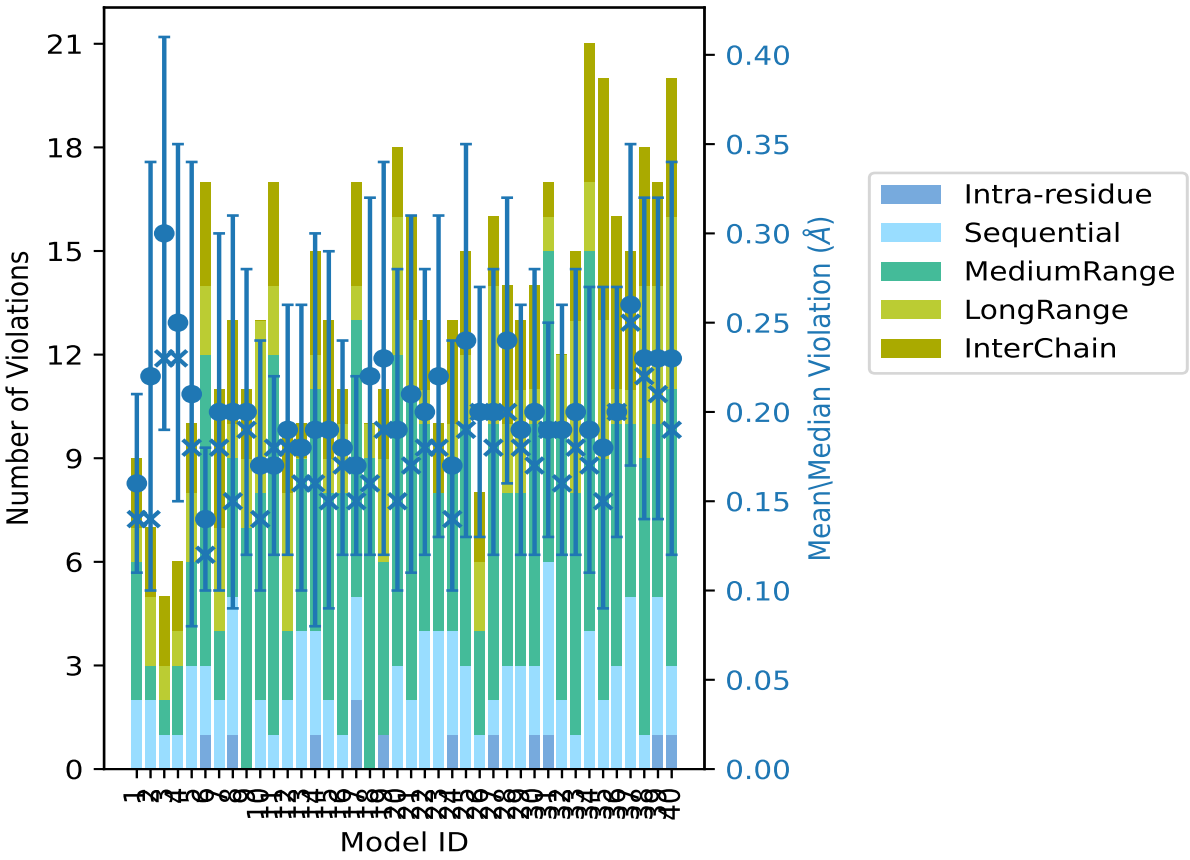
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	2	2	4	2	10	0.19	0.32	0.07	0.18
13	0	4	5	0	1	10	0.18	0.4	0.08	0.16
14	1	3	7	1	3	15	0.19	0.46	0.11	0.16
15	0	2	6	1	4	13	0.19	0.49	0.1	0.15
16	0	1	7	2	1	11	0.18	0.36	0.06	0.17
17	2	3	8	1	3	17	0.17	0.26	0.05	0.15
18	0	0	9	1	0	10	0.22	0.42	0.1	0.16
19	1	0	5	3	2	11	0.23	0.46	0.11	0.19
20	0	3	9	4	2	18	0.19	0.43	0.09	0.15
21	0	2	9	2	3	16	0.21	0.4	0.1	0.17
22	0	4	6	1	2	13	0.2	0.32	0.08	0.18
23	0	4	4	0	2	10	0.22	0.39	0.09	0.18
24	1	3	5	1	3	13	0.17	0.34	0.07	0.14
25	0	3	7	2	3	15	0.24	0.49	0.11	0.19
26	0	1	3	2	2	8	0.2	0.29	0.07	0.2
27	1	1	8	4	2	16	0.2	0.43	0.08	0.18
28	0	3	5	2	4	14	0.24	0.38	0.08	0.2
29	0	3	5	3	2	13	0.19	0.35	0.07	0.18
30	1	2	7	1	3	14	0.2	0.41	0.08	0.17
31	1	5	9	1	1	17	0.19	0.29	0.06	0.19
32	0	2	8	2	0	12	0.19	0.4	0.07	0.16
33	0	1	7	5	2	15	0.2	0.41	0.08	0.18
34	0	4	11	2	4	21	0.19	0.34	0.08	0.17
35	0	2	7	4	7	20	0.18	0.42	0.09	0.15
36	0	3	7	1	5	16	0.2	0.34	0.07	0.2
37	0	5	5	1	4	15	0.26	0.45	0.09	0.25
38	0	1	8	5	4	18	0.23	0.43	0.09	0.22
39	1	4	5	4	3	17	0.23	0.46	0.09	0.21
40	1	2	8	5	4	20	0.23	0.49	0.11	0.19

[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, 457(IR:171, SQ:128, MR:86, LR:31, IC:41) 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]	%
4	11	7	5	14	41	1	2.5
1	3	5	3	2	14	2	5.0
2	7	2	0	1	12	3	7.5
0	0	3	2	2	7	4	10.0
0	2	4	3	1	10	5	12.5
0	2	0	4	0	6	6	15.0

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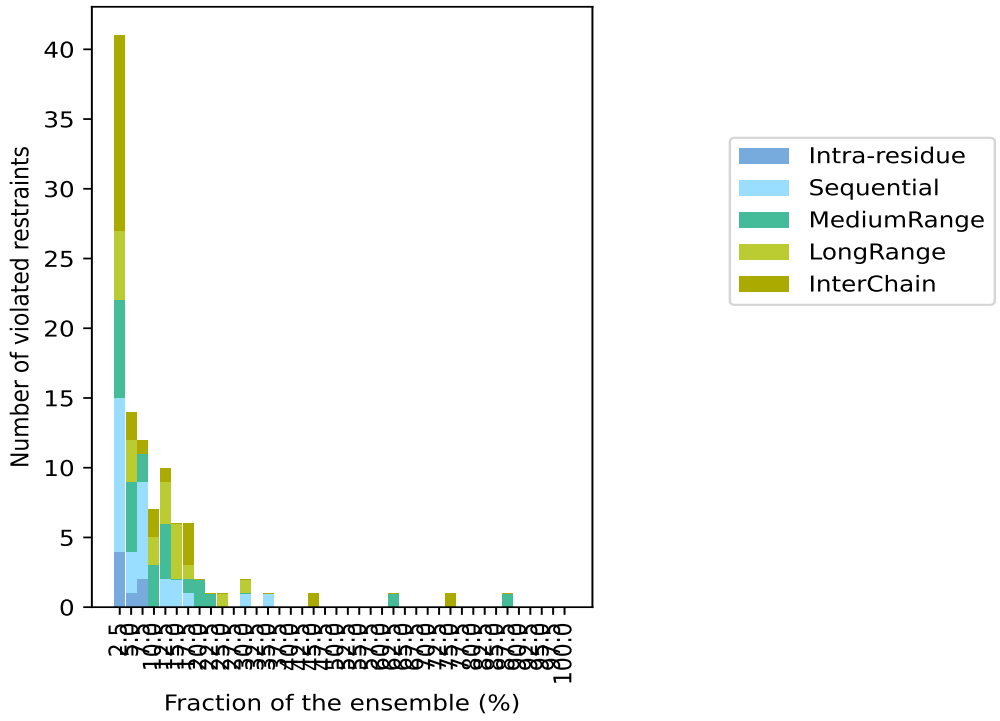
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	1	1	1	3	6	7	17.5
0	0	2	0	0	2	8	20.0
0	0	1	0	0	1	9	22.5
0	0	0	1	0	1	10	25.0
0	0	0	0	0	0	11	27.5
0	1	0	1	0	2	12	30.0
0	0	0	0	0	0	13	32.5
0	1	0	0	0	1	14	35.0
0	0	0	0	0	0	15	37.5
0	0	0	0	0	0	16	40.0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

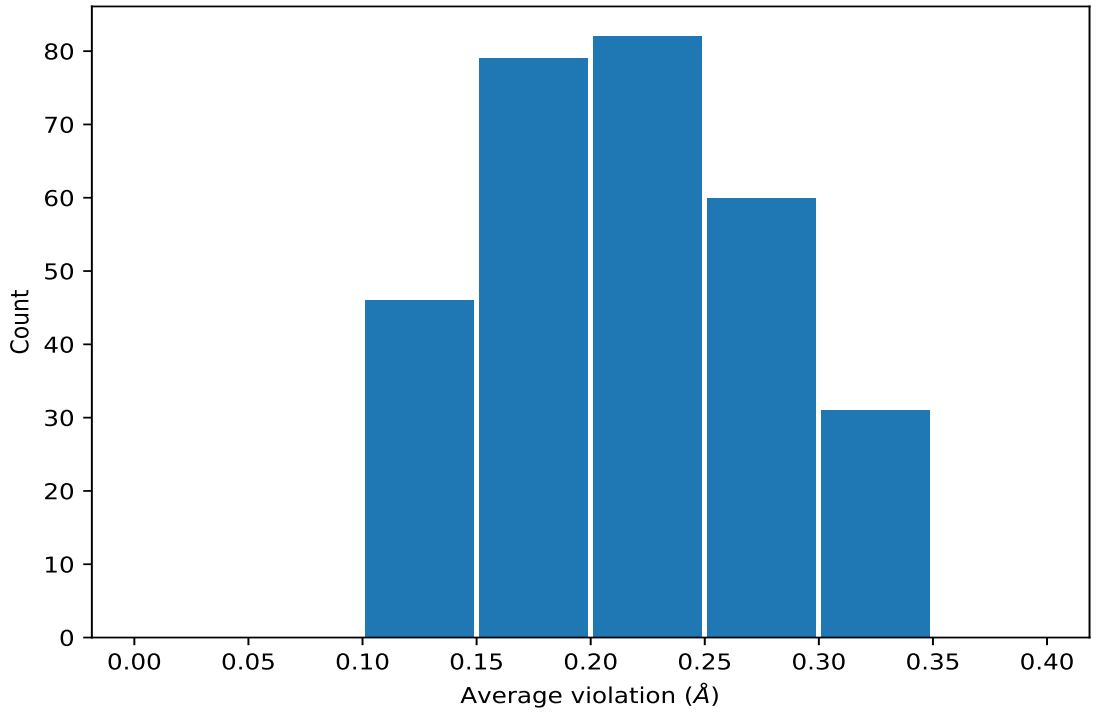
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	35	0.33	0.1	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	35	0.33	0.1	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	35	0.33	0.1	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	35	0.33	0.1	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	35	0.33	0.1	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	35	0.33	0.1	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	35	0.33	0.1	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	35	0.33	0.1	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	35	0.33	0.1	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	35	0.33	0.1	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	35	0.33	0.1	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	35	0.33	0.1	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	35	0.33	0.1	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	35	0.33	0.1	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	35	0.33	0.1	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	35	0.33	0.1	0.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	35	0.33	0.1	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	35	0.33	0.1	0.34
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	30	0.2	0.06	0.18
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	30	0.2	0.06	0.18
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	30	0.2	0.06	0.18
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	25	0.17	0.05	0.17
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	25	0.17	0.05	0.17
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	25	0.17	0.05	0.17
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	18	0.27	0.12	0.24
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	18	0.27	0.12	0.24
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	18	0.27	0.12	0.24
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	18	0.27	0.12	0.24
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	18	0.27	0.12	0.24
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	18	0.27	0.12	0.24
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	16	0.15	0.03	0.15
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG11	14	0.28	0.11	0.29
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG12	14	0.28	0.11	0.29
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG13	14	0.28	0.11	0.29
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG21	14	0.28	0.11	0.29
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG22	14	0.28	0.11	0.29
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG23	14	0.28	0.11	0.29
(3,21)	1:A:15:GLN:O	1:A:18:ASN:H	14	0.18	0.06	0.16
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE1	12	0.28	0.11	0.28
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE2	12	0.28	0.11	0.28
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE1	12	0.28	0.11	0.28
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE2	12	0.28	0.11	0.28
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE1	12	0.28	0.11	0.28
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE2	12	0.28	0.11	0.28
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE1	12	0.28	0.11	0.28
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE2	12	0.28	0.11	0.28
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE1	12	0.28	0.11	0.28
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE2	12	0.28	0.11	0.28
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE1	12	0.28	0.11	0.28
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE2	12	0.28	0.11	0.28
(1,17)	2:B:48:VAL:HG21	2:B:49:CYS:H	12	0.17	0.04	0.16
(1,17)	2:B:48:VAL:HG22	2:B:49:CYS:H	12	0.17	0.04	0.16
(1,17)	2:B:48:VAL:HG23	2:B:49:CYS:H	12	0.17	0.04	0.16
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB2	10	0.22	0.08	0.22
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB3	10	0.22	0.08	0.22
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB2	10	0.22	0.08	0.22
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB3	10	0.22	0.08	0.22
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB2	10	0.22	0.08	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB3	10	0.22	0.08	0.22
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB2	10	0.22	0.08	0.22
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB3	10	0.22	0.08	0.22
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB2	10	0.22	0.08	0.22
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB3	10	0.22	0.08	0.22
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB2	10	0.22	0.08	0.22
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB3	10	0.22	0.08	0.22
(3,17)	1:A:17:GLU:O	1:A:20:CYS:H	10	0.14	0.02	0.14
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD11	9	0.19	0.06	0.2
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD12	9	0.19	0.06	0.2
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD13	9	0.19	0.06	0.2
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD11	8	0.24	0.08	0.22
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD12	8	0.24	0.08	0.22
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD13	8	0.24	0.08	0.22
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD21	8	0.24	0.08	0.22
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD22	8	0.24	0.08	0.22
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD23	8	0.24	0.08	0.22
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE1	8	0.2	0.07	0.18
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE2	8	0.2	0.07	0.18
(1,18)	2:B:48:VAL:HG11	2:B:49:CYS:H	7	0.24	0.04	0.27
(1,18)	2:B:48:VAL:HG12	2:B:49:CYS:H	7	0.24	0.04	0.27
(1,18)	2:B:48:VAL:HG13	2:B:49:CYS:H	7	0.24	0.04	0.27
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG21	7	0.21	0.07	0.18
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG22	7	0.21	0.07	0.18
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG23	7	0.21	0.07	0.18
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD11	7	0.2	0.07	0.17
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD12	7	0.2	0.07	0.17
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD13	7	0.2	0.07	0.17
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD21	7	0.2	0.07	0.17
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD22	7	0.2	0.07	0.17
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD23	7	0.2	0.07	0.17
(1,210)	1:A:16:LEU:HD21	1:A:19:TYR:HD1	7	0.18	0.06	0.15
(1,210)	1:A:16:LEU:HD21	1:A:19:TYR:HD2	7	0.18	0.06	0.15
(1,210)	1:A:16:LEU:HD22	1:A:19:TYR:HD1	7	0.18	0.06	0.15
(1,210)	1:A:16:LEU:HD22	1:A:19:TYR:HD2	7	0.18	0.06	0.15
(1,210)	1:A:16:LEU:HD23	1:A:19:TYR:HD1	7	0.18	0.06	0.15
(1,210)	1:A:16:LEU:HD23	1:A:19:TYR:HD2	7	0.18	0.06	0.15
(1,6)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	7	0.16	0.02	0.15
(1,6)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	7	0.16	0.02	0.15
(1,6)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	7	0.16	0.02	0.15
(1,229)	1:A:2:ILE:HG12	1:A:19:TYR:HE1	7	0.15	0.02	0.14
(1,229)	1:A:2:ILE:HG12	1:A:19:TYR:HE2	7	0.15	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG21	6	0.24	0.1	0.2
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG22	6	0.24	0.1	0.2
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG23	6	0.24	0.1	0.2
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG21	6	0.24	0.1	0.2
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG22	6	0.24	0.1	0.2
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG23	6	0.24	0.1	0.2
(1,537)	2:B:49:CYS:HB2	2:B:50:GLY:H	6	0.22	0.06	0.2
(1,537)	2:B:49:CYS:HB3	2:B:50:GLY:H	6	0.22	0.06	0.2
(1,227)	1:A:2:ILE:HG21	1:A:19:TYR:HE1	6	0.2	0.08	0.18
(1,227)	1:A:2:ILE:HG21	1:A:19:TYR:HE2	6	0.2	0.08	0.18
(1,227)	1:A:2:ILE:HG22	1:A:19:TYR:HE1	6	0.2	0.08	0.18
(1,227)	1:A:2:ILE:HG22	1:A:19:TYR:HE2	6	0.2	0.08	0.18
(1,227)	1:A:2:ILE:HG23	1:A:19:TYR:HE1	6	0.2	0.08	0.18
(1,227)	1:A:2:ILE:HG23	1:A:19:TYR:HE2	6	0.2	0.08	0.18
(1,45)	1:A:2:ILE:H	1:A:19:TYR:HE1	6	0.2	0.07	0.18
(1,45)	1:A:2:ILE:H	1:A:19:TYR:HE2	6	0.2	0.07	0.18
(3,5)	2:B:44:ALA:O	2:B:48:VAL:H	6	0.15	0.04	0.14
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG11	6	0.15	0.05	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG12	6	0.15	0.05	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG13	6	0.15	0.05	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG21	6	0.15	0.05	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG22	6	0.15	0.05	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG23	6	0.15	0.05	0.13
(1,384)	2:B:32:VAL:HG11	2:B:33:ASN:HB2	6	0.15	0.03	0.15
(1,384)	2:B:32:VAL:HG11	2:B:33:ASN:HB3	6	0.15	0.03	0.15
(1,384)	2:B:32:VAL:HG12	2:B:33:ASN:HB2	6	0.15	0.03	0.15
(1,384)	2:B:32:VAL:HG12	2:B:33:ASN:HB3	6	0.15	0.03	0.15
(1,384)	2:B:32:VAL:HG13	2:B:33:ASN:HB2	6	0.15	0.03	0.15
(1,384)	2:B:32:VAL:HG13	2:B:33:ASN:HB3	6	0.15	0.03	0.15
(1,384)	2:B:32:VAL:HG21	2:B:33:ASN:HB2	6	0.15	0.03	0.15
(1,384)	2:B:32:VAL:HG21	2:B:33:ASN:HB3	6	0.15	0.03	0.15
(1,384)	2:B:32:VAL:HG22	2:B:33:ASN:HB2	6	0.15	0.03	0.15
(1,384)	2:B:32:VAL:HG22	2:B:33:ASN:HB3	6	0.15	0.03	0.15
(1,384)	2:B:32:VAL:HG23	2:B:33:ASN:HB2	6	0.15	0.03	0.15
(1,384)	2:B:32:VAL:HG23	2:B:33:ASN:HB3	6	0.15	0.03	0.15
(3,7)	2:B:43:GLU:O	2:B:47:LEU:H	6	0.14	0.03	0.15
(3,31)	1:A:1:GLY:O	1:A:5:GLN:H	6	0.14	0.02	0.13
(3,3)	2:B:45:LEU:O	2:B:49:CYS:H	6	0.13	0.02	0.13
(1,563)	1:A:13:LEU:HD11	2:B:31:PHE:HE1	5	0.29	0.05	0.29
(1,563)	1:A:13:LEU:HD11	2:B:31:PHE:HE2	5	0.29	0.05	0.29
(1,563)	1:A:13:LEU:HD12	2:B:31:PHE:HE1	5	0.29	0.05	0.29
(1,563)	1:A:13:LEU:HD12	2:B:31:PHE:HE2	5	0.29	0.05	0.29

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,563)	1:A:13:LEU:HD13	2:B:31:PHE:HE1	5	0.29	0.05	0.29
(1,563)	1:A:13:LEU:HD13	2:B:31:PHE:HE2	5	0.29	0.05	0.29
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD11	5	0.26	0.12	0.19
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD12	5	0.26	0.12	0.19
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD13	5	0.26	0.12	0.19
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD21	5	0.26	0.12	0.19
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD22	5	0.26	0.12	0.19
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD23	5	0.26	0.12	0.19
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD11	5	0.26	0.12	0.19
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD12	5	0.26	0.12	0.19
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD13	5	0.26	0.12	0.19
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD21	5	0.26	0.12	0.19
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD22	5	0.26	0.12	0.19
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD23	5	0.26	0.12	0.19
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG11	5	0.23	0.13	0.21
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG12	5	0.23	0.13	0.21
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG13	5	0.23	0.13	0.21
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG11	5	0.23	0.13	0.21
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG12	5	0.23	0.13	0.21
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG13	5	0.23	0.13	0.21
(3,1)	2:B:46:TYR:O	2:B:50:GLY:H	5	0.21	0.07	0.19
(1,416)	1:A:12:SER:HB2	1:A:14:TYR:HD1	5	0.19	0.05	0.19
(1,416)	1:A:12:SER:HB2	1:A:14:TYR:HD2	5	0.19	0.05	0.19
(1,416)	1:A:12:SER:HB3	1:A:14:TYR:HD1	5	0.19	0.05	0.19
(1,416)	1:A:12:SER:HB3	1:A:14:TYR:HD2	5	0.19	0.05	0.19
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG11	5	0.18	0.06	0.17
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG12	5	0.18	0.06	0.17
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG13	5	0.18	0.06	0.17
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG21	5	0.18	0.06	0.17
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG22	5	0.18	0.06	0.17
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG23	5	0.18	0.06	0.17
(1,375)	2:B:45:LEU:HA	2:B:48:VAL:HB	5	0.17	0.03	0.19
(1,493)	2:B:39:SER:HB2	2:B:40:HIS:HD2	5	0.17	0.06	0.15
(1,493)	2:B:39:SER:HB3	2:B:40:HIS:HD2	5	0.17	0.06	0.15
(1,225)	2:B:45:LEU:HG	2:B:54:PHE:HE1	5	0.17	0.07	0.14
(1,225)	2:B:45:LEU:HG	2:B:54:PHE:HE2	5	0.17	0.07	0.14
(1,327)	2:B:43:GLU:H	2:B:45:LEU:HB2	5	0.16	0.03	0.15
(1,338)	2:B:42:VAL:HB	2:B:54:PHE:HE1	5	0.14	0.03	0.14
(1,338)	2:B:42:VAL:HB	2:B:54:PHE:HE2	5	0.14	0.03	0.14
(3,11)	2:B:41:LEU:O	2:B:45:LEU:H	5	0.12	0.01	0.12
(1,354)	1:A:4:GLU:HG2	1:A:8:THR:HG21	4	0.3	0.12	0.34
(1,354)	1:A:4:GLU:HG2	1:A:8:THR:HG22	4	0.3	0.12	0.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,354)	1:A:4:GLU:HG2	1:A:8:THR:HG23	4	0.3	0.12	0.34
(1,354)	1:A:4:GLU:HG3	1:A:8:THR:HG21	4	0.3	0.12	0.34
(1,354)	1:A:4:GLU:HG3	1:A:8:THR:HG22	4	0.3	0.12	0.34
(1,354)	1:A:4:GLU:HG3	1:A:8:THR:HG23	4	0.3	0.12	0.34
(1,211)	1:A:19:TYR:HD1	2:B:45:LEU:HD21	4	0.22	0.07	0.22
(1,211)	1:A:19:TYR:HD1	2:B:45:LEU:HD22	4	0.22	0.07	0.22
(1,211)	1:A:19:TYR:HD1	2:B:45:LEU:HD23	4	0.22	0.07	0.22
(1,211)	1:A:19:TYR:HD2	2:B:45:LEU:HD21	4	0.22	0.07	0.22
(1,211)	1:A:19:TYR:HD2	2:B:45:LEU:HD22	4	0.22	0.07	0.22
(1,211)	1:A:19:TYR:HD2	2:B:45:LEU:HD23	4	0.22	0.07	0.22
(1,25)	2:B:36:LEU:HD11	2:B:45:LEU:H	4	0.2	0.06	0.21
(1,25)	2:B:36:LEU:HD12	2:B:45:LEU:H	4	0.2	0.06	0.21
(1,25)	2:B:36:LEU:HD13	2:B:45:LEU:H	4	0.2	0.06	0.21
(1,25)	2:B:36:LEU:HD21	2:B:45:LEU:H	4	0.2	0.06	0.21
(1,25)	2:B:36:LEU:HD22	2:B:45:LEU:H	4	0.2	0.06	0.21
(1,25)	2:B:36:LEU:HD23	2:B:45:LEU:H	4	0.2	0.06	0.21
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD11	4	0.2	0.09	0.2
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD12	4	0.2	0.09	0.2
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD13	4	0.2	0.09	0.2
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD21	4	0.2	0.09	0.2
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD22	4	0.2	0.09	0.2
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD23	4	0.2	0.09	0.2
(1,209)	1:A:2:ILE:HG21	1:A:19:TYR:HD1	4	0.17	0.03	0.18
(1,209)	1:A:2:ILE:HG21	1:A:19:TYR:HD2	4	0.17	0.03	0.18
(1,209)	1:A:2:ILE:HG22	1:A:19:TYR:HD1	4	0.17	0.03	0.18
(1,209)	1:A:2:ILE:HG22	1:A:19:TYR:HD2	4	0.17	0.03	0.18
(1,209)	1:A:2:ILE:HG23	1:A:19:TYR:HD1	4	0.17	0.03	0.18
(1,209)	1:A:2:ILE:HG23	1:A:19:TYR:HD2	4	0.17	0.03	0.18
(1,5)	1:A:10:ILE:HD11	2:B:35:HIS:HE1	4	0.17	0.08	0.12
(1,5)	1:A:10:ILE:HD12	2:B:35:HIS:HE1	4	0.17	0.08	0.12
(1,5)	1:A:10:ILE:HD13	2:B:35:HIS:HE1	4	0.17	0.08	0.12
(1,127)	2:B:37:CYS:H	2:B:40:HIS:HB3	4	0.14	0.03	0.14
(3,15)	2:B:39:SER:O	2:B:43:GLU:H	4	0.14	0.02	0.13
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD11	3	0.35	0.02	0.35
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD12	3	0.35	0.02	0.35
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD13	3	0.35	0.02	0.35
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD21	3	0.35	0.02	0.35
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD22	3	0.35	0.02	0.35
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD23	3	0.35	0.02	0.35
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD11	3	0.35	0.02	0.35
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD12	3	0.35	0.02	0.35
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD13	3	0.35	0.02	0.35

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD21	3	0.35	0.02	0.35
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD22	3	0.35	0.02	0.35
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD23	3	0.35	0.02	0.35
(1,155)	2:B:54:PHE:H	2:B:55:PHE:H	3	0.31	0.07	0.34
(1,301)	1:A:10:ILE:HD11	2:B:33:ASN:HB2	3	0.27	0.16	0.16
(1,301)	1:A:10:ILE:HD11	2:B:33:ASN:HB3	3	0.27	0.16	0.16
(1,301)	1:A:10:ILE:HD12	2:B:33:ASN:HB2	3	0.27	0.16	0.16
(1,301)	1:A:10:ILE:HD12	2:B:33:ASN:HB3	3	0.27	0.16	0.16
(1,301)	1:A:10:ILE:HD13	2:B:33:ASN:HB2	3	0.27	0.16	0.16
(1,301)	1:A:10:ILE:HD13	2:B:33:ASN:HB3	3	0.27	0.16	0.16
(1,566)	1:A:7:CYS:HA	1:A:8:THR:HG21	3	0.23	0.04	0.21
(1,566)	1:A:7:CYS:HA	1:A:8:THR:HG22	3	0.23	0.04	0.21
(1,566)	1:A:7:CYS:HA	1:A:8:THR:HG23	3	0.23	0.04	0.21
(1,178)	2:B:50:GLY:H	2:B:51:GLU:H	3	0.22	0.1	0.2
(1,242)	2:B:54:PHE:H	2:B:54:PHE:HE1	3	0.18	0.08	0.12
(1,242)	2:B:54:PHE:H	2:B:54:PHE:HE2	3	0.18	0.08	0.12
(1,136)	2:B:42:VAL:HG11	2:B:43:GLU:H	3	0.17	0.03	0.16
(1,136)	2:B:42:VAL:HG12	2:B:43:GLU:H	3	0.17	0.03	0.16
(1,136)	2:B:42:VAL:HG13	2:B:43:GLU:H	3	0.17	0.03	0.16
(1,337)	1:A:16:LEU:HG	1:A:19:TYR:HE1	3	0.17	0.02	0.18
(1,337)	1:A:16:LEU:HG	1:A:19:TYR:HE2	3	0.17	0.02	0.18
(1,104)	1:A:20:CYS:HA	1:A:21:ASN:H	3	0.16	0.02	0.16
(3,27)	1:A:3:VAL:O	1:A:7:CYS:H	3	0.14	0.04	0.12
(1,282)	1:A:13:LEU:HA	1:A:13:LEU:HD21	3	0.14	0.02	0.14
(1,282)	1:A:13:LEU:HA	1:A:13:LEU:HD22	3	0.14	0.02	0.14
(1,282)	1:A:13:LEU:HA	1:A:13:LEU:HD23	3	0.14	0.02	0.14
(1,233)	2:B:46:TYR:HE1	2:B:47:LEU:HA	3	0.14	0.03	0.13
(1,233)	2:B:46:TYR:HE2	2:B:47:LEU:HA	3	0.14	0.03	0.13
(1,191)	2:B:54:PHE:HA	2:B:55:PHE:H	3	0.13	0.01	0.14
(3,20)	1:A:16:LEU:O	1:A:19:TYR:N	3	0.13	0.01	0.13
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD11	2	0.26	0.05	0.26
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD12	2	0.26	0.05	0.26
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD13	2	0.26	0.05	0.26
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD21	2	0.26	0.05	0.26
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD22	2	0.26	0.05	0.26
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD23	2	0.26	0.05	0.26
(1,228)	1:A:2:ILE:HG13	1:A:19:TYR:HE1	2	0.24	0.04	0.24
(1,228)	1:A:2:ILE:HG13	1:A:19:TYR:HE2	2	0.24	0.04	0.24
(1,43)	2:B:46:TYR:HE1	2:B:53:GLY:H	2	0.19	0.01	0.19
(1,43)	2:B:46:TYR:HE2	2:B:53:GLY:H	2	0.19	0.01	0.19
(1,253)	2:B:48:VAL:HG21	2:B:49:CYS:HA	2	0.18	0.03	0.18
(1,253)	2:B:48:VAL:HG22	2:B:49:CYS:HA	2	0.18	0.03	0.18

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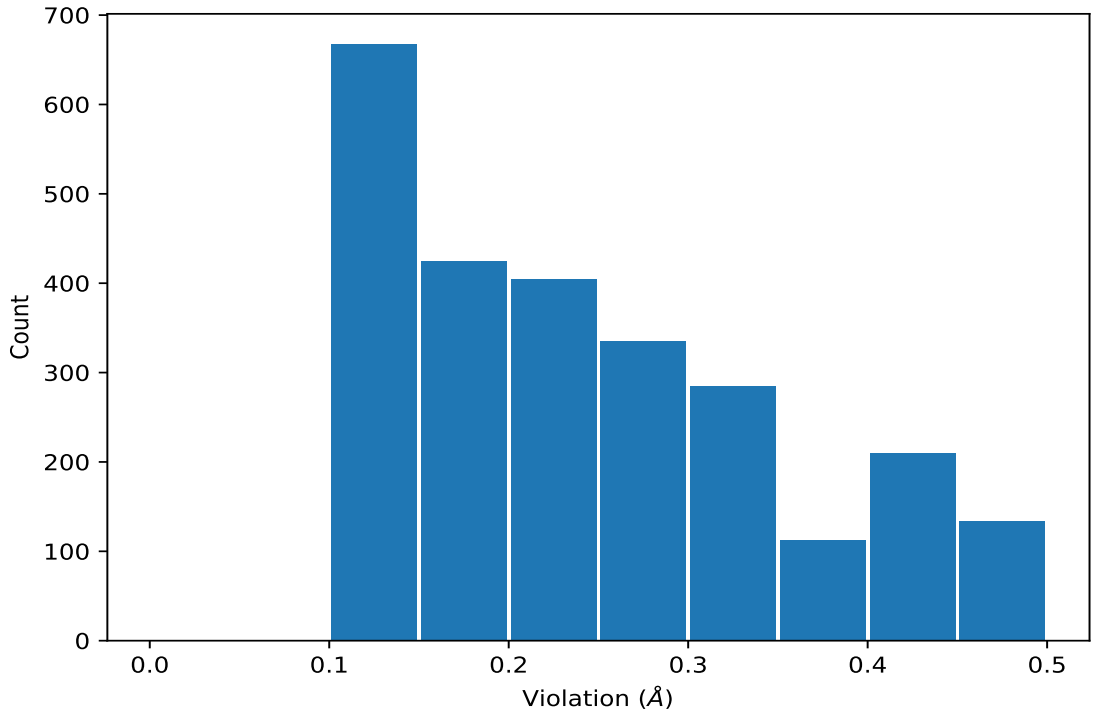
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,253)	2:B:48:VAL:HG23	2:B:49:CYS:HA	2	0.18	0.03	0.18
(1,433)	1:A:15:GLN:HA	1:A:18:ASN:HD21	2	0.17	0.02	0.17
(1,433)	1:A:15:GLN:HA	1:A:18:ASN:HD22	2	0.17	0.02	0.17
(1,326)	2:B:43:GLU:H	2:B:45:LEU:HB3	2	0.16	0.04	0.16
(1,483)	2:B:36:LEU:HB2	2:B:40:HIS:HB2	2	0.16	0.02	0.16
(1,483)	2:B:36:LEU:HB2	2:B:40:HIS:HB3	2	0.16	0.02	0.16
(1,483)	2:B:36:LEU:HB3	2:B:40:HIS:HB2	2	0.16	0.02	0.16
(1,483)	2:B:36:LEU:HB3	2:B:40:HIS:HB3	2	0.16	0.02	0.16
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG11	2	0.16	0.02	0.16
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG12	2	0.16	0.02	0.16
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG13	2	0.16	0.02	0.16
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG21	2	0.16	0.02	0.16
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG22	2	0.16	0.02	0.16
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG23	2	0.16	0.02	0.16
(1,352)	1:A:4:GLU:HA	1:A:8:THR:HG21	2	0.16	0.02	0.16
(1,352)	1:A:4:GLU:HA	1:A:8:THR:HG22	2	0.16	0.02	0.16
(1,352)	1:A:4:GLU:HA	1:A:8:THR:HG23	2	0.16	0.02	0.16
(1,422)	1:A:13:LEU:HB2	2:B:31:PHE:HD1	2	0.16	0.05	0.16
(1,422)	1:A:13:LEU:HB2	2:B:31:PHE:HD2	2	0.16	0.05	0.16
(1,422)	1:A:13:LEU:HB3	2:B:31:PHE:HD1	2	0.16	0.05	0.16
(1,422)	1:A:13:LEU:HB3	2:B:31:PHE:HD2	2	0.16	0.05	0.16
(1,330)	2:B:45:LEU:HB2	2:B:54:PHE:HE1	2	0.16	0.01	0.16
(1,330)	2:B:45:LEU:HB2	2:B:54:PHE:HE2	2	0.16	0.01	0.16
(1,84)	2:B:54:PHE:HB2	2:B:55:PHE:H	2	0.15	0.04	0.15
(3,6)	2:B:44:ALA:O	2:B:48:VAL:N	2	0.14	0.02	0.14
(1,377)	1:A:13:LEU:HA	1:A:13:LEU:HD11	2	0.12	0.02	0.12
(1,377)	1:A:13:LEU:HA	1:A:13:LEU:HD12	2	0.12	0.02	0.12
(1,377)	1:A:13:LEU:HA	1:A:13:LEU:HD13	2	0.12	0.02	0.12
(1,142)	2:B:42:VAL:HB	2:B:43:GLU:H	2	0.12	0.01	0.12
(3,13)	2:B:40:HIS:O	2:B:44:ALA:H	2	0.12	0.0	0.12

[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)
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	5	0.5
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	5	0.5
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	5	0.5
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	5	0.5
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	5	0.5
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	5	0.5
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	5	0.5
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	5	0.5
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	5	0.5
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	5	0.5
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	5	0.5
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	5	0.5
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	5	0.5
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	5	0.5
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	5	0.5
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	5	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	5	0.5
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	5	0.5
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE1	3	0.49
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE2	3	0.49
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE1	3	0.49
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE2	3	0.49
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE1	3	0.49
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE2	3	0.49
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE1	3	0.49
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE2	3	0.49
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE1	3	0.49
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE2	3	0.49
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE1	3	0.49
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE2	3	0.49
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	25	0.49
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	25	0.49
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	25	0.49
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	25	0.49
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	25	0.49
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	25	0.49
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	40	0.49
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	40	0.49
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	40	0.49
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	40	0.49
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	40	0.49
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	40	0.49
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	2	0.49
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	2	0.49
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	2	0.49
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	2	0.49
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	2	0.49
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	2	0.49
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	2	0.49
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	2	0.49
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	2	0.49
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	2	0.49
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	2	0.49
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	2	0.49
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	2	0.49
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	2	0.49
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	2	0.49
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	2	0.49
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	2	0.49
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	15	0.49
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	15	0.49
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	15	0.49
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	15	0.49
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	15	0.49
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	15	0.49
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	15	0.49
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	15	0.49
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	15	0.49
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	15	0.49
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	15	0.49
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	15	0.49
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	15	0.49
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	15	0.49
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	15	0.49
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	15	0.49
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	15	0.49
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	15	0.49
(1,301)	1:A:10:ILE:HD11	2:B:33:ASN:HB2	7	0.49
(1,301)	1:A:10:ILE:HD11	2:B:33:ASN:HB3	7	0.49
(1,301)	1:A:10:ILE:HD12	2:B:33:ASN:HB2	7	0.49
(1,301)	1:A:10:ILE:HD12	2:B:33:ASN:HB3	7	0.49
(1,301)	1:A:10:ILE:HD13	2:B:33:ASN:HB2	7	0.49
(1,301)	1:A:10:ILE:HD13	2:B:33:ASN:HB3	7	0.49
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	14	0.46
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	14	0.46
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	14	0.46
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	14	0.46
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	14	0.46
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	14	0.46
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	14	0.46
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	14	0.46
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	14	0.46
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	14	0.46
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	14	0.46
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	14	0.46
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	14	0.46
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	14	0.46
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	14	0.46
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	14	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	14	0.46
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	14	0.46
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG11	8	0.46
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG12	8	0.46
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG13	8	0.46
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG21	8	0.46
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG22	8	0.46
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG23	8	0.46
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG11	40	0.46
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG12	40	0.46
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG13	40	0.46
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG11	40	0.46
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG12	40	0.46
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG13	40	0.46
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG21	19	0.46
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG22	19	0.46
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG23	19	0.46
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG21	19	0.46
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG22	19	0.46
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG23	19	0.46
(1,232)	1:A:2:ILE:HA	1:A:19:TYR:HE1	39	0.46
(1,232)	1:A:2:ILE:HA	1:A:19:TYR:HE2	39	0.46
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD11	37	0.45
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD12	37	0.45
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD13	37	0.45
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD21	37	0.45
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD22	37	0.45
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD23	37	0.45
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD11	37	0.45
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD12	37	0.45
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD13	37	0.45
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD21	37	0.45
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD22	37	0.45
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD23	37	0.45
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG11	4	0.44
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG12	4	0.44
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG13	4	0.44
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG21	4	0.44
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG22	4	0.44
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG23	4	0.44
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB2	27	0.43
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB3	27	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB2	27	0.43
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB3	27	0.43
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB2	27	0.43
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB3	27	0.43
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB2	27	0.43
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB3	27	0.43
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB2	27	0.43
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB3	27	0.43
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB2	27	0.43
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB3	27	0.43
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	20	0.43
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	20	0.43
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	20	0.43
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	20	0.43
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	20	0.43
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	20	0.43
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	20	0.43
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	20	0.43
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	20	0.43
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	20	0.43
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	20	0.43
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	20	0.43
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	20	0.43
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	20	0.43
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	20	0.43
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	20	0.43
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	20	0.43
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	20	0.43
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	38	0.43
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	38	0.43
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	38	0.43
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	38	0.43
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	38	0.43
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	38	0.43
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	38	0.43
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	38	0.43
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	38	0.43
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	38	0.43
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	38	0.43
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	38	0.43
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	38	0.43
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	38	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	38	0.43
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	38	0.43
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	38	0.43
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	38	0.43
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE1	5	0.42
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE2	5	0.42
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE1	5	0.42
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE2	5	0.42
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE1	5	0.42
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE2	5	0.42
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE1	5	0.42
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE2	5	0.42
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE1	5	0.42
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE2	5	0.42
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE1	5	0.42
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE2	5	0.42
(1,450)	1:A:16:LEU:HD11	2:B:44:ALA:HB1	35	0.42
(1,450)	1:A:16:LEU:HD11	2:B:44:ALA:HB2	35	0.42
(1,450)	1:A:16:LEU:HD11	2:B:44:ALA:HB3	35	0.42
(1,450)	1:A:16:LEU:HD12	2:B:44:ALA:HB1	35	0.42
(1,450)	1:A:16:LEU:HD12	2:B:44:ALA:HB2	35	0.42
(1,450)	1:A:16:LEU:HD12	2:B:44:ALA:HB3	35	0.42
(1,450)	1:A:16:LEU:HD13	2:B:44:ALA:HB1	35	0.42
(1,450)	1:A:16:LEU:HD13	2:B:44:ALA:HB2	35	0.42
(1,450)	1:A:16:LEU:HD13	2:B:44:ALA:HB3	35	0.42
(1,450)	1:A:16:LEU:HD21	2:B:44:ALA:HB1	35	0.42
(1,450)	1:A:16:LEU:HD21	2:B:44:ALA:HB2	35	0.42
(1,450)	1:A:16:LEU:HD21	2:B:44:ALA:HB3	35	0.42
(1,450)	1:A:16:LEU:HD22	2:B:44:ALA:HB1	35	0.42
(1,450)	1:A:16:LEU:HD22	2:B:44:ALA:HB2	35	0.42
(1,450)	1:A:16:LEU:HD22	2:B:44:ALA:HB3	35	0.42
(1,450)	1:A:16:LEU:HD23	2:B:44:ALA:HB1	35	0.42
(1,450)	1:A:16:LEU:HD23	2:B:44:ALA:HB2	35	0.42
(1,450)	1:A:16:LEU:HD23	2:B:44:ALA:HB3	35	0.42
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	18	0.42
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	18	0.42
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	18	0.42
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	18	0.42
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	18	0.42
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	18	0.42
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	18	0.42
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	18	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	18	0.42
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	18	0.42
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	18	0.42
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	18	0.42
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	18	0.42
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	18	0.42
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	18	0.42
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	18	0.42
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	18	0.42
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	18	0.42
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	25	0.42
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	25	0.42
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	25	0.42
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	25	0.42
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	25	0.42
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	25	0.42
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	25	0.42
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	25	0.42
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	25	0.42
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	25	0.42
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	25	0.42
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	25	0.42
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	25	0.42
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	25	0.42
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	25	0.42
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	25	0.42
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	25	0.42
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	25	0.42
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	14	0.41
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	14	0.41
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	14	0.41
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	14	0.41
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	14	0.41
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	14	0.41
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	33	0.41
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	33	0.41
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	33	0.41
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	33	0.41
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	33	0.41
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	33	0.41
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	30	0.41
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	30	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	30	0.41
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	30	0.41
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	30	0.41
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	30	0.41
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	30	0.41
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	30	0.41
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	30	0.41
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	30	0.41
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	30	0.41
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	30	0.41
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	30	0.41
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	30	0.41
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	30	0.41
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	30	0.41
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	30	0.41
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	30	0.41
(1,354)	1:A:4:GLU:HG2	1:A:8:THR:HG21	37	0.41
(1,354)	1:A:4:GLU:HG2	1:A:8:THR:HG22	37	0.41
(1,354)	1:A:4:GLU:HG2	1:A:8:THR:HG23	37	0.41
(1,354)	1:A:4:GLU:HG3	1:A:8:THR:HG21	37	0.41
(1,354)	1:A:4:GLU:HG3	1:A:8:THR:HG22	37	0.41
(1,354)	1:A:4:GLU:HG3	1:A:8:THR:HG23	37	0.41
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	13	0.4
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	13	0.4
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	13	0.4
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	13	0.4
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	13	0.4
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	13	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	13	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	13	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	13	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	13	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	13	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	13	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	13	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	13	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	13	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	13	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	13	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	13	0.4
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	21	0.4
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	21	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	21	0.4
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	21	0.4
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	21	0.4
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	21	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	21	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	21	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	21	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	21	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	21	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	21	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	21	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	21	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	21	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	21	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	21	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	21	0.4
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	32	0.4
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	32	0.4
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	32	0.4
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	32	0.4
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	32	0.4
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	32	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	32	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	32	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	32	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	32	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	32	0.4
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	32	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	32	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	32	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	32	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	32	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	32	0.4
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	32	0.4
(1,354)	1:A:4:GLU:HG2	1:A:8:THR:HG21	18	0.39
(1,354)	1:A:4:GLU:HG2	1:A:8:THR:HG22	18	0.39
(1,354)	1:A:4:GLU:HG2	1:A:8:THR:HG23	18	0.39
(1,354)	1:A:4:GLU:HG3	1:A:8:THR:HG21	18	0.39
(1,354)	1:A:4:GLU:HG3	1:A:8:THR:HG22	18	0.39
(1,354)	1:A:4:GLU:HG3	1:A:8:THR:HG23	18	0.39
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG11	21	0.39
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG12	21	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG13	21	0.39
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG21	21	0.39
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG22	21	0.39
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG23	21	0.39
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG11	23	0.39
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG12	23	0.39
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG13	23	0.39
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG21	23	0.39
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG22	23	0.39
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG23	23	0.39
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	8	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	8	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	8	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	8	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	8	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	8	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	8	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	8	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	8	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	8	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	8	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	8	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	8	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	8	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	8	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	8	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	8	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	8	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	19	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	19	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	19	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	19	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	19	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	19	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	19	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	19	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	19	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	19	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	19	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	19	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	19	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	19	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	19	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	19	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	19	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	28	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	28	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	28	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	28	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	28	0.38
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	28	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	28	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	28	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	28	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	28	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	28	0.38
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	28	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	28	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	28	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	28	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	28	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	28	0.38
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	28	0.38
(1,155)	2:B:54:PHE:H	2:B:55:PHE:H	28	0.38
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE1	21	0.37
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE2	21	0.37
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE1	21	0.37
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE2	21	0.37
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE1	21	0.37
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE2	21	0.37
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE1	21	0.37
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE2	21	0.37
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE1	21	0.37
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE2	21	0.37
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE1	21	0.37
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE2	21	0.37
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD11	37	0.37
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD12	37	0.37
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD13	37	0.37
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD21	37	0.37
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD22	37	0.37
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD23	37	0.37
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD11	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD12	9	0.37
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD13	9	0.37
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD21	9	0.37
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD22	9	0.37
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD23	9	0.37
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD11	9	0.37
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD12	9	0.37
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD13	9	0.37
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD21	9	0.37
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD22	9	0.37
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD23	9	0.37
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG21	40	0.37
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG22	40	0.37
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG23	40	0.37
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG11	16	0.36
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG12	16	0.36
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG13	16	0.36
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG21	16	0.36
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG22	16	0.36
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG23	16	0.36
(1,537)	2:B:49:CYS:HB2	2:B:50:GLY:H	38	0.35
(1,537)	2:B:49:CYS:HB3	2:B:50:GLY:H	38	0.35
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	23	0.35
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	23	0.35
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	23	0.35
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	23	0.35
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	23	0.35
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	23	0.35
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	23	0.35
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	23	0.35
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	23	0.35
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	23	0.35
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	23	0.35
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	23	0.35
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	23	0.35
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	23	0.35
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	23	0.35
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	23	0.35
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	23	0.35
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	23	0.35
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD11	25	0.35
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD12	25	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD13	25	0.35
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD21	25	0.35
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD22	25	0.35
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD23	25	0.35
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD11	25	0.35
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD12	25	0.35
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD13	25	0.35
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD21	25	0.35
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD22	25	0.35
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD23	25	0.35
(1,178)	2:B:50:GLY:H	2:B:51:GLU:H	29	0.35
(1,563)	1:A:13:LEU:HD11	2:B:31:PHE:HE1	27	0.34
(1,563)	1:A:13:LEU:HD11	2:B:31:PHE:HE2	27	0.34
(1,563)	1:A:13:LEU:HD12	2:B:31:PHE:HE1	27	0.34
(1,563)	1:A:13:LEU:HD12	2:B:31:PHE:HE2	27	0.34
(1,563)	1:A:13:LEU:HD13	2:B:31:PHE:HE1	27	0.34
(1,563)	1:A:13:LEU:HD13	2:B:31:PHE:HE2	27	0.34
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE1	39	0.34
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE2	39	0.34
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE1	39	0.34
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE2	39	0.34
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE1	39	0.34
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE2	39	0.34
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE1	39	0.34
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE2	39	0.34
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE1	39	0.34
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE2	39	0.34
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE1	39	0.34
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE2	39	0.34
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE1	38	0.34
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE2	38	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	3	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	3	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	3	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	3	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	3	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	3	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	3	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	3	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	3	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	3	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	3	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	3	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	3	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	3	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	3	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	3	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	3	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	24	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	24	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	24	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	24	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	24	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	24	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	24	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	24	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	24	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	24	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	24	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	24	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	24	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	24	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	24	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	24	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	24	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	24	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	36	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	36	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	36	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	36	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	36	0.34
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	36	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	36	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	36	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	36	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	36	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	36	0.34
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	36	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	36	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	36	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	36	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	36	0.34
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	36	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	36	0.34
(1,259)	1:A:10:ILE:HD11	2:B:34:GLN:HA	35	0.34
(1,259)	1:A:10:ILE:HD12	2:B:34:GLN:HA	35	0.34
(1,259)	1:A:10:ILE:HD13	2:B:34:GLN:HA	35	0.34
(1,227)	1:A:2:ILE:HG21	1:A:19:TYR:HE1	35	0.34
(1,227)	1:A:2:ILE:HG21	1:A:19:TYR:HE2	35	0.34
(1,227)	1:A:2:ILE:HG22	1:A:19:TYR:HE1	35	0.34
(1,227)	1:A:2:ILE:HG22	1:A:19:TYR:HE2	35	0.34
(1,227)	1:A:2:ILE:HG23	1:A:19:TYR:HE1	35	0.34
(1,227)	1:A:2:ILE:HG23	1:A:19:TYR:HE2	35	0.34
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD11	28	0.34
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD12	28	0.34
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD13	28	0.34
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD21	28	0.34
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD22	28	0.34
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD23	28	0.34
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD11	28	0.34
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD12	28	0.34
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD13	28	0.34
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD21	28	0.34
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD22	28	0.34
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD23	28	0.34
(1,155)	2:B:54:PHE:H	2:B:55:PHE:H	34	0.34
(1,563)	1:A:13:LEU:HD11	2:B:31:PHE:HE1	20	0.33
(1,563)	1:A:13:LEU:HD11	2:B:31:PHE:HE2	20	0.33
(1,563)	1:A:13:LEU:HD12	2:B:31:PHE:HE1	20	0.33
(1,563)	1:A:13:LEU:HD12	2:B:31:PHE:HE2	20	0.33
(1,563)	1:A:13:LEU:HD13	2:B:31:PHE:HE1	20	0.33
(1,563)	1:A:13:LEU:HD13	2:B:31:PHE:HE2	20	0.33
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	36	0.33
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	36	0.33
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	36	0.33
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	33	0.33
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	33	0.33
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	33	0.33
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	33	0.33
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	33	0.33
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	33	0.33
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	33	0.33
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	33	0.33
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	33	0.33
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	33	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	33	0.33
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	33	0.33
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	33	0.33
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	33	0.33
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	33	0.33
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	33	0.33
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	33	0.33
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	33	0.33
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD11	39	0.33
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD12	39	0.33
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD13	39	0.33
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD21	39	0.33
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD22	39	0.33
(1,302)	2:B:43:GLU:HG2	2:B:47:LEU:HD23	39	0.33
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD11	39	0.33
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD12	39	0.33
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD13	39	0.33
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD21	39	0.33
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD22	39	0.33
(1,302)	2:B:43:GLU:HG3	2:B:47:LEU:HD23	39	0.33
(3,21)	1:A:15:GLN:O	1:A:18:ASN:H	39	0.32
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	28	0.32
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	28	0.32
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	28	0.32
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD11	22	0.32
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD12	22	0.32
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD13	22	0.32
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD21	22	0.32
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD22	22	0.32
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD23	22	0.32
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	22	0.32
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	22	0.32
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	22	0.32
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	22	0.32
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	22	0.32
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	22	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	10	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	10	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	10	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	10	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	10	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	10	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	10	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	10	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	10	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	10	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	10	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	10	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	10	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	10	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	10	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	10	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	10	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	12	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	12	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	12	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	12	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	12	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	12	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	12	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	12	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	12	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	12	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	12	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	12	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	12	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	12	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	12	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	12	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	12	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	12	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	39	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	39	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	39	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	39	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	39	0.32
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	39	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	39	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	39	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	39	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	39	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	39	0.32
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	39	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	39	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	39	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	39	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	39	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	39	0.32
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	39	0.32
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG11	22	0.32
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG12	22	0.32
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG13	22	0.32
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG21	22	0.32
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG22	22	0.32
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG23	22	0.32
(1,211)	1:A:19:TYR:HD1	2:B:45:LEU:HD21	34	0.32
(1,211)	1:A:19:TYR:HD1	2:B:45:LEU:HD22	34	0.32
(1,211)	1:A:19:TYR:HD1	2:B:45:LEU:HD23	34	0.32
(1,211)	1:A:19:TYR:HD2	2:B:45:LEU:HD21	34	0.32
(1,211)	1:A:19:TYR:HD2	2:B:45:LEU:HD22	34	0.32
(1,211)	1:A:19:TYR:HD2	2:B:45:LEU:HD23	34	0.32
(1,5)	1:A:10:ILE:HD11	2:B:35:HIS:HE1	37	0.31
(1,5)	1:A:10:ILE:HD12	2:B:35:HIS:HE1	37	0.31
(1,5)	1:A:10:ILE:HD13	2:B:35:HIS:HE1	37	0.31
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD11	34	0.31
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD12	34	0.31
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD13	34	0.31
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD21	34	0.31
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD22	34	0.31
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD23	34	0.31
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD11	34	0.31
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD12	34	0.31
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD13	34	0.31
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD21	34	0.31
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD22	34	0.31
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD23	34	0.31
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	29	0.31
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	29	0.31
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	29	0.31
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	29	0.31
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	29	0.31
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	29	0.31
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	29	0.31
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	29	0.31
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	29	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	29	0.31
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	29	0.31
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	29	0.31
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	29	0.31
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	29	0.31
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	29	0.31
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	29	0.31
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	29	0.31
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	29	0.31
(1,225)	2:B:45:LEU:HG	2:B:54:PHE:HE1	38	0.31
(1,225)	2:B:45:LEU:HG	2:B:54:PHE:HE2	38	0.31
(3,1)	2:B:46:TYR:O	2:B:50:GLY:H	38	0.3
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	14	0.3
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	14	0.3
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	14	0.3
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE1	34	0.3
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE2	34	0.3
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE1	34	0.3
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE2	34	0.3
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE1	34	0.3
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE2	34	0.3
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE1	34	0.3
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE2	34	0.3
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE1	34	0.3
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE2	34	0.3
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE1	34	0.3
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE2	34	0.3
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD11	11	0.3
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD12	11	0.3
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD13	11	0.3
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD21	11	0.3
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD22	11	0.3
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD23	11	0.3
(1,45)	1:A:2:ILE:H	1:A:19:TYR:HE1	18	0.3
(1,45)	1:A:2:ILE:H	1:A:19:TYR:HE2	18	0.3
(1,354)	1:A:4:GLU:HG2	1:A:8:THR:HG21	25	0.3
(1,354)	1:A:4:GLU:HG2	1:A:8:THR:HG22	25	0.3
(1,354)	1:A:4:GLU:HG2	1:A:8:THR:HG23	25	0.3
(1,354)	1:A:4:GLU:HG3	1:A:8:THR:HG21	25	0.3
(1,354)	1:A:4:GLU:HG3	1:A:8:THR:HG22	25	0.3
(1,354)	1:A:4:GLU:HG3	1:A:8:THR:HG23	25	0.3
(1,112)	1:A:10:ILE:HD11	2:B:35:HIS:HD2	35	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,112)	1:A:10:ILE:HD12	2:B:35:HIS:HD2	35	0.3
(1,112)	1:A:10:ILE:HD13	2:B:35:HIS:HD2	35	0.3
(1,563)	1:A:13:LEU:HD11	2:B:31:PHE:HE1	8	0.29
(1,563)	1:A:13:LEU:HD11	2:B:31:PHE:HE2	8	0.29
(1,563)	1:A:13:LEU:HD12	2:B:31:PHE:HE1	8	0.29
(1,563)	1:A:13:LEU:HD12	2:B:31:PHE:HE2	8	0.29
(1,563)	1:A:13:LEU:HD13	2:B:31:PHE:HE1	8	0.29
(1,563)	1:A:13:LEU:HD13	2:B:31:PHE:HE2	8	0.29
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	15	0.29
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	15	0.29
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	15	0.29
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE1	38	0.29
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE2	38	0.29
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE1	38	0.29
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE2	38	0.29
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE1	38	0.29
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE2	38	0.29
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE1	38	0.29
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE2	38	0.29
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE1	38	0.29
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE2	38	0.29
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE1	38	0.29
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE2	38	0.29
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	37	0.29
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	37	0.29
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	37	0.29
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	37	0.29
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	37	0.29
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	37	0.29
(1,45)	1:A:2:ILE:H	1:A:19:TYR:HE1	30	0.29
(1,45)	1:A:2:ILE:H	1:A:19:TYR:HE2	30	0.29
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG11	25	0.29
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG12	25	0.29
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG13	25	0.29
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG21	25	0.29
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG22	25	0.29
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG23	25	0.29
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD11	24	0.29
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD12	24	0.29
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD13	24	0.29
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD21	24	0.29
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD22	24	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD23	24	0.29
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD11	31	0.29
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD12	31	0.29
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD13	31	0.29
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD21	31	0.29
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD22	31	0.29
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD23	31	0.29
(1,242)	2:B:54:PHE:H	2:B:54:PHE:HE1	19	0.29
(1,242)	2:B:54:PHE:H	2:B:54:PHE:HE2	19	0.29
(1,210)	1:A:16:LEU:HD21	1:A:19:TYR:HD1	26	0.29
(1,210)	1:A:16:LEU:HD21	1:A:19:TYR:HD2	26	0.29
(1,210)	1:A:16:LEU:HD22	1:A:19:TYR:HD1	26	0.29
(1,210)	1:A:16:LEU:HD22	1:A:19:TYR:HD2	26	0.29
(1,210)	1:A:16:LEU:HD23	1:A:19:TYR:HD1	26	0.29
(1,210)	1:A:16:LEU:HD23	1:A:19:TYR:HD2	26	0.29
(1,566)	1:A:7:CYS:HA	1:A:8:THR:HG21	23	0.28
(1,566)	1:A:7:CYS:HA	1:A:8:THR:HG22	23	0.28
(1,566)	1:A:7:CYS:HA	1:A:8:THR:HG23	23	0.28
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	21	0.28
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	21	0.28
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	21	0.28
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	37	0.28
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	37	0.28
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	37	0.28
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG11	10	0.28
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG12	10	0.28
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG13	10	0.28
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG21	10	0.28
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG22	10	0.28
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG23	10	0.28
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	20	0.28
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	20	0.28
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	20	0.28
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	20	0.28
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	20	0.28
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	20	0.28
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	4	0.28
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	4	0.28
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	4	0.28
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	4	0.28
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	4	0.28
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	4	0.28
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	4	0.28
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	4	0.28
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	4	0.28
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	4	0.28
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	4	0.28
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	4	0.28
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	4	0.28
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	4	0.28
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	4	0.28
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	4	0.28
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	4	0.28
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD11	9	0.28
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD12	9	0.28
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD13	9	0.28
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	39	0.28
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	39	0.28
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	39	0.28
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG11	28	0.28
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG12	28	0.28
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG13	28	0.28
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG21	28	0.28
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG22	28	0.28
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG23	28	0.28
(1,228)	1:A:2:ILE:HG13	1:A:19:TYR:HE1	26	0.28
(1,228)	1:A:2:ILE:HG13	1:A:19:TYR:HE2	26	0.28
(1,18)	2:B:48:VAL:HG11	2:B:49:CYS:H	31	0.28
(1,18)	2:B:48:VAL:HG12	2:B:49:CYS:H	31	0.28
(1,18)	2:B:48:VAL:HG13	2:B:49:CYS:H	31	0.28
(3,1)	2:B:46:TYR:O	2:B:50:GLY:H	33	0.27
(1,563)	1:A:13:LEU:HD11	2:B:31:PHE:HE1	6	0.27
(1,563)	1:A:13:LEU:HD11	2:B:31:PHE:HE2	6	0.27
(1,563)	1:A:13:LEU:HD12	2:B:31:PHE:HE1	6	0.27
(1,563)	1:A:13:LEU:HD12	2:B:31:PHE:HE2	6	0.27
(1,563)	1:A:13:LEU:HD13	2:B:31:PHE:HE1	6	0.27
(1,563)	1:A:13:LEU:HD13	2:B:31:PHE:HE2	6	0.27
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	1	0.27
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	1	0.27
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	1	0.27
(1,493)	2:B:39:SER:HB2	2:B:40:HIS:HD2	31	0.27
(1,493)	2:B:39:SER:HB3	2:B:40:HIS:HD2	31	0.27
(1,416)	1:A:12:SER:HB2	1:A:14:TYR:HD1	40	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,416)	1:A:12:SER:HB2	1:A:14:TYR:HD2	40	0.27
(1,416)	1:A:12:SER:HB3	1:A:14:TYR:HD1	40	0.27
(1,416)	1:A:12:SER:HB3	1:A:14:TYR:HD2	40	0.27
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	34	0.27
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	34	0.27
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	34	0.27
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	34	0.27
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	34	0.27
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	34	0.27
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	34	0.27
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	34	0.27
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	34	0.27
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	34	0.27
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	34	0.27
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	34	0.27
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	34	0.27
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	34	0.27
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	34	0.27
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	34	0.27
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	34	0.27
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	34	0.27
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	40	0.27
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	40	0.27
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	40	0.27
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	40	0.27
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	40	0.27
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	40	0.27
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	40	0.27
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	40	0.27
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	40	0.27
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	40	0.27
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	40	0.27
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	40	0.27
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	40	0.27
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	40	0.27
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	40	0.27
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	40	0.27
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	40	0.27
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	40	0.27
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD11	40	0.27
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD12	40	0.27
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD13	40	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	33	0.27
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	33	0.27
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	33	0.27
(1,25)	2:B:36:LEU:HD11	2:B:45:LEU:H	36	0.27
(1,25)	2:B:36:LEU:HD12	2:B:45:LEU:H	36	0.27
(1,25)	2:B:36:LEU:HD13	2:B:45:LEU:H	36	0.27
(1,25)	2:B:36:LEU:HD21	2:B:45:LEU:H	36	0.27
(1,25)	2:B:36:LEU:HD22	2:B:45:LEU:H	36	0.27
(1,25)	2:B:36:LEU:HD23	2:B:45:LEU:H	36	0.27
(1,18)	2:B:48:VAL:HG11	2:B:49:CYS:H	13	0.27
(1,18)	2:B:48:VAL:HG12	2:B:49:CYS:H	13	0.27
(1,18)	2:B:48:VAL:HG13	2:B:49:CYS:H	13	0.27
(1,18)	2:B:48:VAL:HG11	2:B:49:CYS:H	20	0.27
(1,18)	2:B:48:VAL:HG12	2:B:49:CYS:H	20	0.27
(1,18)	2:B:48:VAL:HG13	2:B:49:CYS:H	20	0.27
(1,18)	2:B:48:VAL:HG11	2:B:49:CYS:H	37	0.27
(1,18)	2:B:48:VAL:HG12	2:B:49:CYS:H	37	0.27
(1,18)	2:B:48:VAL:HG13	2:B:49:CYS:H	37	0.27
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE1	40	0.26
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE2	40	0.26
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE1	40	0.26
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE2	40	0.26
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE1	40	0.26
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE2	40	0.26
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE1	40	0.26
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE2	40	0.26
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE1	40	0.26
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE2	40	0.26
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE1	40	0.26
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE2	40	0.26
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB2	2	0.26
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB3	2	0.26
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB2	2	0.26
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB3	2	0.26
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB2	2	0.26
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB3	2	0.26
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB2	2	0.26
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB3	2	0.26
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB2	2	0.26
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB3	2	0.26
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB2	2	0.26
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB3	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD11	19	0.26
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD12	19	0.26
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD13	19	0.26
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD21	19	0.26
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD22	19	0.26
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD23	19	0.26
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	17	0.26
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	17	0.26
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	17	0.26
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	17	0.26
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	17	0.26
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	17	0.26
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD11	4	0.26
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD12	4	0.26
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD13	4	0.26
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD21	4	0.26
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD22	4	0.26
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD23	4	0.26
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD11	23	0.26
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD12	23	0.26
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD13	23	0.26
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD21	23	0.26
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD22	23	0.26
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD23	23	0.26
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	28	0.26
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	28	0.26
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	28	0.26
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG11	22	0.26
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG12	22	0.26
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG13	22	0.26
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG11	22	0.26
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG12	22	0.26
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG13	22	0.26
(1,227)	1:A:2:ILE:HG21	1:A:19:TYR:HE1	40	0.26
(1,227)	1:A:2:ILE:HG21	1:A:19:TYR:HE2	40	0.26
(1,227)	1:A:2:ILE:HG22	1:A:19:TYR:HE1	40	0.26
(1,227)	1:A:2:ILE:HG22	1:A:19:TYR:HE2	40	0.26
(1,227)	1:A:2:ILE:HG23	1:A:19:TYR:HE1	40	0.26
(1,227)	1:A:2:ILE:HG23	1:A:19:TYR:HE2	40	0.26
(1,211)	1:A:19:TYR:HD1	2:B:45:LEU:HD21	38	0.26
(1,211)	1:A:19:TYR:HD1	2:B:45:LEU:HD22	38	0.26
(1,211)	1:A:19:TYR:HD1	2:B:45:LEU:HD23	38	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,211)	1:A:19:TYR:HD2	2:B:45:LEU:HD21	38	0.26
(1,211)	1:A:19:TYR:HD2	2:B:45:LEU:HD22	38	0.26
(1,211)	1:A:19:TYR:HD2	2:B:45:LEU:HD23	38	0.26
(3,21)	1:A:15:GLN:O	1:A:18:ASN:H	17	0.25
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	12	0.25
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	12	0.25
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	12	0.25
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	12	0.25
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	12	0.25
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	12	0.25
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	9	0.25
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	9	0.25
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	9	0.25
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	9	0.25
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	9	0.25
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	9	0.25
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	9	0.25
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	9	0.25
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	9	0.25
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	9	0.25
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	9	0.25
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	9	0.25
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	9	0.25
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	9	0.25
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	9	0.25
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	9	0.25
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	9	0.25
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	9	0.25
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	31	0.25
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	31	0.25
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	31	0.25
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	31	0.25
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	31	0.25
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	31	0.25
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	31	0.25
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	31	0.25
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	31	0.25
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	31	0.25
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	31	0.25
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	31	0.25
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	31	0.25
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	31	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	31	0.25
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	31	0.25
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	31	0.25
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	31	0.25
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD11	37	0.25
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD12	37	0.25
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD13	37	0.25
(1,17)	2:B:48:VAL:HG21	2:B:49:CYS:H	30	0.25
(1,17)	2:B:48:VAL:HG22	2:B:49:CYS:H	30	0.25
(1,17)	2:B:48:VAL:HG23	2:B:49:CYS:H	30	0.25
(3,21)	1:A:15:GLN:O	1:A:18:ASN:H	1	0.24
(3,21)	1:A:15:GLN:O	1:A:18:ASN:H	20	0.24
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	39	0.24
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	39	0.24
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	39	0.24
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB2	9	0.24
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB3	9	0.24
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB2	9	0.24
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB3	9	0.24
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB2	9	0.24
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB3	9	0.24
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB2	9	0.24
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB3	9	0.24
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB2	9	0.24
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB3	9	0.24
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB2	9	0.24
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB3	9	0.24
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG11	27	0.24
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG12	27	0.24
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG13	27	0.24
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG21	27	0.24
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG22	27	0.24
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG23	27	0.24
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE1	27	0.24
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE2	27	0.24
(1,394)	1:A:2:ILE:HG21	2:B:45:LEU:HD11	39	0.24
(1,394)	1:A:2:ILE:HG21	2:B:45:LEU:HD12	39	0.24
(1,394)	1:A:2:ILE:HG21	2:B:45:LEU:HD13	39	0.24
(1,394)	1:A:2:ILE:HG21	2:B:45:LEU:HD21	39	0.24
(1,394)	1:A:2:ILE:HG21	2:B:45:LEU:HD22	39	0.24
(1,394)	1:A:2:ILE:HG21	2:B:45:LEU:HD23	39	0.24
(1,394)	1:A:2:ILE:HG22	2:B:45:LEU:HD11	39	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,394)	1:A:2:ILE:HG22	2:B:45:LEU:HD12	39	0.24
(1,394)	1:A:2:ILE:HG22	2:B:45:LEU:HD13	39	0.24
(1,394)	1:A:2:ILE:HG22	2:B:45:LEU:HD21	39	0.24
(1,394)	1:A:2:ILE:HG22	2:B:45:LEU:HD22	39	0.24
(1,394)	1:A:2:ILE:HG22	2:B:45:LEU:HD23	39	0.24
(1,394)	1:A:2:ILE:HG23	2:B:45:LEU:HD11	39	0.24
(1,394)	1:A:2:ILE:HG23	2:B:45:LEU:HD12	39	0.24
(1,394)	1:A:2:ILE:HG23	2:B:45:LEU:HD13	39	0.24
(1,394)	1:A:2:ILE:HG23	2:B:45:LEU:HD21	39	0.24
(1,394)	1:A:2:ILE:HG23	2:B:45:LEU:HD22	39	0.24
(1,394)	1:A:2:ILE:HG23	2:B:45:LEU:HD23	39	0.24
(1,379)	1:A:13:LEU:HD21	2:B:31:PHE:HB2	17	0.24
(1,379)	1:A:13:LEU:HD21	2:B:31:PHE:HB3	17	0.24
(1,379)	1:A:13:LEU:HD22	2:B:31:PHE:HB2	17	0.24
(1,379)	1:A:13:LEU:HD22	2:B:31:PHE:HB3	17	0.24
(1,379)	1:A:13:LEU:HD23	2:B:31:PHE:HB2	17	0.24
(1,379)	1:A:13:LEU:HD23	2:B:31:PHE:HB3	17	0.24
(1,300)	1:A:10:ILE:HG21	2:B:33:ASN:HB2	7	0.24
(1,300)	1:A:10:ILE:HG21	2:B:33:ASN:HB3	7	0.24
(1,300)	1:A:10:ILE:HG22	2:B:33:ASN:HB2	7	0.24
(1,300)	1:A:10:ILE:HG22	2:B:33:ASN:HB3	7	0.24
(1,300)	1:A:10:ILE:HG23	2:B:33:ASN:HB2	7	0.24
(1,300)	1:A:10:ILE:HG23	2:B:33:ASN:HB3	7	0.24
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG21	12	0.24
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG22	12	0.24
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG23	12	0.24
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG21	12	0.24
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG22	12	0.24
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG23	12	0.24
(1,17)	2:B:48:VAL:HG21	2:B:49:CYS:H	17	0.24
(1,17)	2:B:48:VAL:HG22	2:B:49:CYS:H	17	0.24
(1,17)	2:B:48:VAL:HG23	2:B:49:CYS:H	17	0.24
(3,5)	2:B:44:ALA:O	2:B:48:VAL:H	27	0.23
(3,21)	1:A:15:GLN:O	1:A:18:ASN:H	38	0.23
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	9	0.23
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	9	0.23
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	9	0.23
(1,537)	2:B:49:CYS:HB2	2:B:50:GLY:H	29	0.23
(1,537)	2:B:49:CYS:HB3	2:B:50:GLY:H	29	0.23
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE1	25	0.23
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE2	25	0.23
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE1	25	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE2	25	0.23
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE1	25	0.23
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE2	25	0.23
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE1	25	0.23
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE2	25	0.23
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE1	25	0.23
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE2	25	0.23
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE1	25	0.23
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE2	25	0.23
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG11	17	0.23
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG12	17	0.23
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG13	17	0.23
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG21	17	0.23
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG22	17	0.23
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG23	17	0.23
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	2	0.23
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	2	0.23
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	2	0.23
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	2	0.23
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	2	0.23
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	2	0.23
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	30	0.23
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	30	0.23
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	30	0.23
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	30	0.23
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	30	0.23
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	30	0.23
(1,391)	2:B:37:CYS:H	2:B:40:HIS:H	32	0.23
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG11	3	0.23
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG12	3	0.23
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG13	3	0.23
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG21	3	0.23
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG22	3	0.23
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG23	3	0.23
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG21	38	0.23
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG22	38	0.23
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG23	38	0.23
(1,267)	1:A:17:GLU:HA	2:B:48:VAL:HG11	24	0.23
(1,267)	1:A:17:GLU:HA	2:B:48:VAL:HG12	24	0.23
(1,267)	1:A:17:GLU:HA	2:B:48:VAL:HG13	24	0.23
(1,25)	2:B:36:LEU:HD11	2:B:45:LEU:H	12	0.23
(1,25)	2:B:36:LEU:HD12	2:B:45:LEU:H	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	2:B:36:LEU:HD13	2:B:45:LEU:H	12	0.23
(1,25)	2:B:36:LEU:HD21	2:B:45:LEU:H	12	0.23
(1,25)	2:B:36:LEU:HD22	2:B:45:LEU:H	12	0.23
(1,25)	2:B:36:LEU:HD23	2:B:45:LEU:H	12	0.23
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	11	0.22
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	30	0.22
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	30	0.22
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	30	0.22
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	33	0.22
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	33	0.22
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	33	0.22
(1,537)	2:B:49:CYS:HB2	2:B:50:GLY:H	22	0.22
(1,537)	2:B:49:CYS:HB3	2:B:50:GLY:H	22	0.22
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB2	7	0.22
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB3	7	0.22
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB2	7	0.22
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB3	7	0.22
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB2	7	0.22
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB3	7	0.22
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB2	7	0.22
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB3	7	0.22
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB2	7	0.22
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB3	7	0.22
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB2	7	0.22
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB3	7	0.22
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB2	26	0.22
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB3	26	0.22
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB2	26	0.22
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB3	26	0.22
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB2	26	0.22
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB3	26	0.22
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB2	26	0.22
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB3	26	0.22
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB2	26	0.22
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB3	26	0.22
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB2	26	0.22
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB3	26	0.22
(1,478)	2:B:34:GLN:HG2	2:B:36:LEU:HD11	31	0.22
(1,478)	2:B:34:GLN:HG2	2:B:36:LEU:HD12	31	0.22
(1,478)	2:B:34:GLN:HG2	2:B:36:LEU:HD13	31	0.22
(1,478)	2:B:34:GLN:HG2	2:B:36:LEU:HD21	31	0.22
(1,478)	2:B:34:GLN:HG2	2:B:36:LEU:HD22	31	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	2:B:34:GLN:HG2	2:B:36:LEU:HD23	31	0.22
(1,478)	2:B:34:GLN:HG3	2:B:36:LEU:HD11	31	0.22
(1,478)	2:B:34:GLN:HG3	2:B:36:LEU:HD12	31	0.22
(1,478)	2:B:34:GLN:HG3	2:B:36:LEU:HD13	31	0.22
(1,478)	2:B:34:GLN:HG3	2:B:36:LEU:HD21	31	0.22
(1,478)	2:B:34:GLN:HG3	2:B:36:LEU:HD22	31	0.22
(1,478)	2:B:34:GLN:HG3	2:B:36:LEU:HD23	31	0.22
(1,458)	1:A:17:GLU:HA	2:B:48:VAL:HG11	38	0.22
(1,458)	1:A:17:GLU:HA	2:B:48:VAL:HG12	38	0.22
(1,458)	1:A:17:GLU:HA	2:B:48:VAL:HG13	38	0.22
(1,458)	1:A:17:GLU:HA	2:B:48:VAL:HG21	38	0.22
(1,458)	1:A:17:GLU:HA	2:B:48:VAL:HG22	38	0.22
(1,458)	1:A:17:GLU:HA	2:B:48:VAL:HG23	38	0.22
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	15	0.22
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	15	0.22
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	15	0.22
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	15	0.22
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	15	0.22
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	15	0.22
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	21	0.22
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	21	0.22
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	21	0.22
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	21	0.22
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	21	0.22
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	21	0.22
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE1	21	0.22
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE2	21	0.22
(1,18)	2:B:48:VAL:HG11	2:B:49:CYS:H	26	0.22
(1,18)	2:B:48:VAL:HG12	2:B:49:CYS:H	26	0.22
(1,18)	2:B:48:VAL:HG13	2:B:49:CYS:H	26	0.22
(1,18)	2:B:48:VAL:HG11	2:B:49:CYS:H	27	0.22
(1,18)	2:B:48:VAL:HG12	2:B:49:CYS:H	27	0.22
(1,18)	2:B:48:VAL:HG13	2:B:49:CYS:H	27	0.22
(1,17)	2:B:48:VAL:HG21	2:B:49:CYS:H	32	0.22
(1,17)	2:B:48:VAL:HG22	2:B:49:CYS:H	32	0.22
(1,17)	2:B:48:VAL:HG23	2:B:49:CYS:H	32	0.22
(1,155)	2:B:54:PHE:H	2:B:55:PHE:H	36	0.22
(1,566)	1:A:7:CYS:HA	1:A:8:THR:HG21	37	0.21
(1,566)	1:A:7:CYS:HA	1:A:8:THR:HG22	37	0.21
(1,566)	1:A:7:CYS:HA	1:A:8:THR:HG23	37	0.21
(1,563)	1:A:13:LEU:HD11	2:B:31:PHE:HE1	3	0.21
(1,563)	1:A:13:LEU:HD11	2:B:31:PHE:HE2	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	1:A:13:LEU:HD12	2:B:31:PHE:HE1	3	0.21
(1,563)	1:A:13:LEU:HD12	2:B:31:PHE:HE2	3	0.21
(1,563)	1:A:13:LEU:HD13	2:B:31:PHE:HE1	3	0.21
(1,563)	1:A:13:LEU:HD13	2:B:31:PHE:HE2	3	0.21
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	19	0.21
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	19	0.21
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	19	0.21
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE1	29	0.21
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE2	29	0.21
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE1	29	0.21
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE2	29	0.21
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE1	29	0.21
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE2	29	0.21
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE1	29	0.21
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE2	29	0.21
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE1	29	0.21
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE2	29	0.21
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE1	29	0.21
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE2	29	0.21
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB2	40	0.21
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB3	40	0.21
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB2	40	0.21
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB3	40	0.21
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB2	40	0.21
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB3	40	0.21
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB2	40	0.21
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB3	40	0.21
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB2	40	0.21
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB3	40	0.21
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB2	40	0.21
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB3	40	0.21
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD11	3	0.21
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD12	3	0.21
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD13	3	0.21
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD21	3	0.21
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD22	3	0.21
(1,444)	1:A:16:LEU:HG	2:B:45:LEU:HD23	3	0.21
(1,422)	1:A:13:LEU:HB2	2:B:31:PHE:HD1	11	0.21
(1,422)	1:A:13:LEU:HB2	2:B:31:PHE:HD2	11	0.21
(1,422)	1:A:13:LEU:HB3	2:B:31:PHE:HD1	11	0.21
(1,422)	1:A:13:LEU:HB3	2:B:31:PHE:HD2	11	0.21
(1,416)	1:A:12:SER:HB2	1:A:14:TYR:HD1	28	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,416)	1:A:12:SER:HB2	1:A:14:TYR:HD2	28	0.21
(1,416)	1:A:12:SER:HB3	1:A:14:TYR:HD1	28	0.21
(1,416)	1:A:12:SER:HB3	1:A:14:TYR:HD2	28	0.21
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	27	0.21
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	27	0.21
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	27	0.21
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	27	0.21
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	27	0.21
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	27	0.21
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	27	0.21
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	27	0.21
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	27	0.21
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	27	0.21
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	27	0.21
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	27	0.21
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	27	0.21
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	27	0.21
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	27	0.21
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	27	0.21
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	27	0.21
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	27	0.21
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD11	16	0.21
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD12	16	0.21
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD13	16	0.21
(1,375)	2:B:45:LEU:HA	2:B:48:VAL:HB	20	0.21
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	12	0.21
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	12	0.21
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	12	0.21
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	15	0.21
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	15	0.21
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	15	0.21
(1,314)	1:A:16:LEU:HD11	2:B:44:ALA:HB1	36	0.21
(1,314)	1:A:16:LEU:HD11	2:B:44:ALA:HB2	36	0.21
(1,314)	1:A:16:LEU:HD11	2:B:44:ALA:HB3	36	0.21
(1,314)	1:A:16:LEU:HD12	2:B:44:ALA:HB1	36	0.21
(1,314)	1:A:16:LEU:HD12	2:B:44:ALA:HB2	36	0.21
(1,314)	1:A:16:LEU:HD12	2:B:44:ALA:HB3	36	0.21
(1,314)	1:A:16:LEU:HD13	2:B:44:ALA:HB1	36	0.21
(1,314)	1:A:16:LEU:HD13	2:B:44:ALA:HB2	36	0.21
(1,314)	1:A:16:LEU:HD13	2:B:44:ALA:HB3	36	0.21
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG11	7	0.21
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG12	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG13	7	0.21
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG11	7	0.21
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG12	7	0.21
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG13	7	0.21
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG21	20	0.21
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG22	20	0.21
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG23	20	0.21
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG21	20	0.21
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG22	20	0.21
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG23	20	0.21
(1,210)	1:A:16:LEU:HD21	1:A:19:TYR:HD1	36	0.21
(1,210)	1:A:16:LEU:HD21	1:A:19:TYR:HD2	36	0.21
(1,210)	1:A:16:LEU:HD22	1:A:19:TYR:HD1	36	0.21
(1,210)	1:A:16:LEU:HD22	1:A:19:TYR:HD2	36	0.21
(1,210)	1:A:16:LEU:HD23	1:A:19:TYR:HD1	36	0.21
(1,210)	1:A:16:LEU:HD23	1:A:19:TYR:HD2	36	0.21
(1,210)	1:A:16:LEU:HD21	1:A:19:TYR:HD1	37	0.21
(1,210)	1:A:16:LEU:HD21	1:A:19:TYR:HD2	37	0.21
(1,210)	1:A:16:LEU:HD22	1:A:19:TYR:HD1	37	0.21
(1,210)	1:A:16:LEU:HD22	1:A:19:TYR:HD2	37	0.21
(1,210)	1:A:16:LEU:HD23	1:A:19:TYR:HD1	37	0.21
(1,210)	1:A:16:LEU:HD23	1:A:19:TYR:HD2	37	0.21
(1,136)	2:B:42:VAL:HG11	2:B:43:GLU:H	39	0.21
(1,136)	2:B:42:VAL:HG12	2:B:43:GLU:H	39	0.21
(1,136)	2:B:42:VAL:HG13	2:B:43:GLU:H	39	0.21
(3,27)	1:A:3:VAL:O	1:A:7:CYS:H	21	0.2
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	10	0.2
(1,566)	1:A:7:CYS:HA	1:A:8:THR:HG21	36	0.2
(1,566)	1:A:7:CYS:HA	1:A:8:THR:HG22	36	0.2
(1,566)	1:A:7:CYS:HA	1:A:8:THR:HG23	36	0.2
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	29	0.2
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	29	0.2
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	29	0.2
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB2	10	0.2
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB3	10	0.2
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB2	10	0.2
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB3	10	0.2
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB2	10	0.2
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB3	10	0.2
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB2	10	0.2
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB3	10	0.2
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB2	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB3	10	0.2
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB2	10	0.2
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB3	10	0.2
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	31	0.2
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	31	0.2
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	31	0.2
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	31	0.2
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	31	0.2
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	31	0.2
(1,43)	2:B:46:TYR:HE1	2:B:53:GLY:H	38	0.2
(1,43)	2:B:46:TYR:HE2	2:B:53:GLY:H	38	0.2
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	11	0.2
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	11	0.2
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	11	0.2
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	11	0.2
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	11	0.2
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	11	0.2
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	11	0.2
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	11	0.2
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	11	0.2
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	11	0.2
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	11	0.2
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	11	0.2
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	11	0.2
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	11	0.2
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	11	0.2
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	11	0.2
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	11	0.2
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	11	0.2
(1,384)	2:B:32:VAL:HG11	2:B:33:ASN:HB2	5	0.2
(1,384)	2:B:32:VAL:HG11	2:B:33:ASN:HB3	5	0.2
(1,384)	2:B:32:VAL:HG12	2:B:33:ASN:HB2	5	0.2
(1,384)	2:B:32:VAL:HG12	2:B:33:ASN:HB3	5	0.2
(1,384)	2:B:32:VAL:HG13	2:B:33:ASN:HB2	5	0.2
(1,384)	2:B:32:VAL:HG13	2:B:33:ASN:HB3	5	0.2
(1,384)	2:B:32:VAL:HG21	2:B:33:ASN:HB2	5	0.2
(1,384)	2:B:32:VAL:HG21	2:B:33:ASN:HB3	5	0.2
(1,384)	2:B:32:VAL:HG22	2:B:33:ASN:HB2	5	0.2
(1,384)	2:B:32:VAL:HG22	2:B:33:ASN:HB3	5	0.2
(1,384)	2:B:32:VAL:HG23	2:B:33:ASN:HB2	5	0.2
(1,384)	2:B:32:VAL:HG23	2:B:33:ASN:HB3	5	0.2
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD11	31	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD12	31	0.2
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD13	31	0.2
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	4	0.2
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	4	0.2
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	4	0.2
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	10	0.2
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	10	0.2
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	10	0.2
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	36	0.2
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	36	0.2
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	36	0.2
(1,327)	2:B:43:GLU:H	2:B:45:LEU:HB2	40	0.2
(1,326)	2:B:43:GLU:H	2:B:45:LEU:HB3	32	0.2
(1,253)	2:B:48:VAL:HG21	2:B:49:CYS:HA	5	0.2
(1,253)	2:B:48:VAL:HG22	2:B:49:CYS:HA	5	0.2
(1,253)	2:B:48:VAL:HG23	2:B:49:CYS:HA	5	0.2
(1,228)	1:A:2:ILE:HG13	1:A:19:TYR:HE1	5	0.2
(1,228)	1:A:2:ILE:HG13	1:A:19:TYR:HE2	5	0.2
(1,227)	1:A:2:ILE:HG21	1:A:19:TYR:HE1	20	0.2
(1,227)	1:A:2:ILE:HG21	1:A:19:TYR:HE2	20	0.2
(1,227)	1:A:2:ILE:HG22	1:A:19:TYR:HE1	20	0.2
(1,227)	1:A:2:ILE:HG22	1:A:19:TYR:HE2	20	0.2
(1,227)	1:A:2:ILE:HG23	1:A:19:TYR:HE1	20	0.2
(1,227)	1:A:2:ILE:HG23	1:A:19:TYR:HE2	20	0.2
(1,209)	1:A:2:ILE:HG21	1:A:19:TYR:HD1	29	0.2
(1,209)	1:A:2:ILE:HG21	1:A:19:TYR:HD2	29	0.2
(1,209)	1:A:2:ILE:HG22	1:A:19:TYR:HD1	29	0.2
(1,209)	1:A:2:ILE:HG22	1:A:19:TYR:HD2	29	0.2
(1,209)	1:A:2:ILE:HG23	1:A:19:TYR:HD1	29	0.2
(1,209)	1:A:2:ILE:HG23	1:A:19:TYR:HD2	29	0.2
(1,209)	1:A:2:ILE:HG21	1:A:19:TYR:HD1	37	0.2
(1,209)	1:A:2:ILE:HG21	1:A:19:TYR:HD2	37	0.2
(1,209)	1:A:2:ILE:HG22	1:A:19:TYR:HD1	37	0.2
(1,209)	1:A:2:ILE:HG22	1:A:19:TYR:HD2	37	0.2
(1,209)	1:A:2:ILE:HG23	1:A:19:TYR:HD1	37	0.2
(1,209)	1:A:2:ILE:HG23	1:A:19:TYR:HD2	37	0.2
(1,178)	2:B:50:GLY:H	2:B:51:GLU:H	37	0.2
(3,7)	2:B:43:GLU:O	2:B:47:LEU:H	34	0.19
(3,5)	2:B:44:ALA:O	2:B:48:VAL:H	28	0.19
(3,21)	1:A:15:GLN:O	1:A:18:ASN:H	11	0.19
(3,1)	2:B:46:TYR:O	2:B:50:GLY:H	22	0.19
(1,84)	2:B:54:PHE:HB2	2:B:55:PHE:H	25	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	36	0.19
(1,6)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	36	0.19
(1,6)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	36	0.19
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	11	0.19
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	11	0.19
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	11	0.19
(1,537)	2:B:49:CYS:HB2	2:B:50:GLY:H	33	0.19
(1,537)	2:B:49:CYS:HB3	2:B:50:GLY:H	33	0.19
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG11	7	0.19
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG12	7	0.19
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG13	7	0.19
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG21	7	0.19
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG22	7	0.19
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG23	7	0.19
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD11	25	0.19
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD12	25	0.19
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD13	25	0.19
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD21	25	0.19
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD22	25	0.19
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD23	25	0.19
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD11	31	0.19
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD12	31	0.19
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD13	31	0.19
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD21	31	0.19
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD22	31	0.19
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD23	31	0.19
(1,493)	2:B:39:SER:HB2	2:B:40:HIS:HD2	14	0.19
(1,493)	2:B:39:SER:HB3	2:B:40:HIS:HD2	14	0.19
(1,483)	2:B:36:LEU:HB2	2:B:40:HIS:HB2	8	0.19
(1,483)	2:B:36:LEU:HB2	2:B:40:HIS:HB3	8	0.19
(1,483)	2:B:36:LEU:HB3	2:B:40:HIS:HB2	8	0.19
(1,483)	2:B:36:LEU:HB3	2:B:40:HIS:HB3	8	0.19
(1,45)	1:A:2:ILE:H	1:A:19:TYR:HE1	35	0.19
(1,45)	1:A:2:ILE:H	1:A:19:TYR:HE2	35	0.19
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE1	25	0.19
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE2	25	0.19
(1,433)	1:A:15:GLN:HA	1:A:18:ASN:HD21	21	0.19
(1,433)	1:A:15:GLN:HA	1:A:18:ASN:HD22	21	0.19
(1,416)	1:A:12:SER:HB2	1:A:14:TYR:HD1	9	0.19
(1,416)	1:A:12:SER:HB2	1:A:14:TYR:HD2	9	0.19
(1,416)	1:A:12:SER:HB3	1:A:14:TYR:HD1	9	0.19
(1,416)	1:A:12:SER:HB3	1:A:14:TYR:HD2	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	2:B:45:LEU:HA	2:B:48:VAL:HB	26	0.19
(1,375)	2:B:45:LEU:HA	2:B:48:VAL:HB	31	0.19
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	19	0.19
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	19	0.19
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	19	0.19
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	25	0.19
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	25	0.19
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	25	0.19
(1,338)	2:B:42:VAL:HB	2:B:54:PHE:HE1	11	0.19
(1,338)	2:B:42:VAL:HB	2:B:54:PHE:HE2	11	0.19
(1,337)	1:A:16:LEU:HG	1:A:19:TYR:HE1	16	0.19
(1,337)	1:A:16:LEU:HG	1:A:19:TYR:HE2	16	0.19
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG11	6	0.19
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG12	6	0.19
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG13	6	0.19
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG21	6	0.19
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG22	6	0.19
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG23	6	0.19
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG21	36	0.19
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG22	36	0.19
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG23	36	0.19
(1,25)	2:B:36:LEU:HD11	2:B:45:LEU:H	28	0.19
(1,25)	2:B:36:LEU:HD12	2:B:45:LEU:H	28	0.19
(1,25)	2:B:36:LEU:HD13	2:B:45:LEU:H	28	0.19
(1,25)	2:B:36:LEU:HD21	2:B:45:LEU:H	28	0.19
(1,25)	2:B:36:LEU:HD22	2:B:45:LEU:H	28	0.19
(1,25)	2:B:36:LEU:HD23	2:B:45:LEU:H	28	0.19
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG21	33	0.19
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG22	33	0.19
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG23	33	0.19
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG21	33	0.19
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG22	33	0.19
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG23	33	0.19
(1,229)	1:A:2:ILE:HG12	1:A:19:TYR:HE1	27	0.19
(1,229)	1:A:2:ILE:HG12	1:A:19:TYR:HE2	27	0.19
(1,211)	1:A:19:TYR:HD1	2:B:45:LEU:HD21	28	0.19
(1,211)	1:A:19:TYR:HD1	2:B:45:LEU:HD22	28	0.19
(1,211)	1:A:19:TYR:HD1	2:B:45:LEU:HD23	28	0.19
(1,211)	1:A:19:TYR:HD2	2:B:45:LEU:HD21	28	0.19
(1,211)	1:A:19:TYR:HD2	2:B:45:LEU:HD22	28	0.19
(1,211)	1:A:19:TYR:HD2	2:B:45:LEU:HD23	28	0.19
(1,17)	2:B:48:VAL:HG21	2:B:49:CYS:H	39	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	2:B:48:VAL:HG22	2:B:49:CYS:H	39	0.19
(1,17)	2:B:48:VAL:HG23	2:B:49:CYS:H	39	0.19
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD11	6	0.19
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD12	6	0.19
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD13	6	0.19
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD21	6	0.19
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD22	6	0.19
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD23	6	0.19
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD11	6	0.19
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD12	6	0.19
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD13	6	0.19
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD21	6	0.19
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD22	6	0.19
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD23	6	0.19
(1,104)	1:A:20:CYS:HA	1:A:21:ASN:H	32	0.19
(3,8)	2:B:43:GLU:O	2:B:47:LEU:N	34	0.18
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	6	0.18
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	16	0.18
(3,17)	1:A:17:GLU:O	1:A:20:CYS:H	30	0.18
(1,6)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	28	0.18
(1,6)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	28	0.18
(1,6)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	28	0.18
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	7	0.18
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	7	0.18
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	7	0.18
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	16	0.18
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	16	0.18
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	16	0.18
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	17	0.18
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	17	0.18
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	17	0.18
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	34	0.18
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	34	0.18
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	34	0.18
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	40	0.18
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	40	0.18
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	40	0.18
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE1	33	0.18
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE2	33	0.18
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE1	33	0.18
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE2	33	0.18
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE1	33	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE2	33	0.18
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE1	33	0.18
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE2	33	0.18
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE1	33	0.18
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE2	33	0.18
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE1	33	0.18
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE2	33	0.18
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD11	18	0.18
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD12	18	0.18
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD13	18	0.18
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD21	18	0.18
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD22	18	0.18
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD23	18	0.18
(1,475)	2:B:34:GLN:H	2:B:34:GLN:HG2	31	0.18
(1,475)	2:B:34:GLN:H	2:B:34:GLN:HG3	31	0.18
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG11	38	0.18
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG12	38	0.18
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG13	38	0.18
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG21	38	0.18
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG22	38	0.18
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG23	38	0.18
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE1	29	0.18
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE2	29	0.18
(1,43)	2:B:46:TYR:HE1	2:B:53:GLY:H	40	0.18
(1,43)	2:B:46:TYR:HE2	2:B:53:GLY:H	40	0.18
(1,420)	1:A:13:LEU:HA	1:A:16:LEU:HD11	34	0.18
(1,420)	1:A:13:LEU:HA	1:A:16:LEU:HD12	34	0.18
(1,420)	1:A:13:LEU:HA	1:A:16:LEU:HD13	34	0.18
(1,420)	1:A:13:LEU:HA	1:A:16:LEU:HD21	34	0.18
(1,420)	1:A:13:LEU:HA	1:A:16:LEU:HD22	34	0.18
(1,420)	1:A:13:LEU:HA	1:A:16:LEU:HD23	34	0.18
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	17	0.18
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	17	0.18
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	17	0.18
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	17	0.18
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	17	0.18
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	17	0.18
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	17	0.18
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	17	0.18
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	17	0.18
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	17	0.18
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	17	0.18
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	17	0.18
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	17	0.18
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	17	0.18
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	17	0.18
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	17	0.18
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	17	0.18
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	1	0.18
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	1	0.18
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	1	0.18
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	23	0.18
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	23	0.18
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	23	0.18
(1,352)	1:A:4:GLU:HA	1:A:8:THR:HG21	11	0.18
(1,352)	1:A:4:GLU:HA	1:A:8:THR:HG22	11	0.18
(1,352)	1:A:4:GLU:HA	1:A:8:THR:HG23	11	0.18
(1,337)	1:A:16:LEU:HG	1:A:19:TYR:HE1	13	0.18
(1,337)	1:A:16:LEU:HG	1:A:19:TYR:HE2	13	0.18
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG11	11	0.18
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG12	11	0.18
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG13	11	0.18
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG21	11	0.18
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG22	11	0.18
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG23	11	0.18
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG11	13	0.18
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG12	13	0.18
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG13	13	0.18
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG21	13	0.18
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG22	13	0.18
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG23	13	0.18
(1,327)	2:B:43:GLU:H	2:B:45:LEU:HB2	33	0.18
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG21	7	0.18
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG22	7	0.18
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG23	7	0.18
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG21	8	0.18
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG22	8	0.18
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG23	8	0.18
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG21	22	0.18
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG22	22	0.18
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG23	22	0.18
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG21	28	0.18
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG22	28	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG23	28	0.18
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG21	28	0.18
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG22	28	0.18
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG23	28	0.18
(1,233)	2:B:46:TYR:HE1	2:B:47:LEU:HA	37	0.18
(1,233)	2:B:46:TYR:HE2	2:B:47:LEU:HA	37	0.18
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD11	17	0.18
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD12	17	0.18
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD13	17	0.18
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD21	17	0.18
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD22	17	0.18
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD23	17	0.18
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD11	17	0.18
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD12	17	0.18
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD13	17	0.18
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD21	17	0.18
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD22	17	0.18
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD23	17	0.18
(1,127)	2:B:37:CYS:H	2:B:40:HIS:HB3	28	0.18
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	19	0.17
(3,17)	1:A:17:GLU:O	1:A:20:CYS:H	16	0.17
(3,17)	1:A:17:GLU:O	1:A:20:CYS:H	18	0.17
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	4	0.17
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	4	0.17
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	4	0.17
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	23	0.17
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	23	0.17
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	23	0.17
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG11	30	0.17
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG12	30	0.17
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG13	30	0.17
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG21	30	0.17
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG22	30	0.17
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG23	30	0.17
(1,463)	1:A:18:ASN:HB2	1:A:19:TYR:HD1	39	0.17
(1,463)	1:A:18:ASN:HB2	1:A:19:TYR:HD2	39	0.17
(1,463)	1:A:18:ASN:HB3	1:A:19:TYR:HD1	39	0.17
(1,463)	1:A:18:ASN:HB3	1:A:19:TYR:HD2	39	0.17
(1,45)	1:A:2:ILE:H	1:A:19:TYR:HE1	29	0.17
(1,45)	1:A:2:ILE:H	1:A:19:TYR:HE2	29	0.17
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD11	6	0.17
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD12	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD13	6	0.17
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD21	6	0.17
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD22	6	0.17
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD23	6	0.17
(1,384)	2:B:32:VAL:HG11	2:B:33:ASN:HB2	30	0.17
(1,384)	2:B:32:VAL:HG11	2:B:33:ASN:HB3	30	0.17
(1,384)	2:B:32:VAL:HG12	2:B:33:ASN:HB2	30	0.17
(1,384)	2:B:32:VAL:HG12	2:B:33:ASN:HB3	30	0.17
(1,384)	2:B:32:VAL:HG13	2:B:33:ASN:HB2	30	0.17
(1,384)	2:B:32:VAL:HG13	2:B:33:ASN:HB3	30	0.17
(1,384)	2:B:32:VAL:HG21	2:B:33:ASN:HB2	30	0.17
(1,384)	2:B:32:VAL:HG21	2:B:33:ASN:HB3	30	0.17
(1,384)	2:B:32:VAL:HG22	2:B:33:ASN:HB2	30	0.17
(1,384)	2:B:32:VAL:HG22	2:B:33:ASN:HB3	30	0.17
(1,384)	2:B:32:VAL:HG23	2:B:33:ASN:HB2	30	0.17
(1,384)	2:B:32:VAL:HG23	2:B:33:ASN:HB3	30	0.17
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	14	0.17
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	14	0.17
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	14	0.17
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	30	0.17
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	30	0.17
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	30	0.17
(1,312)	1:A:16:LEU:HD11	2:B:45:LEU:HB2	39	0.17
(1,312)	1:A:16:LEU:HD12	2:B:45:LEU:HB2	39	0.17
(1,312)	1:A:16:LEU:HD13	2:B:45:LEU:HB2	39	0.17
(1,282)	1:A:13:LEU:HA	1:A:13:LEU:HD21	27	0.17
(1,282)	1:A:13:LEU:HA	1:A:13:LEU:HD22	27	0.17
(1,282)	1:A:13:LEU:HA	1:A:13:LEU:HD23	27	0.17
(1,229)	1:A:2:ILE:HG12	1:A:19:TYR:HE1	32	0.17
(1,229)	1:A:2:ILE:HG12	1:A:19:TYR:HE2	32	0.17
(1,17)	2:B:48:VAL:HG21	2:B:49:CYS:H	8	0.17
(1,17)	2:B:48:VAL:HG22	2:B:49:CYS:H	8	0.17
(1,17)	2:B:48:VAL:HG23	2:B:49:CYS:H	8	0.17
(1,17)	2:B:48:VAL:HG21	2:B:49:CYS:H	34	0.17
(1,17)	2:B:48:VAL:HG22	2:B:49:CYS:H	34	0.17
(1,17)	2:B:48:VAL:HG23	2:B:49:CYS:H	34	0.17
(1,118)	2:B:33:ASN:HA	2:B:34:GLN:H	36	0.17
(3,7)	2:B:43:GLU:O	2:B:47:LEU:H	11	0.16
(3,7)	2:B:43:GLU:O	2:B:47:LEU:H	22	0.16
(3,31)	1:A:1:GLY:O	1:A:5:GLN:H	9	0.16
(3,31)	1:A:1:GLY:O	1:A:5:GLN:H	35	0.16
(3,3)	2:B:45:LEU:O	2:B:49:CYS:H	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,3)	2:B:45:LEU:O	2:B:49:CYS:H	18	0.16
(3,21)	1:A:15:GLN:O	1:A:18:ASN:H	14	0.16
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	1	0.16
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	29	0.16
(3,15)	2:B:39:SER:O	2:B:43:GLU:H	32	0.16
(3,1)	2:B:46:TYR:O	2:B:50:GLY:H	5	0.16
(1,6)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	14	0.16
(1,6)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	14	0.16
(1,6)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	14	0.16
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	25	0.16
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	25	0.16
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	25	0.16
(1,537)	2:B:49:CYS:HB2	2:B:50:GLY:H	23	0.16
(1,537)	2:B:49:CYS:HB3	2:B:50:GLY:H	23	0.16
(1,537)	2:B:49:CYS:HB2	2:B:50:GLY:H	25	0.16
(1,537)	2:B:49:CYS:HB3	2:B:50:GLY:H	25	0.16
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB2	16	0.16
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB3	16	0.16
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB2	16	0.16
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB3	16	0.16
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB2	16	0.16
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB3	16	0.16
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB2	16	0.16
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB3	16	0.16
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB2	16	0.16
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB3	16	0.16
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB2	16	0.16
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB3	16	0.16
(1,472)	2:B:31:PHE:HD1	2:B:48:VAL:HG11	35	0.16
(1,472)	2:B:31:PHE:HD1	2:B:48:VAL:HG12	35	0.16
(1,472)	2:B:31:PHE:HD1	2:B:48:VAL:HG13	35	0.16
(1,472)	2:B:31:PHE:HD1	2:B:48:VAL:HG21	35	0.16
(1,472)	2:B:31:PHE:HD1	2:B:48:VAL:HG22	35	0.16
(1,472)	2:B:31:PHE:HD1	2:B:48:VAL:HG23	35	0.16
(1,472)	2:B:31:PHE:HD2	2:B:48:VAL:HG11	35	0.16
(1,472)	2:B:31:PHE:HD2	2:B:48:VAL:HG12	35	0.16
(1,472)	2:B:31:PHE:HD2	2:B:48:VAL:HG13	35	0.16
(1,472)	2:B:31:PHE:HD2	2:B:48:VAL:HG21	35	0.16
(1,472)	2:B:31:PHE:HD2	2:B:48:VAL:HG22	35	0.16
(1,472)	2:B:31:PHE:HD2	2:B:48:VAL:HG23	35	0.16
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE1	33	0.16
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE2	33	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	35	0.16
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	35	0.16
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	35	0.16
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	35	0.16
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	35	0.16
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	35	0.16
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	35	0.16
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	35	0.16
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	35	0.16
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	35	0.16
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	35	0.16
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	35	0.16
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	35	0.16
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	35	0.16
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	35	0.16
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	35	0.16
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	35	0.16
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	35	0.16
(1,384)	2:B:32:VAL:HG11	2:B:33:ASN:HB2	13	0.16
(1,384)	2:B:32:VAL:HG11	2:B:33:ASN:HB3	13	0.16
(1,384)	2:B:32:VAL:HG12	2:B:33:ASN:HB2	13	0.16
(1,384)	2:B:32:VAL:HG12	2:B:33:ASN:HB3	13	0.16
(1,384)	2:B:32:VAL:HG13	2:B:33:ASN:HB2	13	0.16
(1,384)	2:B:32:VAL:HG13	2:B:33:ASN:HB3	13	0.16
(1,384)	2:B:32:VAL:HG21	2:B:33:ASN:HB2	13	0.16
(1,384)	2:B:32:VAL:HG21	2:B:33:ASN:HB3	13	0.16
(1,384)	2:B:32:VAL:HG22	2:B:33:ASN:HB2	13	0.16
(1,384)	2:B:32:VAL:HG22	2:B:33:ASN:HB3	13	0.16
(1,384)	2:B:32:VAL:HG23	2:B:33:ASN:HB2	13	0.16
(1,384)	2:B:32:VAL:HG23	2:B:33:ASN:HB3	13	0.16
(1,375)	2:B:45:LEU:HA	2:B:48:VAL:HB	27	0.16
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	16	0.16
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	16	0.16
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	16	0.16
(1,330)	2:B:45:LEU:HB2	2:B:54:PHE:HE1	38	0.16
(1,330)	2:B:45:LEU:HB2	2:B:54:PHE:HE2	38	0.16
(1,301)	1:A:10:ILE:HD11	2:B:33:ASN:HB2	30	0.16
(1,301)	1:A:10:ILE:HD11	2:B:33:ASN:HB3	30	0.16
(1,301)	1:A:10:ILE:HD12	2:B:33:ASN:HB2	30	0.16
(1,301)	1:A:10:ILE:HD12	2:B:33:ASN:HB3	30	0.16
(1,301)	1:A:10:ILE:HD13	2:B:33:ASN:HB2	30	0.16
(1,301)	1:A:10:ILE:HD13	2:B:33:ASN:HB3	30	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:A:10:ILE:HD11	2:B:33:ASN:HB2	35	0.16
(1,301)	1:A:10:ILE:HD11	2:B:33:ASN:HB3	35	0.16
(1,301)	1:A:10:ILE:HD12	2:B:33:ASN:HB2	35	0.16
(1,301)	1:A:10:ILE:HD12	2:B:33:ASN:HB3	35	0.16
(1,301)	1:A:10:ILE:HD13	2:B:33:ASN:HB2	35	0.16
(1,301)	1:A:10:ILE:HD13	2:B:33:ASN:HB3	35	0.16
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG21	24	0.16
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG22	24	0.16
(1,246)	2:B:31:PHE:HE1	2:B:48:VAL:HG23	24	0.16
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG21	24	0.16
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG22	24	0.16
(1,246)	2:B:31:PHE:HE2	2:B:48:VAL:HG23	24	0.16
(1,234)	1:A:14:TYR:HA	1:A:14:TYR:HE1	39	0.16
(1,234)	1:A:14:TYR:HA	1:A:14:TYR:HE2	39	0.16
(1,229)	1:A:2:ILE:HG12	1:A:19:TYR:HE1	9	0.16
(1,229)	1:A:2:ILE:HG12	1:A:19:TYR:HE2	9	0.16
(1,209)	1:A:2:ILE:HG21	1:A:19:TYR:HD1	11	0.16
(1,209)	1:A:2:ILE:HG21	1:A:19:TYR:HD2	11	0.16
(1,209)	1:A:2:ILE:HG22	1:A:19:TYR:HD1	11	0.16
(1,209)	1:A:2:ILE:HG22	1:A:19:TYR:HD2	11	0.16
(1,209)	1:A:2:ILE:HG23	1:A:19:TYR:HD1	11	0.16
(1,209)	1:A:2:ILE:HG23	1:A:19:TYR:HD2	11	0.16
(1,189)	2:B:46:TYR:H	2:B:54:PHE:HE1	31	0.16
(1,189)	2:B:46:TYR:H	2:B:54:PHE:HE2	31	0.16
(1,17)	2:B:48:VAL:HG21	2:B:49:CYS:H	15	0.16
(1,17)	2:B:48:VAL:HG22	2:B:49:CYS:H	15	0.16
(1,17)	2:B:48:VAL:HG23	2:B:49:CYS:H	15	0.16
(1,163)	2:B:46:TYR:HA	2:B:46:TYR:HE1	14	0.16
(1,163)	2:B:46:TYR:HA	2:B:46:TYR:HE2	14	0.16
(1,136)	2:B:42:VAL:HG11	2:B:43:GLU:H	31	0.16
(1,136)	2:B:42:VAL:HG12	2:B:43:GLU:H	31	0.16
(1,136)	2:B:42:VAL:HG13	2:B:43:GLU:H	31	0.16
(1,12)	1:A:10:ILE:HD11	2:B:34:GLN:H	29	0.16
(1,12)	1:A:10:ILE:HD12	2:B:34:GLN:H	29	0.16
(1,12)	1:A:10:ILE:HD13	2:B:34:GLN:H	29	0.16
(1,111)	1:A:13:LEU:HD11	2:B:31:PHE:HD1	6	0.16
(1,111)	1:A:13:LEU:HD11	2:B:31:PHE:HD2	6	0.16
(1,111)	1:A:13:LEU:HD12	2:B:31:PHE:HD1	6	0.16
(1,111)	1:A:13:LEU:HD12	2:B:31:PHE:HD2	6	0.16
(1,111)	1:A:13:LEU:HD13	2:B:31:PHE:HD1	6	0.16
(1,111)	1:A:13:LEU:HD13	2:B:31:PHE:HD2	6	0.16
(1,104)	1:A:20:CYS:HA	1:A:21:ASN:H	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	2:B:44:ALA:O	2:B:48:VAL:N	27	0.15
(3,5)	2:B:44:ALA:O	2:B:48:VAL:H	34	0.15
(3,21)	1:A:15:GLN:O	1:A:18:ASN:H	24	0.15
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	20	0.15
(3,17)	1:A:17:GLU:O	1:A:20:CYS:H	17	0.15
(3,17)	1:A:17:GLU:O	1:A:20:CYS:H	27	0.15
(1,6)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	15	0.15
(1,6)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	15	0.15
(1,6)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	15	0.15
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	13	0.15
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	13	0.15
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	13	0.15
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	35	0.15
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	35	0.15
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	35	0.15
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB2	8	0.15
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB3	8	0.15
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB2	8	0.15
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB3	8	0.15
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB2	8	0.15
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB3	8	0.15
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB2	8	0.15
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB3	8	0.15
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB2	8	0.15
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB3	8	0.15
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB2	8	0.15
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB3	8	0.15
(1,493)	2:B:39:SER:HB2	2:B:40:HIS:HD2	35	0.15
(1,493)	2:B:39:SER:HB3	2:B:40:HIS:HD2	35	0.15
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	11	0.15
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	11	0.15
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	11	0.15
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	11	0.15
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	11	0.15
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	11	0.15
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD11	8	0.15
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD12	8	0.15
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD13	8	0.15
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD21	8	0.15
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD22	8	0.15
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD23	8	0.15
(1,433)	1:A:15:GLN:HA	1:A:18:ASN:HD21	40	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:A:15:GLN:HA	1:A:18:ASN:HD22	40	0.15
(1,416)	1:A:12:SER:HB2	1:A:14:TYR:HD1	21	0.15
(1,416)	1:A:12:SER:HB2	1:A:14:TYR:HD2	21	0.15
(1,416)	1:A:12:SER:HB3	1:A:14:TYR:HD1	21	0.15
(1,416)	1:A:12:SER:HB3	1:A:14:TYR:HD2	21	0.15
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD11	21	0.15
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD12	21	0.15
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD13	21	0.15
(1,365)	1:A:12:SER:HB3	1:A:13:LEU:H	31	0.15
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	9	0.15
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	9	0.15
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	9	0.15
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	32	0.15
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	32	0.15
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	32	0.15
(1,330)	2:B:45:LEU:HB2	2:B:54:PHE:HE1	33	0.15
(1,330)	2:B:45:LEU:HB2	2:B:54:PHE:HE2	33	0.15
(1,327)	2:B:43:GLU:H	2:B:45:LEU:HB2	27	0.15
(1,324)	2:B:50:GLY:HA2	2:B:51:GLU:HA	23	0.15
(1,324)	2:B:50:GLY:HA3	2:B:51:GLU:HA	23	0.15
(1,253)	2:B:48:VAL:HG21	2:B:49:CYS:HA	22	0.15
(1,253)	2:B:48:VAL:HG22	2:B:49:CYS:HA	22	0.15
(1,253)	2:B:48:VAL:HG23	2:B:49:CYS:HA	22	0.15
(1,227)	1:A:2:ILE:HG21	1:A:19:TYR:HE1	6	0.15
(1,227)	1:A:2:ILE:HG21	1:A:19:TYR:HE2	6	0.15
(1,227)	1:A:2:ILE:HG22	1:A:19:TYR:HE1	6	0.15
(1,227)	1:A:2:ILE:HG22	1:A:19:TYR:HE2	6	0.15
(1,227)	1:A:2:ILE:HG23	1:A:19:TYR:HE1	6	0.15
(1,227)	1:A:2:ILE:HG23	1:A:19:TYR:HE2	6	0.15
(1,225)	2:B:45:LEU:HG	2:B:54:PHE:HE1	16	0.15
(1,225)	2:B:45:LEU:HG	2:B:54:PHE:HE2	16	0.15
(1,210)	1:A:16:LEU:HD21	1:A:19:TYR:HD1	32	0.15
(1,210)	1:A:16:LEU:HD21	1:A:19:TYR:HD2	32	0.15
(1,210)	1:A:16:LEU:HD22	1:A:19:TYR:HD1	32	0.15
(1,210)	1:A:16:LEU:HD22	1:A:19:TYR:HD2	32	0.15
(1,210)	1:A:16:LEU:HD23	1:A:19:TYR:HD1	32	0.15
(1,210)	1:A:16:LEU:HD23	1:A:19:TYR:HD2	32	0.15
(1,187)	2:B:46:TYR:H	2:B:54:PHE:HD1	12	0.15
(1,187)	2:B:46:TYR:H	2:B:54:PHE:HD2	12	0.15
(1,18)	2:B:48:VAL:HG11	2:B:49:CYS:H	24	0.15
(1,18)	2:B:48:VAL:HG12	2:B:49:CYS:H	24	0.15
(1,18)	2:B:48:VAL:HG13	2:B:49:CYS:H	24	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	2:B:48:VAL:HG21	2:B:49:CYS:H	21	0.15
(1,17)	2:B:48:VAL:HG22	2:B:49:CYS:H	21	0.15
(1,17)	2:B:48:VAL:HG23	2:B:49:CYS:H	21	0.15
(1,13)	2:B:32:VAL:HG11	2:B:33:ASN:H	7	0.15
(1,13)	2:B:32:VAL:HG12	2:B:33:ASN:H	7	0.15
(1,13)	2:B:32:VAL:HG13	2:B:33:ASN:H	7	0.15
(1,13)	2:B:32:VAL:HG21	2:B:33:ASN:H	7	0.15
(1,13)	2:B:32:VAL:HG22	2:B:33:ASN:H	7	0.15
(1,13)	2:B:32:VAL:HG23	2:B:33:ASN:H	7	0.15
(1,127)	2:B:37:CYS:H	2:B:40:HIS:HB3	40	0.15
(3,9)	2:B:42:VAL:O	2:B:46:TYR:H	35	0.14
(3,4)	2:B:45:LEU:O	2:B:49:CYS:N	18	0.14
(3,31)	1:A:1:GLY:O	1:A:5:GLN:H	32	0.14
(3,21)	1:A:15:GLN:O	1:A:18:ASN:H	8	0.14
(3,20)	1:A:16:LEU:O	1:A:19:TYR:N	11	0.14
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	17	0.14
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	39	0.14
(3,15)	2:B:39:SER:O	2:B:43:GLU:H	23	0.14
(3,11)	2:B:41:LEU:O	2:B:45:LEU:H	38	0.14
(1,6)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	21	0.14
(1,6)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	21	0.14
(1,6)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	21	0.14
(1,6)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	37	0.14
(1,6)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	37	0.14
(1,6)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	37	0.14
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	27	0.14
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	27	0.14
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	27	0.14
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG11	21	0.14
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG12	21	0.14
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG13	21	0.14
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG21	21	0.14
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG22	21	0.14
(1,520)	2:B:45:LEU:HB2	2:B:48:VAL:HG23	21	0.14
(1,511)	2:B:42:VAL:HG11	2:B:54:PHE:HE1	35	0.14
(1,511)	2:B:42:VAL:HG11	2:B:54:PHE:HE2	35	0.14
(1,511)	2:B:42:VAL:HG12	2:B:54:PHE:HE1	35	0.14
(1,511)	2:B:42:VAL:HG12	2:B:54:PHE:HE2	35	0.14
(1,511)	2:B:42:VAL:HG13	2:B:54:PHE:HE1	35	0.14
(1,511)	2:B:42:VAL:HG13	2:B:54:PHE:HE2	35	0.14
(1,511)	2:B:42:VAL:HG21	2:B:54:PHE:HE1	35	0.14
(1,511)	2:B:42:VAL:HG21	2:B:54:PHE:HE2	35	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	2:B:42:VAL:HG22	2:B:54:PHE:HE1	35	0.14
(1,511)	2:B:42:VAL:HG22	2:B:54:PHE:HE2	35	0.14
(1,511)	2:B:42:VAL:HG23	2:B:54:PHE:HE1	35	0.14
(1,511)	2:B:42:VAL:HG23	2:B:54:PHE:HE2	35	0.14
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD11	10	0.14
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD12	10	0.14
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD13	10	0.14
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD21	10	0.14
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD22	10	0.14
(1,500)	2:B:41:LEU:HG	2:B:45:LEU:HD23	10	0.14
(1,483)	2:B:36:LEU:HB2	2:B:40:HIS:HB2	20	0.14
(1,483)	2:B:36:LEU:HB2	2:B:40:HIS:HB3	20	0.14
(1,483)	2:B:36:LEU:HB3	2:B:40:HIS:HB2	20	0.14
(1,483)	2:B:36:LEU:HB3	2:B:40:HIS:HB3	20	0.14
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD11	24	0.14
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD12	24	0.14
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD13	24	0.14
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD21	24	0.14
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD22	24	0.14
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD23	24	0.14
(1,413)	1:A:12:SER:HA	1:A:13:LEU:HB2	40	0.14
(1,413)	1:A:12:SER:HA	1:A:13:LEU:HB3	40	0.14
(1,384)	2:B:32:VAL:HG11	2:B:33:ASN:HB2	1	0.14
(1,384)	2:B:32:VAL:HG11	2:B:33:ASN:HB3	1	0.14
(1,384)	2:B:32:VAL:HG12	2:B:33:ASN:HB2	1	0.14
(1,384)	2:B:32:VAL:HG12	2:B:33:ASN:HB3	1	0.14
(1,384)	2:B:32:VAL:HG13	2:B:33:ASN:HB2	1	0.14
(1,384)	2:B:32:VAL:HG13	2:B:33:ASN:HB3	1	0.14
(1,384)	2:B:32:VAL:HG21	2:B:33:ASN:HB2	1	0.14
(1,384)	2:B:32:VAL:HG21	2:B:33:ASN:HB3	1	0.14
(1,384)	2:B:32:VAL:HG22	2:B:33:ASN:HB2	1	0.14
(1,384)	2:B:32:VAL:HG22	2:B:33:ASN:HB3	1	0.14
(1,384)	2:B:32:VAL:HG23	2:B:33:ASN:HB2	1	0.14
(1,384)	2:B:32:VAL:HG23	2:B:33:ASN:HB3	1	0.14
(1,377)	1:A:13:LEU:HA	1:A:13:LEU:HD11	17	0.14
(1,377)	1:A:13:LEU:HA	1:A:13:LEU:HD12	17	0.14
(1,377)	1:A:13:LEU:HA	1:A:13:LEU:HD13	17	0.14
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD11	20	0.14
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD12	20	0.14
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD13	20	0.14
(1,352)	1:A:4:GLU:HA	1:A:8:THR:HG21	36	0.14
(1,352)	1:A:4:GLU:HA	1:A:8:THR:HG22	36	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,352)	1:A:4:GLU:HA	1:A:8:THR:HG23	36	0.14
(1,347)	2:B:32:VAL:HA	2:B:33:ASN:HB2	7	0.14
(1,347)	2:B:32:VAL:HA	2:B:33:ASN:HB3	7	0.14
(1,338)	2:B:42:VAL:HB	2:B:54:PHE:HE1	10	0.14
(1,338)	2:B:42:VAL:HB	2:B:54:PHE:HE2	10	0.14
(1,338)	2:B:42:VAL:HB	2:B:54:PHE:HE1	15	0.14
(1,338)	2:B:42:VAL:HB	2:B:54:PHE:HE2	15	0.14
(1,337)	1:A:16:LEU:HG	1:A:19:TYR:HE1	18	0.14
(1,337)	1:A:16:LEU:HG	1:A:19:TYR:HE2	18	0.14
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG11	2	0.14
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG12	2	0.14
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG13	2	0.14
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG21	2	0.14
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG22	2	0.14
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG23	2	0.14
(1,327)	2:B:43:GLU:H	2:B:45:LEU:HB2	15	0.14
(1,282)	1:A:13:LEU:HA	1:A:13:LEU:HD21	30	0.14
(1,282)	1:A:13:LEU:HA	1:A:13:LEU:HD22	30	0.14
(1,282)	1:A:13:LEU:HA	1:A:13:LEU:HD23	30	0.14
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG21	35	0.14
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG22	35	0.14
(1,276)	1:A:17:GLU:HA	2:B:48:VAL:HG23	35	0.14
(1,229)	1:A:2:ILE:HG12	1:A:19:TYR:HE1	19	0.14
(1,229)	1:A:2:ILE:HG12	1:A:19:TYR:HE2	19	0.14
(1,229)	1:A:2:ILE:HG12	1:A:19:TYR:HE1	25	0.14
(1,229)	1:A:2:ILE:HG12	1:A:19:TYR:HE2	25	0.14
(1,227)	1:A:2:ILE:HG21	1:A:19:TYR:HE1	19	0.14
(1,227)	1:A:2:ILE:HG21	1:A:19:TYR:HE2	19	0.14
(1,227)	1:A:2:ILE:HG22	1:A:19:TYR:HE1	19	0.14
(1,227)	1:A:2:ILE:HG22	1:A:19:TYR:HE2	19	0.14
(1,227)	1:A:2:ILE:HG23	1:A:19:TYR:HE1	19	0.14
(1,227)	1:A:2:ILE:HG23	1:A:19:TYR:HE2	19	0.14
(1,225)	2:B:45:LEU:HG	2:B:54:PHE:HE1	4	0.14
(1,225)	2:B:45:LEU:HG	2:B:54:PHE:HE2	4	0.14
(1,210)	1:A:16:LEU:HD21	1:A:19:TYR:HD1	18	0.14
(1,210)	1:A:16:LEU:HD21	1:A:19:TYR:HD2	18	0.14
(1,210)	1:A:16:LEU:HD22	1:A:19:TYR:HD1	18	0.14
(1,210)	1:A:16:LEU:HD22	1:A:19:TYR:HD2	18	0.14
(1,210)	1:A:16:LEU:HD23	1:A:19:TYR:HD1	18	0.14
(1,210)	1:A:16:LEU:HD23	1:A:19:TYR:HD2	18	0.14
(1,191)	2:B:54:PHE:HA	2:B:55:PHE:H	15	0.14
(1,191)	2:B:54:PHE:HA	2:B:55:PHE:H	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	2:B:48:VAL:HG21	2:B:49:CYS:H	2	0.14
(1,17)	2:B:48:VAL:HG22	2:B:49:CYS:H	2	0.14
(1,17)	2:B:48:VAL:HG23	2:B:49:CYS:H	2	0.14
(1,17)	2:B:48:VAL:HG21	2:B:49:CYS:H	14	0.14
(1,17)	2:B:48:VAL:HG22	2:B:49:CYS:H	14	0.14
(1,17)	2:B:48:VAL:HG23	2:B:49:CYS:H	14	0.14
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD11	40	0.14
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD12	40	0.14
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD13	40	0.14
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD21	40	0.14
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD22	40	0.14
(1,166)	2:B:46:TYR:HE1	2:B:47:LEU:HD23	40	0.14
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD11	40	0.14
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD12	40	0.14
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD13	40	0.14
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD21	40	0.14
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD22	40	0.14
(1,166)	2:B:46:TYR:HE2	2:B:47:LEU:HD23	40	0.14
(1,136)	2:B:42:VAL:HG11	2:B:43:GLU:H	8	0.14
(1,136)	2:B:42:VAL:HG12	2:B:43:GLU:H	8	0.14
(1,136)	2:B:42:VAL:HG13	2:B:43:GLU:H	8	0.14
(1,104)	1:A:20:CYS:HA	1:A:21:ASN:H	20	0.14
(3,7)	2:B:43:GLU:O	2:B:47:LEU:H	37	0.13
(3,3)	2:B:45:LEU:O	2:B:49:CYS:H	20	0.13
(3,3)	2:B:45:LEU:O	2:B:49:CYS:H	36	0.13
(3,25)	1:A:12:SER:O	1:A:16:LEU:H	30	0.13
(3,20)	1:A:16:LEU:O	1:A:19:TYR:N	6	0.13
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	35	0.13
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	40	0.13
(3,17)	1:A:17:GLU:O	1:A:20:CYS:H	14	0.13
(3,17)	1:A:17:GLU:O	1:A:20:CYS:H	34	0.13
(3,17)	1:A:17:GLU:O	1:A:20:CYS:H	40	0.13
(3,11)	2:B:41:LEU:O	2:B:45:LEU:H	21	0.13
(1,6)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	1	0.13
(1,6)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	1	0.13
(1,6)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	1	0.13
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	12	0.13
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	12	0.13
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	12	0.13
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	26	0.13
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	26	0.13
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	26	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE1	7	0.13
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE2	7	0.13
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE1	7	0.13
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE2	7	0.13
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE1	7	0.13
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE2	7	0.13
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE1	7	0.13
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE2	7	0.13
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE1	7	0.13
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE2	7	0.13
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE1	7	0.13
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE2	7	0.13
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG11	18	0.13
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG12	18	0.13
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG13	18	0.13
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG21	18	0.13
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG22	18	0.13
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG23	18	0.13
(1,5)	1:A:10:ILE:HD11	2:B:35:HIS:HE1	40	0.13
(1,5)	1:A:10:ILE:HD12	2:B:35:HIS:HE1	40	0.13
(1,5)	1:A:10:ILE:HD13	2:B:35:HIS:HE1	40	0.13
(1,493)	2:B:39:SER:HB2	2:B:40:HIS:HD2	29	0.13
(1,493)	2:B:39:SER:HB3	2:B:40:HIS:HD2	29	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG11	2	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG12	2	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG13	2	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG21	2	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG22	2	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG23	2	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG11	12	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG12	12	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG13	12	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG21	12	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG22	12	0.13
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG23	12	0.13
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD11	32	0.13
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD12	32	0.13
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD13	32	0.13
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	35	0.13
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	35	0.13
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	35	0.13
(1,326)	2:B:43:GLU:H	2:B:45:LEU:HB3	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	2:B:46:TYR:HE1	2:B:47:LEU:HA	24	0.13
(1,233)	2:B:46:TYR:HE2	2:B:47:LEU:HA	24	0.13
(1,225)	2:B:45:LEU:HG	2:B:54:PHE:HE1	39	0.13
(1,225)	2:B:45:LEU:HG	2:B:54:PHE:HE2	39	0.13
(1,209)	1:A:2:ILE:HG21	1:A:19:TYR:HD1	33	0.13
(1,209)	1:A:2:ILE:HG21	1:A:19:TYR:HD2	33	0.13
(1,209)	1:A:2:ILE:HG22	1:A:19:TYR:HD1	33	0.13
(1,209)	1:A:2:ILE:HG22	1:A:19:TYR:HD2	33	0.13
(1,209)	1:A:2:ILE:HG23	1:A:19:TYR:HD1	33	0.13
(1,209)	1:A:2:ILE:HG23	1:A:19:TYR:HD2	33	0.13
(1,142)	2:B:42:VAL:HB	2:B:43:GLU:H	12	0.13
(3,6)	2:B:44:ALA:O	2:B:48:VAL:N	34	0.12
(3,5)	2:B:44:ALA:O	2:B:48:VAL:H	15	0.12
(3,5)	2:B:44:ALA:O	2:B:48:VAL:H	22	0.12
(3,31)	1:A:1:GLY:O	1:A:5:GLN:H	1	0.12
(3,31)	1:A:1:GLY:O	1:A:5:GLN:H	34	0.12
(3,29)	1:A:2:ILE:O	1:A:6:CYS:H	11	0.12
(3,27)	1:A:3:VAL:O	1:A:7:CYS:H	17	0.12
(3,21)	1:A:15:GLN:O	1:A:18:ASN:H	15	0.12
(3,21)	1:A:15:GLN:O	1:A:18:ASN:H	31	0.12
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	23	0.12
(3,18)	1:A:17:GLU:O	1:A:20:CYS:N	30	0.12
(3,17)	1:A:17:GLU:O	1:A:20:CYS:H	35	0.12
(3,15)	2:B:39:SER:O	2:B:43:GLU:H	27	0.12
(3,15)	2:B:39:SER:O	2:B:43:GLU:H	36	0.12
(3,13)	2:B:40:HIS:O	2:B:44:ALA:H	31	0.12
(3,12)	2:B:41:LEU:O	2:B:45:LEU:N	38	0.12
(3,11)	2:B:41:LEU:O	2:B:45:LEU:H	6	0.12
(3,11)	2:B:41:LEU:O	2:B:45:LEU:H	34	0.12
(3,1)	2:B:46:TYR:O	2:B:50:GLY:H	25	0.12
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	2	0.12
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	2	0.12
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	2	0.12
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	38	0.12
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	38	0.12
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	38	0.12
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE1	1	0.12
(1,535)	2:B:48:VAL:HG11	2:B:54:PHE:HE2	1	0.12
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE1	1	0.12
(1,535)	2:B:48:VAL:HG12	2:B:54:PHE:HE2	1	0.12
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE1	1	0.12
(1,535)	2:B:48:VAL:HG13	2:B:54:PHE:HE2	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE1	1	0.12
(1,535)	2:B:48:VAL:HG21	2:B:54:PHE:HE2	1	0.12
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE1	1	0.12
(1,535)	2:B:48:VAL:HG22	2:B:54:PHE:HE2	1	0.12
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE1	1	0.12
(1,535)	2:B:48:VAL:HG23	2:B:54:PHE:HE2	1	0.12
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB2	17	0.12
(1,523)	2:B:45:LEU:HD11	2:B:54:PHE:HB3	17	0.12
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB2	17	0.12
(1,523)	2:B:45:LEU:HD12	2:B:54:PHE:HB3	17	0.12
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB2	17	0.12
(1,523)	2:B:45:LEU:HD13	2:B:54:PHE:HB3	17	0.12
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB2	17	0.12
(1,523)	2:B:45:LEU:HD21	2:B:54:PHE:HB3	17	0.12
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB2	17	0.12
(1,523)	2:B:45:LEU:HD22	2:B:54:PHE:HB3	17	0.12
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB2	17	0.12
(1,523)	2:B:45:LEU:HD23	2:B:54:PHE:HB3	17	0.12
(1,5)	1:A:10:ILE:HD11	2:B:35:HIS:HE1	15	0.12
(1,5)	1:A:10:ILE:HD12	2:B:35:HIS:HE1	15	0.12
(1,5)	1:A:10:ILE:HD13	2:B:35:HIS:HE1	15	0.12
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG11	10	0.12
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG12	10	0.12
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG13	10	0.12
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG21	10	0.12
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG22	10	0.12
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG23	10	0.12
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	26	0.12
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	26	0.12
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	26	0.12
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	26	0.12
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	26	0.12
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	26	0.12
(1,45)	1:A:2:ILE:H	1:A:19:TYR:HE1	10	0.12
(1,45)	1:A:2:ILE:H	1:A:19:TYR:HE2	10	0.12
(1,45)	1:A:2:ILE:H	1:A:19:TYR:HE1	39	0.12
(1,45)	1:A:2:ILE:H	1:A:19:TYR:HE2	39	0.12
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE1	14	0.12
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE2	14	0.12
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	16	0.12
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	16	0.12
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	16	0.12
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	16	0.12
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	16	0.12
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	16	0.12
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	16	0.12
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	16	0.12
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	16	0.12
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	16	0.12
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	16	0.12
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	16	0.12
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	16	0.12
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	16	0.12
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	16	0.12
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	16	0.12
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	16	0.12
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD11	6	0.12
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD12	6	0.12
(1,376)	1:A:13:LEU:HA	1:A:16:LEU:HD13	6	0.12
(1,375)	2:B:45:LEU:HA	2:B:48:VAL:HB	13	0.12
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	6	0.12
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	6	0.12
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	6	0.12
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	11	0.12
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	11	0.12
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	11	0.12
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	17	0.12
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	17	0.12
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	17	0.12
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	29	0.12
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	29	0.12
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	29	0.12
(1,344)	2:B:32:VAL:HG11	2:B:34:GLN:H	13	0.12
(1,344)	2:B:32:VAL:HG12	2:B:34:GLN:H	13	0.12
(1,344)	2:B:32:VAL:HG13	2:B:34:GLN:H	13	0.12
(1,344)	2:B:32:VAL:HG21	2:B:34:GLN:H	13	0.12
(1,344)	2:B:32:VAL:HG22	2:B:34:GLN:H	13	0.12
(1,344)	2:B:32:VAL:HG23	2:B:34:GLN:H	13	0.12
(1,338)	2:B:42:VAL:HB	2:B:54:PHE:HE1	14	0.12
(1,338)	2:B:42:VAL:HB	2:B:54:PHE:HE2	14	0.12
(1,338)	2:B:42:VAL:HB	2:B:54:PHE:HE1	20	0.12
(1,338)	2:B:42:VAL:HB	2:B:54:PHE:HE2	20	0.12
(1,299)	1:A:6:CYS:HB3	2:B:41:LEU:HD21	28	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:A:6:CYS:HB3	2:B:41:LEU:HD22	28	0.12
(1,299)	1:A:6:CYS:HB3	2:B:41:LEU:HD23	28	0.12
(1,254)	2:B:48:VAL:HG11	2:B:49:CYS:HA	31	0.12
(1,254)	2:B:48:VAL:HG12	2:B:49:CYS:HA	31	0.12
(1,254)	2:B:48:VAL:HG13	2:B:49:CYS:HA	31	0.12
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG11	21	0.12
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG12	21	0.12
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG13	21	0.12
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG11	21	0.12
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG12	21	0.12
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG13	21	0.12
(1,242)	2:B:54:PHE:H	2:B:54:PHE:HE1	8	0.12
(1,242)	2:B:54:PHE:H	2:B:54:PHE:HE2	8	0.12
(1,242)	2:B:54:PHE:H	2:B:54:PHE:HE1	40	0.12
(1,242)	2:B:54:PHE:H	2:B:54:PHE:HE2	40	0.12
(1,229)	1:A:2:ILE:HG12	1:A:19:TYR:HE1	10	0.12
(1,229)	1:A:2:ILE:HG12	1:A:19:TYR:HE2	10	0.12
(1,229)	1:A:2:ILE:HG12	1:A:19:TYR:HE1	20	0.12
(1,229)	1:A:2:ILE:HG12	1:A:19:TYR:HE2	20	0.12
(1,227)	1:A:2:ILE:HG21	1:A:19:TYR:HE1	34	0.12
(1,227)	1:A:2:ILE:HG21	1:A:19:TYR:HE2	34	0.12
(1,227)	1:A:2:ILE:HG22	1:A:19:TYR:HE1	34	0.12
(1,227)	1:A:2:ILE:HG22	1:A:19:TYR:HE2	34	0.12
(1,227)	1:A:2:ILE:HG23	1:A:19:TYR:HE1	34	0.12
(1,227)	1:A:2:ILE:HG23	1:A:19:TYR:HE2	34	0.12
(1,219)	2:B:59:LYS:HA	2:B:60:THR:H	22	0.12
(1,218)	2:B:58:PRO:HG2	2:B:59:LYS:H	14	0.12
(1,218)	2:B:58:PRO:HG3	2:B:59:LYS:H	14	0.12
(1,211)	1:A:19:TYR:HD1	2:B:45:LEU:HD21	24	0.12
(1,211)	1:A:19:TYR:HD1	2:B:45:LEU:HD22	24	0.12
(1,211)	1:A:19:TYR:HD1	2:B:45:LEU:HD23	24	0.12
(1,211)	1:A:19:TYR:HD2	2:B:45:LEU:HD21	24	0.12
(1,211)	1:A:19:TYR:HD2	2:B:45:LEU:HD22	24	0.12
(1,211)	1:A:19:TYR:HD2	2:B:45:LEU:HD23	24	0.12
(1,210)	1:A:16:LEU:HD21	1:A:19:TYR:HD1	5	0.12
(1,210)	1:A:16:LEU:HD21	1:A:19:TYR:HD2	5	0.12
(1,210)	1:A:16:LEU:HD22	1:A:19:TYR:HD1	5	0.12
(1,210)	1:A:16:LEU:HD22	1:A:19:TYR:HD2	5	0.12
(1,210)	1:A:16:LEU:HD23	1:A:19:TYR:HD1	5	0.12
(1,210)	1:A:16:LEU:HD23	1:A:19:TYR:HD2	5	0.12
(1,180)	2:B:52:GLN:H	2:B:53:GLY:H	34	0.12
(1,17)	2:B:48:VAL:HG21	2:B:49:CYS:H	35	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	2:B:48:VAL:HG22	2:B:49:CYS:H	35	0.12
(1,17)	2:B:48:VAL:HG23	2:B:49:CYS:H	35	0.12
(1,127)	2:B:37:CYS:H	2:B:40:HIS:HB3	36	0.12
(1,110)	1:A:13:LEU:HD21	2:B:31:PHE:HD1	5	0.12
(1,110)	1:A:13:LEU:HD21	2:B:31:PHE:HD2	5	0.12
(1,110)	1:A:13:LEU:HD22	2:B:31:PHE:HD1	5	0.12
(1,110)	1:A:13:LEU:HD22	2:B:31:PHE:HD2	5	0.12
(1,110)	1:A:13:LEU:HD23	2:B:31:PHE:HD1	5	0.12
(1,110)	1:A:13:LEU:HD23	2:B:31:PHE:HD2	5	0.12
(3,7)	2:B:43:GLU:O	2:B:47:LEU:H	24	0.11
(3,7)	2:B:43:GLU:O	2:B:47:LEU:H	35	0.11
(3,5)	2:B:44:ALA:O	2:B:48:VAL:H	33	0.11
(3,31)	1:A:1:GLY:O	1:A:5:GLN:H	22	0.11
(3,3)	2:B:45:LEU:O	2:B:49:CYS:H	13	0.11
(3,3)	2:B:45:LEU:O	2:B:49:CYS:H	26	0.11
(3,27)	1:A:3:VAL:O	1:A:7:CYS:H	38	0.11
(3,21)	1:A:15:GLN:O	1:A:18:ASN:H	6	0.11
(3,21)	1:A:15:GLN:O	1:A:18:ASN:H	29	0.11
(3,21)	1:A:15:GLN:O	1:A:18:ASN:H	33	0.11
(3,20)	1:A:16:LEU:O	1:A:19:TYR:N	20	0.11
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	21	0.11
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	31	0.11
(3,19)	1:A:16:LEU:O	1:A:19:TYR:H	34	0.11
(3,17)	1:A:17:GLU:O	1:A:20:CYS:H	10	0.11
(3,13)	2:B:40:HIS:O	2:B:44:ALA:H	6	0.11
(3,11)	2:B:41:LEU:O	2:B:45:LEU:H	24	0.11
(1,84)	2:B:54:PHE:HB2	2:B:55:PHE:H	5	0.11
(1,557)	1:A:10:ILE:HG21	2:B:35:HIS:HE1	5	0.11
(1,557)	1:A:10:ILE:HG22	2:B:35:HIS:HE1	5	0.11
(1,557)	1:A:10:ILE:HG23	2:B:35:HIS:HE1	5	0.11
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG11	14	0.11
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG12	14	0.11
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG13	14	0.11
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG21	14	0.11
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG22	14	0.11
(1,514)	2:B:44:ALA:HA	2:B:48:VAL:HG23	14	0.11
(1,5)	1:A:10:ILE:HD11	2:B:35:HIS:HE1	36	0.11
(1,5)	1:A:10:ILE:HD12	2:B:35:HIS:HE1	36	0.11
(1,5)	1:A:10:ILE:HD13	2:B:35:HIS:HE1	36	0.11
(1,494)	2:B:39:SER:HB2	2:B:42:VAL:HG11	14	0.11
(1,494)	2:B:39:SER:HB2	2:B:42:VAL:HG12	14	0.11
(1,494)	2:B:39:SER:HB2	2:B:42:VAL:HG13	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,494)	2:B:39:SER:HB2	2:B:42:VAL:HG21	14	0.11
(1,494)	2:B:39:SER:HB2	2:B:42:VAL:HG22	14	0.11
(1,494)	2:B:39:SER:HB2	2:B:42:VAL:HG23	14	0.11
(1,494)	2:B:39:SER:HB3	2:B:42:VAL:HG11	14	0.11
(1,494)	2:B:39:SER:HB3	2:B:42:VAL:HG12	14	0.11
(1,494)	2:B:39:SER:HB3	2:B:42:VAL:HG13	14	0.11
(1,494)	2:B:39:SER:HB3	2:B:42:VAL:HG21	14	0.11
(1,494)	2:B:39:SER:HB3	2:B:42:VAL:HG22	14	0.11
(1,494)	2:B:39:SER:HB3	2:B:42:VAL:HG23	14	0.11
(1,493)	2:B:39:SER:HB2	2:B:40:HIS:HD2	1	0.11
(1,493)	2:B:39:SER:HB3	2:B:40:HIS:HD2	1	0.11
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG11	33	0.11
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG12	33	0.11
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG13	33	0.11
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG21	33	0.11
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG22	33	0.11
(1,473)	2:B:31:PHE:HZ	2:B:48:VAL:HG23	33	0.11
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	9	0.11
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	9	0.11
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	9	0.11
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	9	0.11
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	9	0.11
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	9	0.11
(1,452)	1:A:16:LEU:HD11	2:B:45:LEU:HG	35	0.11
(1,452)	1:A:16:LEU:HD12	2:B:45:LEU:HG	35	0.11
(1,452)	1:A:16:LEU:HD13	2:B:45:LEU:HG	35	0.11
(1,452)	1:A:16:LEU:HD21	2:B:45:LEU:HG	35	0.11
(1,452)	1:A:16:LEU:HD22	2:B:45:LEU:HG	35	0.11
(1,452)	1:A:16:LEU:HD23	2:B:45:LEU:HG	35	0.11
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD11	25	0.11
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD12	25	0.11
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD13	25	0.11
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD21	25	0.11
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD22	25	0.11
(1,440)	1:A:16:LEU:HA	2:B:45:LEU:HD23	25	0.11
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE1	6	0.11
(1,44)	1:A:16:LEU:H	1:A:19:TYR:HE2	6	0.11
(1,422)	1:A:13:LEU:HB2	2:B:31:PHE:HD1	19	0.11
(1,422)	1:A:13:LEU:HB2	2:B:31:PHE:HD2	19	0.11
(1,422)	1:A:13:LEU:HB3	2:B:31:PHE:HD1	19	0.11
(1,422)	1:A:13:LEU:HB3	2:B:31:PHE:HD2	19	0.11
(1,416)	1:A:12:SER:HB2	1:A:14:TYR:HD1	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,416)	1:A:12:SER:HB2	1:A:14:TYR:HD2	7	0.11
(1,416)	1:A:12:SER:HB3	1:A:14:TYR:HD1	7	0.11
(1,416)	1:A:12:SER:HB3	1:A:14:TYR:HD2	7	0.11
(1,393)	2:B:31:PHE:HZ	2:B:33:ASN:HA	11	0.11
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD11	6	0.11
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD12	6	0.11
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD13	6	0.11
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD21	6	0.11
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD22	6	0.11
(1,387)	2:B:44:ALA:HB1	2:B:47:LEU:HD23	6	0.11
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD11	6	0.11
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD12	6	0.11
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD13	6	0.11
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD21	6	0.11
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD22	6	0.11
(1,387)	2:B:44:ALA:HB2	2:B:47:LEU:HD23	6	0.11
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD11	6	0.11
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD12	6	0.11
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD13	6	0.11
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD21	6	0.11
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD22	6	0.11
(1,387)	2:B:44:ALA:HB3	2:B:47:LEU:HD23	6	0.11
(1,384)	2:B:32:VAL:HG11	2:B:33:ASN:HB2	8	0.11
(1,384)	2:B:32:VAL:HG11	2:B:33:ASN:HB3	8	0.11
(1,384)	2:B:32:VAL:HG12	2:B:33:ASN:HB2	8	0.11
(1,384)	2:B:32:VAL:HG12	2:B:33:ASN:HB3	8	0.11
(1,384)	2:B:32:VAL:HG13	2:B:33:ASN:HB2	8	0.11
(1,384)	2:B:32:VAL:HG13	2:B:33:ASN:HB3	8	0.11
(1,384)	2:B:32:VAL:HG21	2:B:33:ASN:HB2	8	0.11
(1,384)	2:B:32:VAL:HG21	2:B:33:ASN:HB3	8	0.11
(1,384)	2:B:32:VAL:HG22	2:B:33:ASN:HB2	8	0.11
(1,384)	2:B:32:VAL:HG22	2:B:33:ASN:HB3	8	0.11
(1,384)	2:B:32:VAL:HG23	2:B:33:ASN:HB2	8	0.11
(1,384)	2:B:32:VAL:HG23	2:B:33:ASN:HB3	8	0.11
(1,384)	2:B:32:VAL:HG11	2:B:33:ASN:HB2	10	0.11
(1,384)	2:B:32:VAL:HG11	2:B:33:ASN:HB3	10	0.11
(1,384)	2:B:32:VAL:HG12	2:B:33:ASN:HB2	10	0.11
(1,384)	2:B:32:VAL:HG12	2:B:33:ASN:HB3	10	0.11
(1,384)	2:B:32:VAL:HG13	2:B:33:ASN:HB2	10	0.11
(1,384)	2:B:32:VAL:HG13	2:B:33:ASN:HB3	10	0.11
(1,384)	2:B:32:VAL:HG21	2:B:33:ASN:HB2	10	0.11
(1,384)	2:B:32:VAL:HG21	2:B:33:ASN:HB3	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,384)	2:B:32:VAL:HG22	2:B:33:ASN:HB2	10	0.11
(1,384)	2:B:32:VAL:HG22	2:B:33:ASN:HB3	10	0.11
(1,384)	2:B:32:VAL:HG23	2:B:33:ASN:HB2	10	0.11
(1,384)	2:B:32:VAL:HG23	2:B:33:ASN:HB3	10	0.11
(1,377)	1:A:13:LEU:HA	1:A:13:LEU:HD11	24	0.11
(1,377)	1:A:13:LEU:HA	1:A:13:LEU:HD12	24	0.11
(1,377)	1:A:13:LEU:HA	1:A:13:LEU:HD13	24	0.11
(1,354)	1:A:4:GLU:HG2	1:A:8:THR:HG21	9	0.11
(1,354)	1:A:4:GLU:HG2	1:A:8:THR:HG22	9	0.11
(1,354)	1:A:4:GLU:HG2	1:A:8:THR:HG23	9	0.11
(1,354)	1:A:4:GLU:HG3	1:A:8:THR:HG21	9	0.11
(1,354)	1:A:4:GLU:HG3	1:A:8:THR:HG22	9	0.11
(1,354)	1:A:4:GLU:HG3	1:A:8:THR:HG23	9	0.11
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	8	0.11
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	8	0.11
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	8	0.11
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	34	0.11
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	34	0.11
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	34	0.11
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG21	38	0.11
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG22	38	0.11
(1,353)	2:B:45:LEU:HA	2:B:48:VAL:HG23	38	0.11
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG11	34	0.11
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG12	34	0.11
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG13	34	0.11
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG21	34	0.11
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG22	34	0.11
(1,328)	2:B:31:PHE:HZ	2:B:32:VAL:HG23	34	0.11
(1,327)	2:B:43:GLU:H	2:B:45:LEU:HB2	11	0.11
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD11	17	0.11
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD12	17	0.11
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD13	17	0.11
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD21	17	0.11
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD22	17	0.11
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD23	17	0.11
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD11	30	0.11
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD12	30	0.11
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD13	30	0.11
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD21	30	0.11
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD22	30	0.11
(1,303)	2:B:34:GLN:HG3	2:B:36:LEU:HD23	30	0.11
(1,282)	1:A:13:LEU:HA	1:A:13:LEU:HD21	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,282)	1:A:13:LEU:HA	1:A:13:LEU:HD22	6	0.11
(1,282)	1:A:13:LEU:HA	1:A:13:LEU:HD23	6	0.11
(1,25)	2:B:36:LEU:HD11	2:B:45:LEU:H	27	0.11
(1,25)	2:B:36:LEU:HD12	2:B:45:LEU:H	27	0.11
(1,25)	2:B:36:LEU:HD13	2:B:45:LEU:H	27	0.11
(1,25)	2:B:36:LEU:HD21	2:B:45:LEU:H	27	0.11
(1,25)	2:B:36:LEU:HD22	2:B:45:LEU:H	27	0.11
(1,25)	2:B:36:LEU:HD23	2:B:45:LEU:H	27	0.11
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG11	32	0.11
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG12	32	0.11
(1,247)	2:B:31:PHE:HE1	2:B:48:VAL:HG13	32	0.11
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG11	32	0.11
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG12	32	0.11
(1,247)	2:B:31:PHE:HE2	2:B:48:VAL:HG13	32	0.11
(1,233)	2:B:46:TYR:HE1	2:B:47:LEU:HA	39	0.11
(1,233)	2:B:46:TYR:HE2	2:B:47:LEU:HA	39	0.11
(1,225)	2:B:45:LEU:HG	2:B:54:PHE:HE1	6	0.11
(1,225)	2:B:45:LEU:HG	2:B:54:PHE:HE2	6	0.11
(1,210)	1:A:16:LEU:HD21	1:A:19:TYR:HD1	20	0.11
(1,210)	1:A:16:LEU:HD21	1:A:19:TYR:HD2	20	0.11
(1,210)	1:A:16:LEU:HD22	1:A:19:TYR:HD1	20	0.11
(1,210)	1:A:16:LEU:HD22	1:A:19:TYR:HD2	20	0.11
(1,210)	1:A:16:LEU:HD23	1:A:19:TYR:HD1	20	0.11
(1,210)	1:A:16:LEU:HD23	1:A:19:TYR:HD2	20	0.11
(1,191)	2:B:54:PHE:HA	2:B:55:PHE:H	17	0.11
(1,178)	2:B:50:GLY:H	2:B:51:GLU:H	24	0.11
(1,17)	2:B:48:VAL:HG21	2:B:49:CYS:H	12	0.11
(1,17)	2:B:48:VAL:HG22	2:B:49:CYS:H	12	0.11
(1,17)	2:B:48:VAL:HG23	2:B:49:CYS:H	12	0.11
(1,150)	2:B:44:ALA:H	2:B:47:LEU:HD11	22	0.11
(1,150)	2:B:44:ALA:H	2:B:47:LEU:HD12	22	0.11
(1,150)	2:B:44:ALA:H	2:B:47:LEU:HD13	22	0.11
(1,150)	2:B:44:ALA:H	2:B:47:LEU:HD21	22	0.11
(1,150)	2:B:44:ALA:H	2:B:47:LEU:HD22	22	0.11
(1,150)	2:B:44:ALA:H	2:B:47:LEU:HD23	22	0.11
(1,142)	2:B:42:VAL:HB	2:B:43:GLU:H	10	0.11
(1,127)	2:B:37:CYS:H	2:B:40:HIS:HB3	16	0.11
(1,105)	1:A:21:ASN:H	1:A:21:ASN:HB2	17	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found