



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 04:57 PM EST

PDB ID : 6ZV2
BMRB ID : 34539
Title : TFIIS N-terminal domain (TND) from human PPP1R10
Authors : Veverka, V.
Deposited on : 2020-07-23

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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

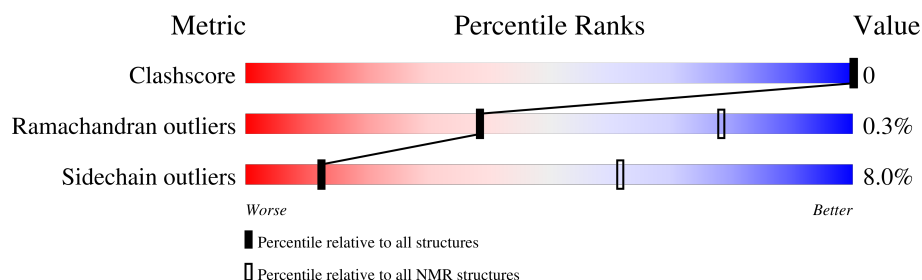
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	154	

2 Ensemble composition and analysis

This entry contains 40 models. Model 33 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:23-A:151 (129)	0.41	33

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 5 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2476 atoms, of which 1269 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Serine/threonine-protein phosphatase 1 regulatory subunit 10.

Mol	Chain	Residues	Atoms						Trace
1	A	154	Total	C	H	N	O	S	0
			2476	765	1269	208	229	5	

There are 7 discrepancies between the modelled and reference sequences:

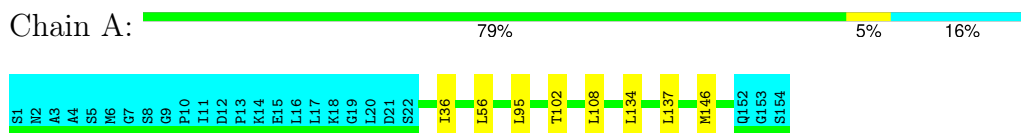
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q96QC0
A	2	ASN	-	expression tag	UNP Q96QC0
A	3	ALA	-	expression tag	UNP Q96QC0
A	4	ALA	-	expression tag	UNP Q96QC0
A	5	SER	-	expression tag	UNP Q96QC0
A	153	GLY	-	expression tag	UNP Q96QC0
A	154	SER	-	expression tag	UNP Q96QC0

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: Serine/threonine-protein phosphatase 1 regulatory subunit 10

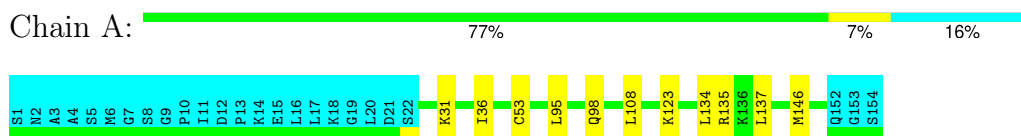


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

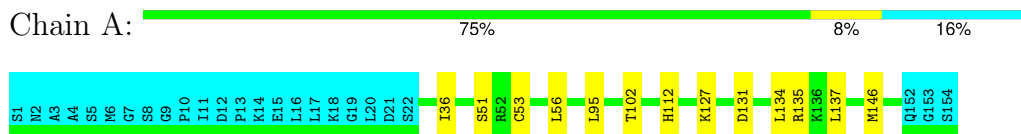
4.2.1 Score per residue for model 1

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



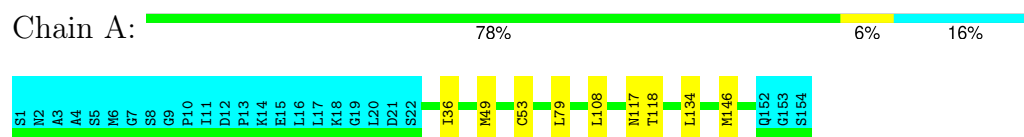
4.2.2 Score per residue for model 2

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



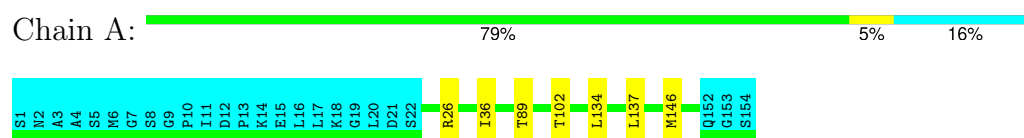
4.2.3 Score per residue for model 3

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



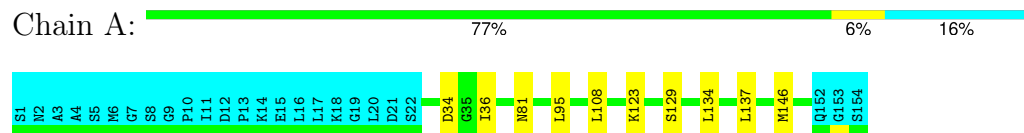
4.2.4 Score per residue for model 4

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



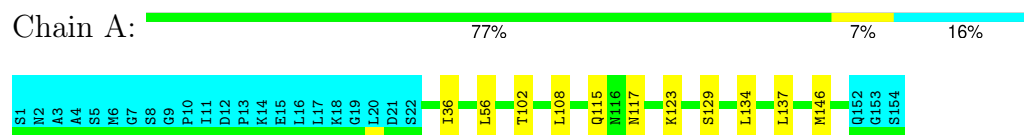
4.2.5 Score per residue for model 5

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



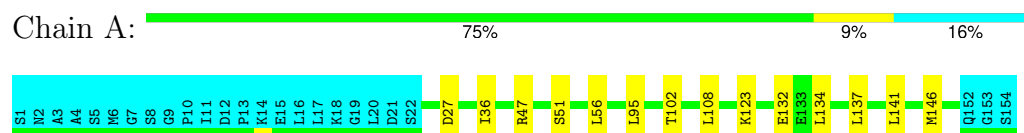
4.2.6 Score per residue for model 6

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



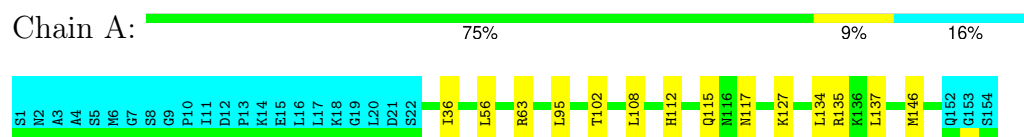
4.2.7 Score per residue for model 7

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



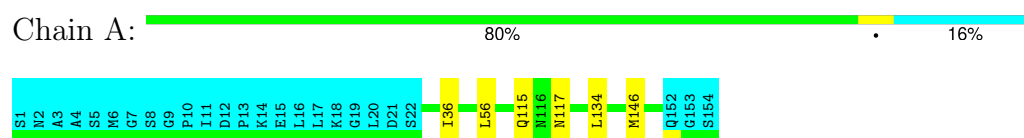
4.2.8 Score per residue for model 8

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



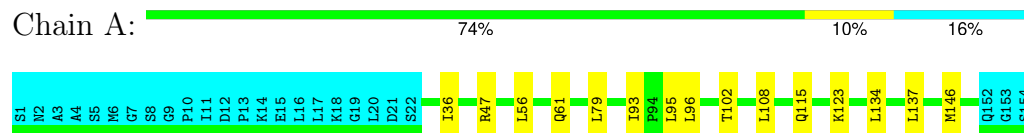
4.2.9 Score per residue for model 9

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



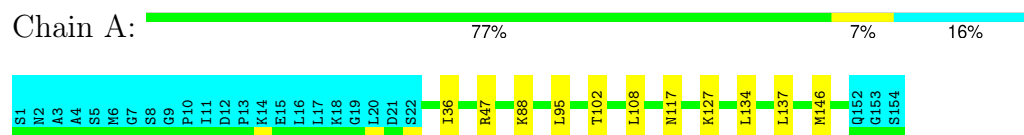
4.2.10 Score per residue for model 10

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



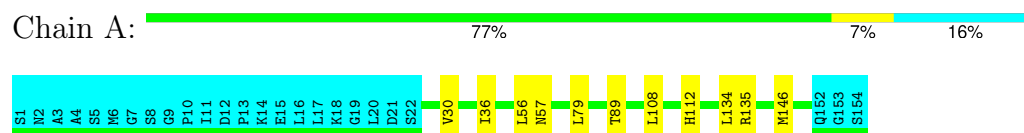
4.2.11 Score per residue for model 11

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



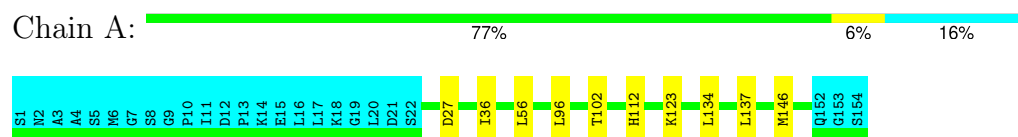
4.2.12 Score per residue for model 12

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



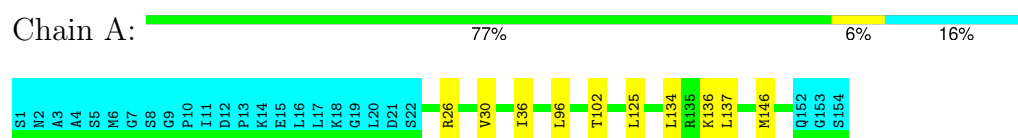
4.2.13 Score per residue for model 13

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



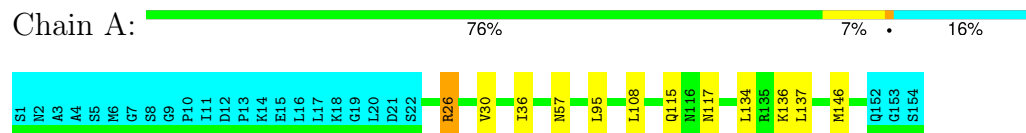
4.2.14 Score per residue for model 14

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



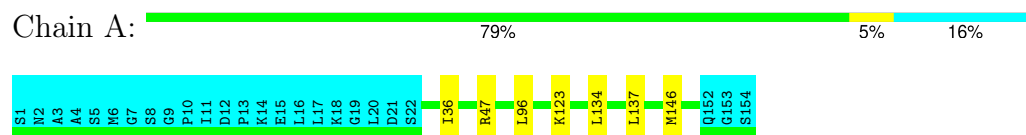
4.2.15 Score per residue for model 15

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



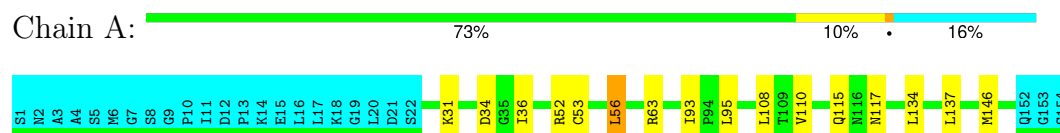
4.2.16 Score per residue for model 16

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



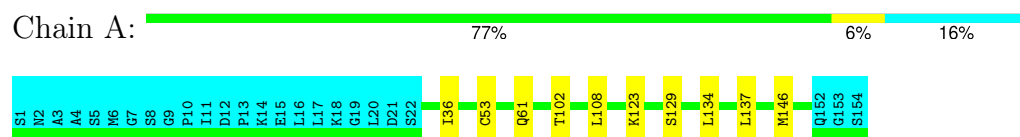
4.2.17 Score per residue for model 17

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



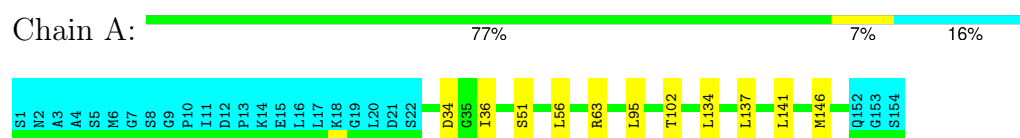
4.2.18 Score per residue for model 18

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



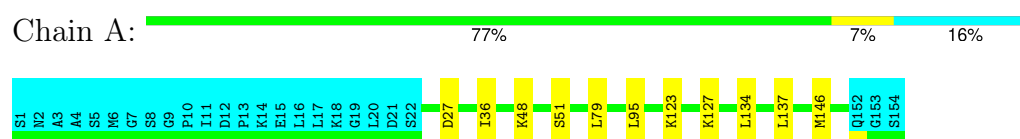
4.2.19 Score per residue for model 19

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



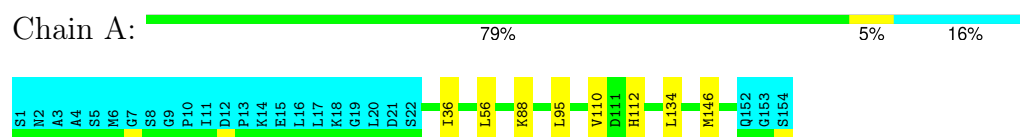
4.2.20 Score per residue for model 20

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



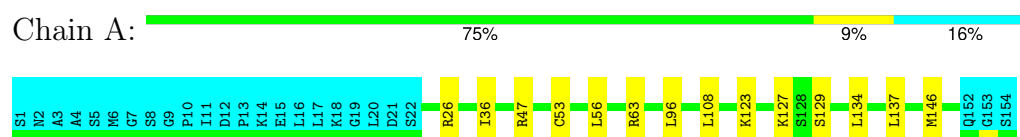
4.2.21 Score per residue for model 21

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



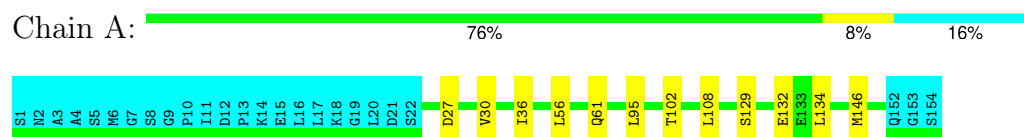
4.2.22 Score per residue for model 22

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



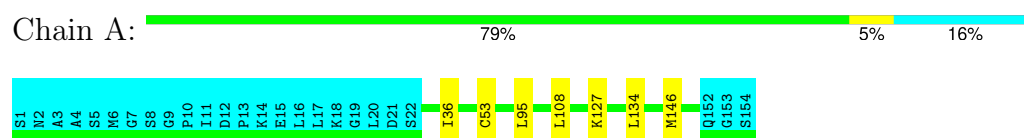
4.2.23 Score per residue for model 23

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



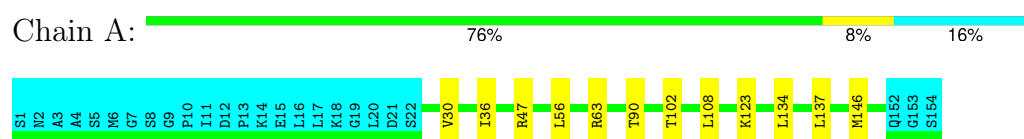
4.2.24 Score per residue for model 24

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



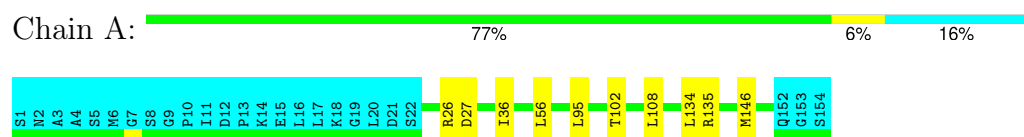
4.2.25 Score per residue for model 25

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



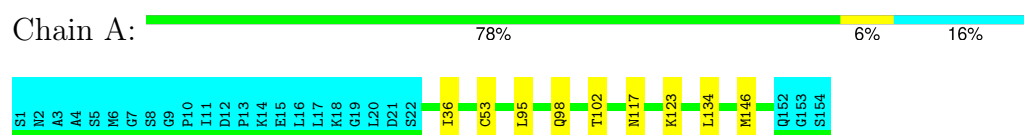
4.2.26 Score per residue for model 26

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



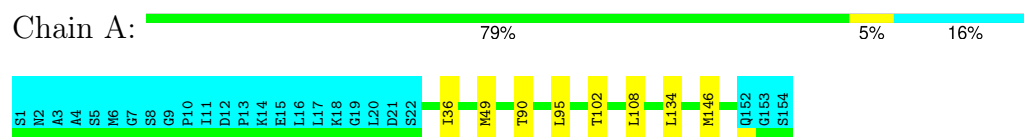
4.2.27 Score per residue for model 27

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



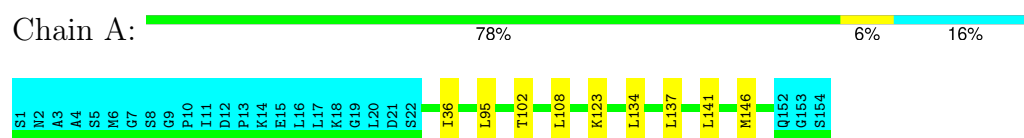
4.2.28 Score per residue for model 28

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



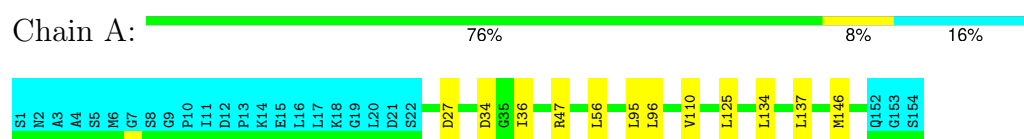
4.2.29 Score per residue for model 29

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



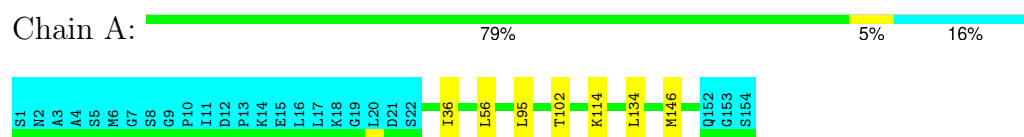
4.2.30 Score per residue for model 30

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



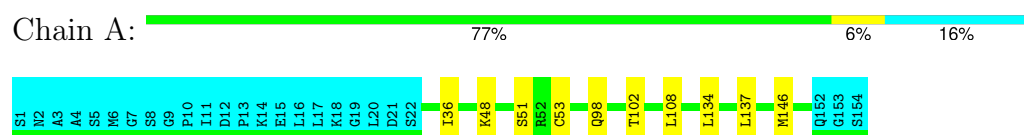
4.2.31 Score per residue for model 31

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



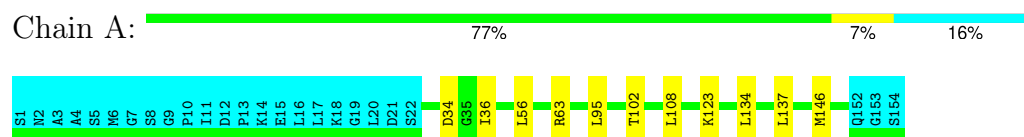
4.2.32 Score per residue for model 32

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



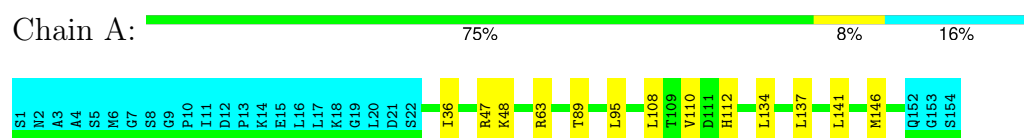
4.2.33 Score per residue for model 33 (medoid)

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



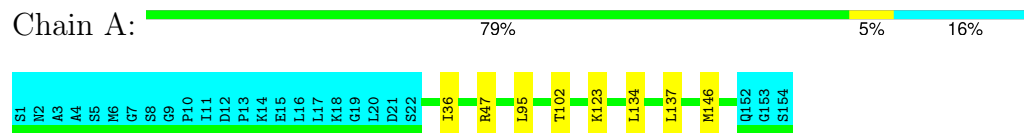
4.2.34 Score per residue for model 34

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



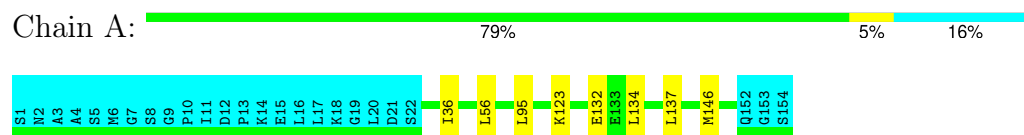
4.2.35 Score per residue for model 35

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



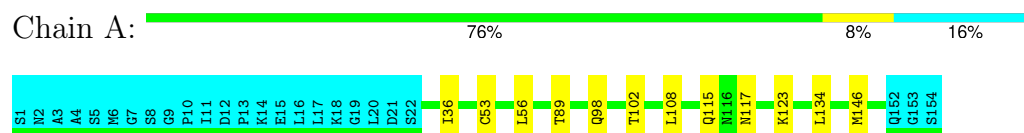
4.2.36 Score per residue for model 36

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



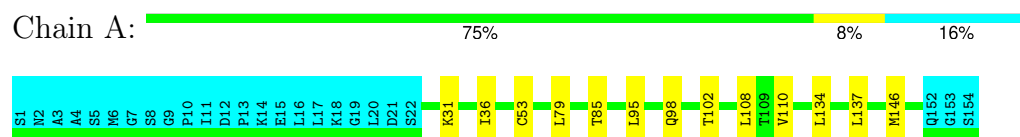
4.2.37 Score per residue for model 37

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



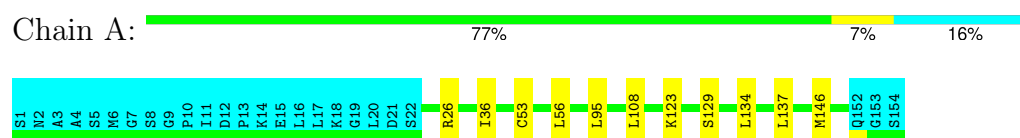
4.2.38 Score per residue for model 38

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



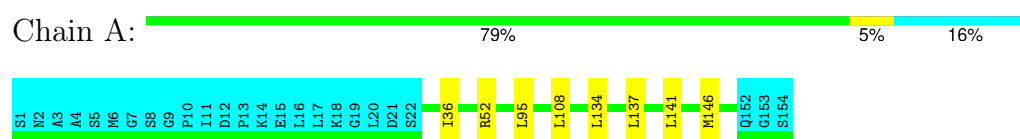
4.2.39 Score per residue for model 39

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



4.2.40 Score per residue for model 40

- Molecule 1: Serine/threonine-protein phosphatase 1 regulatory subunit 10



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, 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 calculation	
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	1943
Number of shifts mapped to atoms	1943
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.58±0.01	0±0/1051 (0.0± 0.0%)	0.69±0.02	0±1/1420 (0.0± 0.1%)
All	All	0.58	0/42040 (0.0%)	0.69	18/56800 (0.0%)

There are no bond-length outliers.

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	26	ARG	NE-CZ-NH1	6.29	123.45	120.30	22	3
1	A	135	ARG	NE-CZ-NH1	6.14	123.37	120.30	1	5
1	A	47	ARG	NE-CZ-NH1	6.05	123.32	120.30	11	4
1	A	63	ARG	NE-CZ-NH1	5.98	123.29	120.30	34	5
1	A	52	ARG	NE-CZ-NH1	5.08	122.84	120.30	40	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1036	1099	1099	0±0
All	All	41440	43960	43960	3

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:96:LEU:HD21	1:A:125:LEU:HD13	0.45	1.89	14	2
1:A:52:ARG:O	1:A:56:LEU:HD22	0.40	2.17	17	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	129/154 (84%)	126±1 (98±1%)	3±1 (2±1%)	0±0 (0±0%)	38	78
All	All	5160/6160 (84%)	5033 (98%)	113 (2%)	14 (0%)	38	78

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	117	ASN	7
1	A	47	ARG	4
1	A	48	LYS	3

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	121/140 (86%)	111±2 (92±2%)	10±2 (8±2%)	12	62
All	All	4840/5600 (86%)	4455 (92%)	385 (8%)	12	62

All 42 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	36	ILE	40
1	A	134	LEU	40
1	A	146	MET	40
1	A	137	LEU	29
1	A	95	LEU	27
1	A	108	LEU	26
1	A	102	THR	23
1	A	56	LEU	21
1	A	123	LYS	18
1	A	53	CYS	12
1	A	115	GLN	7
1	A	112	HIS	6
1	A	127	LYS	6
1	A	129	SER	6
1	A	27	ASP	6
1	A	98	GLN	5
1	A	51	SER	5
1	A	79	LEU	5
1	A	34	ASP	5
1	A	141	LEU	5
1	A	30	VAL	5
1	A	110	VAL	5
1	A	26	ARG	4
1	A	89	THR	4
1	A	96	LEU	4
1	A	31	LYS	3
1	A	132	GLU	3
1	A	61	GLN	3
1	A	49	MET	2
1	A	93	ILE	2
1	A	88	LYS	2
1	A	117	ASN	2
1	A	57	ASN	2
1	A	136	LYS	2
1	A	63	ARG	2
1	A	90	THR	2
1	A	131	ASP	1
1	A	118	THR	1
1	A	81	ASN	1
1	A	47	ARG	1
1	A	114	LYS	1
1	A	85	THR	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping

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

Total number of shifts	1943
Number of shifts mapped to atoms	1943
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	149	-0.55 ± 0.16	Should be checked
$^{13}\text{C}_\beta$	140	0.21 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	148	-0.45 ± 0.10	None needed (< 0.5 ppm)
^{15}N	139	0.19 ± 0.19	None needed (< 0.5 ppm)

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 90%, i.e. 1686 atoms were assigned a chemical shift out of a possible 1864. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	621/643 (97%)	250/259 (97%)	251/258 (97%)	120/126 (95%)
Sidechain	993/1126 (88%)	681/735 (93%)	299/347 (86%)	13/44 (30%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	72/95 (76%)	42/47 (89%)	28/44 (64%)	2/4 (50%)
Overall	1686/1864 (90%)	973/1041 (93%)	578/649 (89%)	135/174 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1939 atoms were assigned a chemical shift out of a possible 2150. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	732/768 (95%)	296/311 (95%)	297/308 (96%)	139/149 (93%)
Sidechain	1135/1287 (88%)	778/840 (93%)	344/399 (86%)	13/48 (27%)
Aromatic	72/95 (76%)	42/47 (89%)	28/44 (64%)	2/4 (50%)
Overall	1939/2150 (90%)	1116/1198 (93%)	669/751 (89%)	154/201 (77%)

7.1.4 Statistically unusual chemical shifts ⓘ

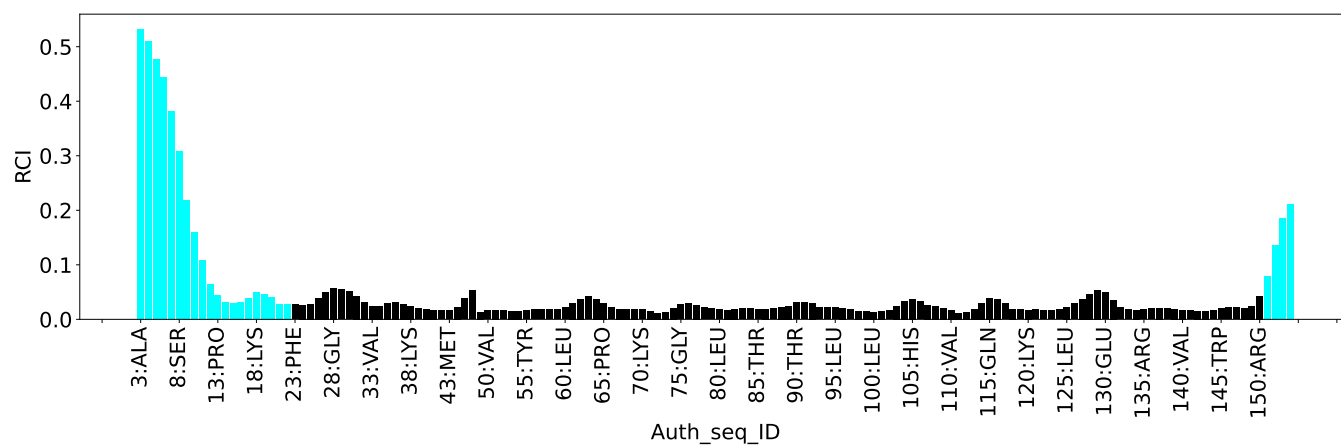
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	62	THR	HG1	5.58	0.08 – 2.19	21.1
1	A	118	THR	HG1	5.36	0.08 – 2.19	20.0
1	A	54	THR	HG1	5.21	0.08 – 2.19	19.3
1	A	102	THR	HG1	4.34	0.08 – 2.19	15.2
1	A	52	ARG	HD3	0.99	1.81 – 4.39	-8.2
1	A	76	GLY	HA3	1.75	2.08 – 5.71	-5.9
1	A	52	ARG	HG3	0.14	0.15 – 2.94	-5.0

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3095
Intra-residue ($ i-j =0$)	791
Sequential ($ i-j =1$)	771
Medium range ($ i-j >1$ and $ i-j <5$)	743
Long range ($ i-j \geq 5$)	790
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	246
Number of unmapped restraints	0
Number of restraints per residue	21.7
Number of long range restraints per residue ¹	5.1

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	6.4	0.2
0.2-0.5 (Medium)	2.7	0.5
>0.5 (Large)	1.1	1.69

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	2.2	5.02
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

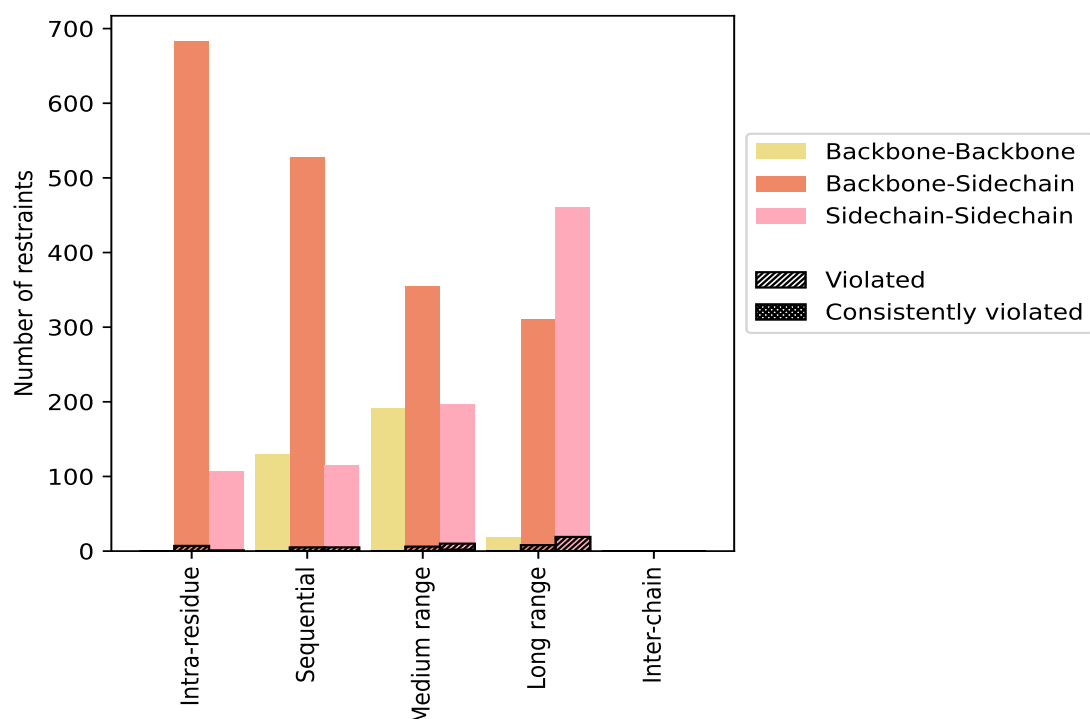
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	791	25.6	8	1.0	0.3	0	0.0	0.0
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	683	22.1	7	1.0	0.2	0	0.0	0.0
Sidechain-Sidechain	107	3.5	1	0.9	0.0	0	0.0	0.0
Sequential ($i-j =1$)	771	24.9	10	1.3	0.3	0	0.0	0.0
Backbone-Backbone	129	4.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	527	17.0	5	0.9	0.2	0	0.0	0.0
Sidechain-Sidechain	115	3.7	5	4.3	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	743	24.0	16	2.2	0.5	2	0.3	0.1
Backbone-Backbone	191	6.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	355	11.5	6	1.7	0.2	0	0.0	0.0
Sidechain-Sidechain	197	6.4	10	5.1	0.3	2	1.0	0.1
Long range ($i-j \geq 5$)	790	25.5	27	3.4	0.9	0	0.0	0.0
Backbone-Backbone	18	0.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	311	10.0	8	2.6	0.3	0	0.0	0.0
Sidechain-Sidechain	461	14.9	19	4.1	0.6	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3095	100.0	61	2.0	2.0	2	0.1	0.1
Backbone-Backbone	339	11.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1876	60.6	26	1.4	0.8	0	0.0	0.0
Sidechain-Sidechain	880	28.4	35	4.0	1.1	2	0.2	0.1

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	5	3	1	0	9	0.35	1.31	0.35	0.23
2	1	5	5	3	0	14	0.24	1.08	0.24	0.16
3	1	3	2	2	0	8	0.33	1.27	0.37	0.17
4	1	4	4	3	0	12	0.24	1.06	0.25	0.15
5	0	3	4	2	0	9	0.32	1.19	0.32	0.23
6	1	3	2	0	0	6	0.34	1.17	0.38	0.17
7	0	3	4	0	0	7	0.35	1.39	0.43	0.19
8	1	4	2	0	0	7	0.4	1.68	0.53	0.16
9	1	5	3	0	0	9	0.3	1.19	0.33	0.14
10	0	3	3	1	0	7	0.36	1.38	0.42	0.17

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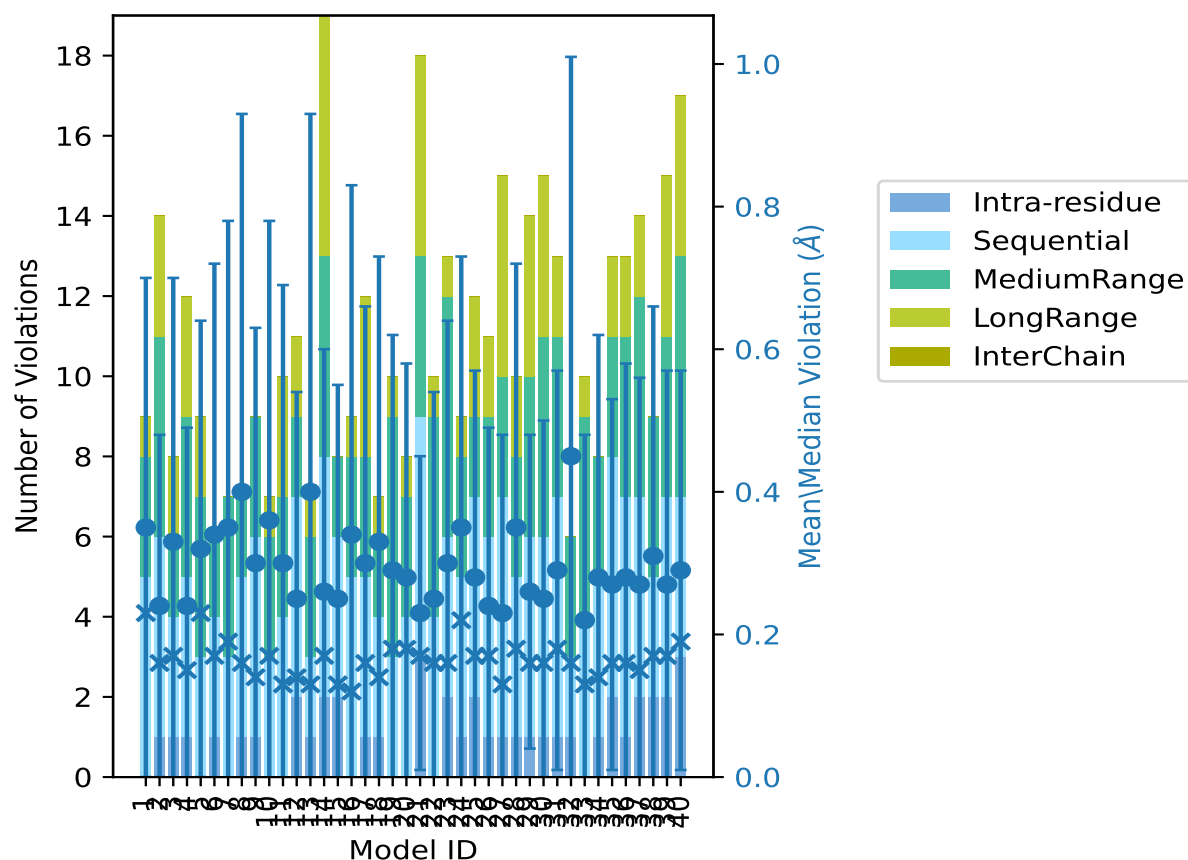
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	4	3	3	0	10	0.3	1.44	0.39	0.13
12	2	5	2	2	0	11	0.25	1.14	0.29	0.14
13	1	2	3	1	0	7	0.4	1.68	0.53	0.13
14	2	6	5	6	0	19	0.26	1.67	0.34	0.17
15	2	4	2	0	0	8	0.25	1.05	0.3	0.13
16	0	5	3	1	0	9	0.34	1.69	0.49	0.12
17	1	4	3	4	0	12	0.3	1.43	0.36	0.16
18	1	3	2	1	0	7	0.33	1.28	0.4	0.14
19	0	3	6	1	0	10	0.29	1.24	0.33	0.18
20	0	4	3	1	0	8	0.28	1.06	0.3	0.18
21	3	6	4	5	0	18	0.23	1.08	0.22	0.17
22	0	4	5	1	0	10	0.25	1.12	0.29	0.16
23	2	4	6	1	0	13	0.3	1.39	0.34	0.16
24	1	4	3	1	0	9	0.35	1.4	0.38	0.22
25	2	5	2	3	0	12	0.28	1.18	0.29	0.17
26	1	5	3	2	0	11	0.24	1.03	0.25	0.17
27	1	6	3	5	0	15	0.23	1.13	0.25	0.13
28	1	4	3	2	0	10	0.35	1.38	0.37	0.18
29	1	5	4	4	0	14	0.26	0.93	0.22	0.16
30	1	5	5	4	0	15	0.25	1.1	0.25	0.16
31	1	6	4	2	0	13	0.29	1.22	0.28	0.18
32	1	2	3	0	0	6	0.45	1.68	0.56	0.16
33	0	4	5	1	0	10	0.22	1.01	0.26	0.13
34	1	4	3	0	0	8	0.28	1.16	0.34	0.14
35	2	6	3	2	0	13	0.27	1.1	0.26	0.16
36	1	6	4	2	0	13	0.28	1.26	0.3	0.16
37	2	5	5	2	0	14	0.27	1.26	0.29	0.15
38	2	3	4	0	0	9	0.31	1.26	0.35	0.17
39	2	5	4	4	0	15	0.27	1.32	0.3	0.17
40	3	4	6	4	0	17	0.29	1.26	0.28	0.19

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3034(IR:783, SQ:761, MR:727, LR:763, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
5	1	5	12	0	23	1	2.5
1	1	4	4	0	10	2	5.0
0	1	2	5	0	8	3	7.5
0	1	0	1	0	2	4	10.0
0	0	0	1	0	1	5	12.5
0	0	0	1	0	1	6	15.0

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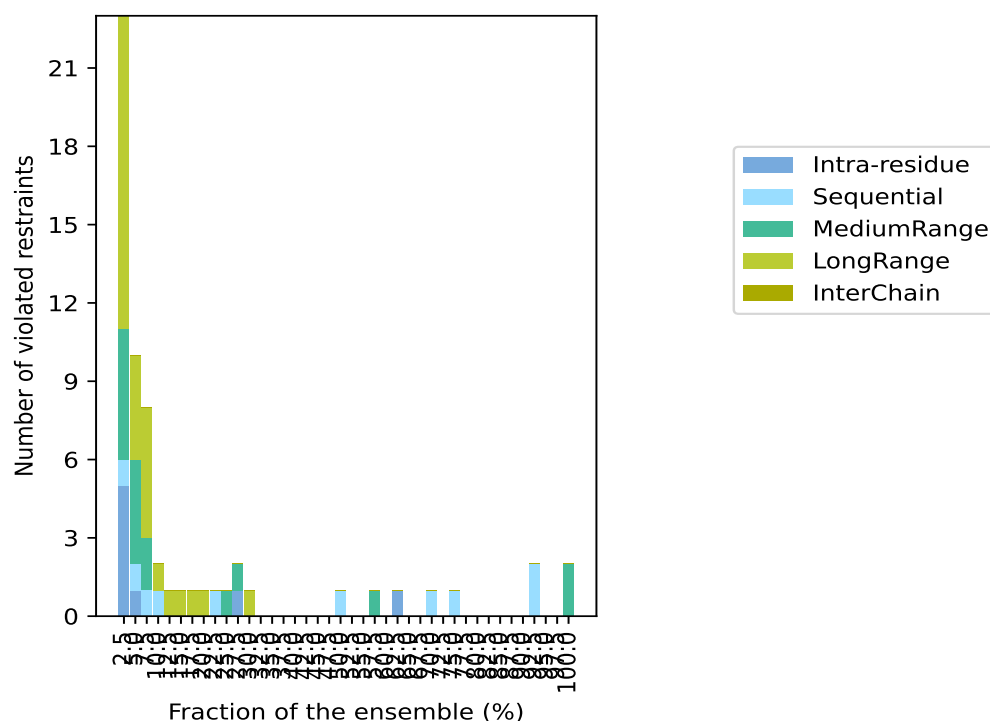
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	1	0	1	7	17.5
0	0	0	1	0	1	8	20.0
0	1	0	0	0	1	9	22.5
0	0	1	0	0	1	10	25.0
1	0	1	0	0	2	11	27.5
0	0	0	1	0	1	12	30.0
0	0	0	0	0	0	13	32.5
0	0	0	0	0	0	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	0	0	18	45.0
0	0	0	0	0	0	19	47.5
0	1	0	0	0	1	20	50.0
0	0	0	0	0	0	21	52.5
0	0	0	0	0	0	22	55.0
0	0	1	0	0	1	23	57.5
0	0	0	0	0	0	24	60.0
1	0	0	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	1	0	0	0	1	28	70.0
0	0	0	0	0	0	29	72.5
0	1	0	0	0	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	0	0	0	0	35	87.5
0	0	0	0	0	0	36	90.0
0	2	0	0	0	2	37	92.5
0	0	0	0	0	0	38	95.0
0	0	0	0	0	0	39	97.5
0	0	2	0	0	2	40	100.0

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

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

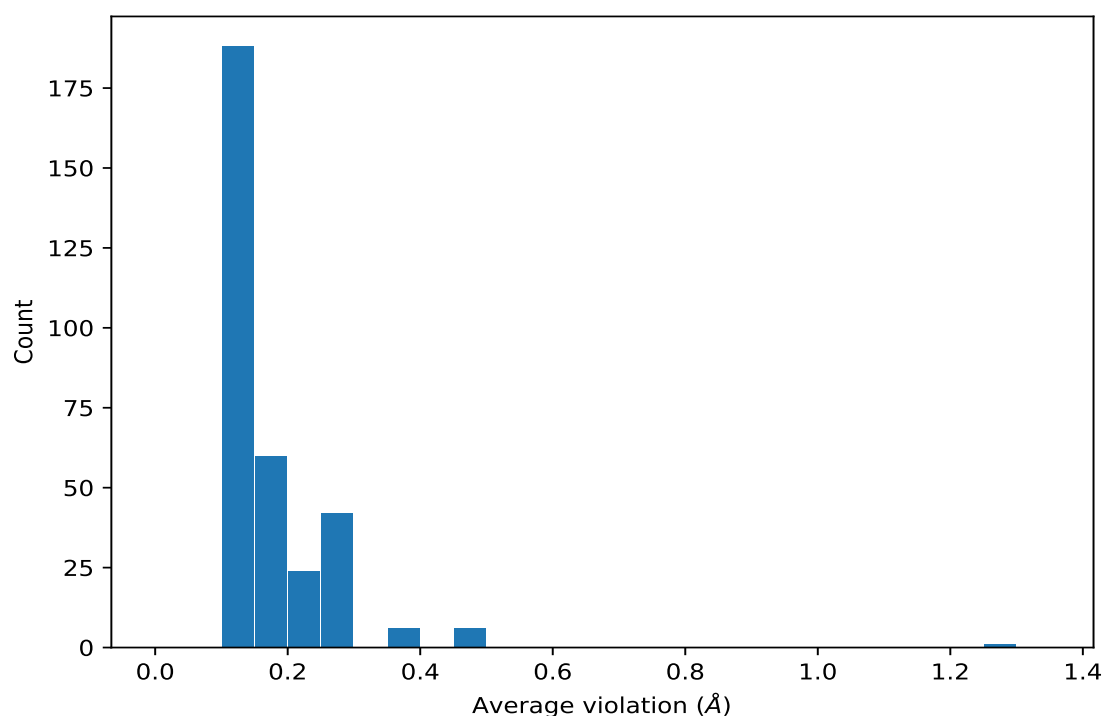
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	40	1.27	0.2	1.25
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	40	0.37	0.11	0.36
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	40	0.37	0.11	0.36
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	40	0.37	0.11	0.36
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	40	0.37	0.11	0.36
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	40	0.37	0.11	0.36
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	40	0.37	0.11	0.36
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	37	0.15	0.03	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	37	0.15	0.03	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	37	0.15	0.03	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	37	0.15	0.03	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	37	0.15	0.03	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	37	0.15	0.03	0.14
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	37	0.14	0.02	0.13
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	37	0.14	0.02	0.13
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	37	0.14	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	37	0.14	0.02	0.13
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	37	0.14	0.02	0.13
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	37	0.14	0.02	0.13
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	30	0.22	0.07	0.2
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	30	0.22	0.07	0.2
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	30	0.22	0.07	0.2
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	30	0.22	0.07	0.2
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	30	0.22	0.07	0.2
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	30	0.22	0.07	0.2
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	30	0.22	0.07	0.2
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	30	0.22	0.07	0.2
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	30	0.22	0.07	0.2
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	30	0.22	0.07	0.2
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	30	0.22	0.07	0.2
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	30	0.22	0.07	0.2
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	28	0.13	0.02	0.13
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	28	0.13	0.02	0.13
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	28	0.13	0.02	0.13
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	25	0.21	0.05	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	25	0.21	0.05	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	25	0.21	0.05	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	25	0.21	0.05	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	25	0.21	0.05	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	25	0.21	0.05	0.21
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	23	0.28	0.11	0.24
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	23	0.28	0.11	0.24
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	23	0.28	0.11	0.24
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	23	0.28	0.11	0.24
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	23	0.28	0.11	0.24
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	23	0.28	0.11	0.24
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	23	0.28	0.11	0.24
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	23	0.28	0.11	0.24
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	23	0.28	0.11	0.24
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	23	0.28	0.11	0.24
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	23	0.28	0.11	0.24
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	23	0.28	0.11	0.24
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	20	0.14	0.03	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	20	0.14	0.03	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	20	0.14	0.03	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	20	0.14	0.03	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	20	0.14	0.03	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	20	0.14	0.03	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2662)	1:84:A:LEU:HD11	1:97:A:GLN:H	12	0.12	0.01	0.11
(1,2662)	1:84:A:LEU:HD12	1:97:A:GLN:H	12	0.12	0.01	0.11
(1,2662)	1:84:A:LEU:HD13	1:97:A:GLN:H	12	0.12	0.01	0.11
(1,2662)	1:84:A:LEU:HD21	1:97:A:GLN:H	12	0.12	0.01	0.11
(1,2662)	1:84:A:LEU:HD22	1:97:A:GLN:H	12	0.12	0.01	0.11
(1,2662)	1:84:A:LEU:HD23	1:97:A:GLN:H	12	0.12	0.01	0.11
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD11	11	0.15	0.02	0.14
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD12	11	0.15	0.02	0.14
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD13	11	0.15	0.02	0.14
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG21	11	0.13	0.03	0.12
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG22	11	0.13	0.03	0.12
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG23	11	0.13	0.03	0.12
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG2	10	0.26	0.04	0.26
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG3	10	0.26	0.04	0.26
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG2	10	0.26	0.04	0.26
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG3	10	0.26	0.04	0.26
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG2	10	0.26	0.04	0.26
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG3	10	0.26	0.04	0.26
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG2	10	0.26	0.04	0.26
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG3	10	0.26	0.04	0.26
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG2	10	0.26	0.04	0.26
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG3	10	0.26	0.04	0.26
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG2	10	0.26	0.04	0.26
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG3	10	0.26	0.04	0.26
(1,2742)	1:96:A:LEU:HD11	1:97:A:GLN:HA	9	0.23	0.07	0.22
(1,2742)	1:96:A:LEU:HD12	1:97:A:GLN:HA	9	0.23	0.07	0.22
(1,2742)	1:96:A:LEU:HD13	1:97:A:GLN:HA	9	0.23	0.07	0.22
(1,2742)	1:96:A:LEU:HD21	1:97:A:GLN:HA	9	0.23	0.07	0.22
(1,2742)	1:96:A:LEU:HD22	1:97:A:GLN:HA	9	0.23	0.07	0.22
(1,2742)	1:96:A:LEU:HD23	1:97:A:GLN:HA	9	0.23	0.07	0.22
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD21	8	0.16	0.05	0.15
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD22	8	0.16	0.05	0.15
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD23	8	0.16	0.05	0.15
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD21	8	0.16	0.05	0.15
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD22	8	0.16	0.05	0.15
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD23	8	0.16	0.05	0.15
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD11	7	0.15	0.02	0.15
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD12	7	0.15	0.02	0.15
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD13	7	0.15	0.02	0.15
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD21	7	0.15	0.02	0.15
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD22	7	0.15	0.02	0.15
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD23	7	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD11	7	0.15	0.02	0.15
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD12	7	0.15	0.02	0.15
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD13	7	0.15	0.02	0.15
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD21	7	0.15	0.02	0.15
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD22	7	0.15	0.02	0.15
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD23	7	0.15	0.02	0.15
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD11	7	0.15	0.02	0.15
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD12	7	0.15	0.02	0.15
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD13	7	0.15	0.02	0.15
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD21	7	0.15	0.02	0.15
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD22	7	0.15	0.02	0.15
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD23	7	0.15	0.02	0.15
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD11	6	0.18	0.07	0.18
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD12	6	0.18	0.07	0.18
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD13	6	0.18	0.07	0.18
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD21	6	0.18	0.07	0.18
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD22	6	0.18	0.07	0.18
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD23	6	0.18	0.07	0.18
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD11	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD12	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD13	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD21	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD22	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD23	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD11	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD12	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD13	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD21	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD22	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD23	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD11	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD12	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD13	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD21	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD22	5	0.12	0.02	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD23	5	0.12	0.02	0.12
(1,2374)	1:42:A:LEU:HD11	1:55:A:TYR:HD1	4	0.12	0.01	0.12
(1,2374)	1:42:A:LEU:HD11	1:55:A:TYR:HD2	4	0.12	0.01	0.12
(1,2374)	1:42:A:LEU:HD12	1:55:A:TYR:HD1	4	0.12	0.01	0.12
(1,2374)	1:42:A:LEU:HD12	1:55:A:TYR:HD2	4	0.12	0.01	0.12
(1,2374)	1:42:A:LEU:HD13	1:55:A:TYR:HD1	4	0.12	0.01	0.12
(1,2374)	1:42:A:LEU:HD13	1:55:A:TYR:HD2	4	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2374)	1:42:A:LEU:HD21	1:55:A:TYR:HD1	4	0.12	0.01	0.12
(1,2374)	1:42:A:LEU:HD21	1:55:A:TYR:HD2	4	0.12	0.01	0.12
(1,2374)	1:42:A:LEU:HD22	1:55:A:TYR:HD1	4	0.12	0.01	0.12
(1,2374)	1:42:A:LEU:HD22	1:55:A:TYR:HD2	4	0.12	0.01	0.12
(1,2374)	1:42:A:LEU:HD23	1:55:A:TYR:HD1	4	0.12	0.01	0.12
(1,2374)	1:42:A:LEU:HD23	1:55:A:TYR:HD2	4	0.12	0.01	0.12
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD11	4	0.12	0.02	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD12	4	0.12	0.02	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD13	4	0.12	0.02	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD21	4	0.12	0.02	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD22	4	0.12	0.02	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD23	4	0.12	0.02	0.11
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD11	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD12	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD13	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD21	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD22	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD23	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD11	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD12	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD13	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD21	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD22	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD23	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD11	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD12	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD13	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD21	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD22	3	0.25	0.02	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD23	3	0.25	0.02	0.24
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD11	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD12	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD13	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD21	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD22	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD23	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD11	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD12	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD13	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD21	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD22	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD23	3	0.19	0.04	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD11	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD12	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD13	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD21	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD22	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD23	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD11	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD12	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD13	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD21	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD22	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD23	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD11	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD12	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD13	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD21	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD22	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD23	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD11	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD12	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD13	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD21	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD22	3	0.19	0.04	0.17
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD23	3	0.19	0.04	0.17
(1,1264)	1:147:A:ALA:HB1	1:151:A:SER:HB2	3	0.12	0.01	0.11
(1,1264)	1:147:A:ALA:HB1	1:151:A:SER:HB3	3	0.12	0.01	0.11
(1,1264)	1:147:A:ALA:HB2	1:151:A:SER:HB2	3	0.12	0.01	0.11
(1,1264)	1:147:A:ALA:HB2	1:151:A:SER:HB3	3	0.12	0.01	0.11
(1,1264)	1:147:A:ALA:HB3	1:151:A:SER:HB2	3	0.12	0.01	0.11
(1,1264)	1:147:A:ALA:HB3	1:151:A:SER:HB3	3	0.12	0.01	0.11
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD11	3	0.12	0.02	0.11
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD12	3	0.12	0.02	0.11
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD13	3	0.12	0.02	0.11
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD21	3	0.12	0.02	0.11
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD22	3	0.12	0.02	0.11
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD23	3	0.12	0.02	0.11
(1,524)	1:62:A:THR:HG21	1:67:A:ILE:HA	3	0.11	0.01	0.11
(1,524)	1:62:A:THR:HG22	1:67:A:ILE:HA	3	0.11	0.01	0.11
(1,524)	1:62:A:THR:HG23	1:67:A:ILE:HA	3	0.11	0.01	0.11
(1,2565)	1:68:A:LEU:HD11	1:107:A:PRO:HD2	3	0.11	0.01	0.11
(1,2565)	1:68:A:LEU:HD12	1:107:A:PRO:HD2	3	0.11	0.01	0.11
(1,2565)	1:68:A:LEU:HD13	1:107:A:PRO:HD2	3	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2565)	1:68:A:LEU:HD21	1:107:A:PRO:HD2	3	0.11	0.01	0.11
(1,2565)	1:68:A:LEU:HD22	1:107:A:PRO:HD2	3	0.11	0.01	0.11
(1,2565)	1:68:A:LEU:HD23	1:107:A:PRO:HD2	3	0.11	0.01	0.11
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD11	3	0.11	0.01	0.11
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD12	3	0.11	0.01	0.11
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD13	3	0.11	0.01	0.11
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD21	3	0.11	0.01	0.11
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD22	3	0.11	0.01	0.11
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD23	3	0.11	0.01	0.11
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD11	3	0.11	0.01	0.11
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD12	3	0.11	0.01	0.11
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD13	3	0.11	0.01	0.11
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD21	3	0.11	0.01	0.11
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD22	3	0.11	0.01	0.11
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD23	3	0.11	0.01	0.11
(1,2970)	1:123:A:LYS:HE2	1:124:A:GLN:HB2	3	0.11	0.01	0.11
(1,2970)	1:123:A:LYS:HE2	1:124:A:GLN:HB3	3	0.11	0.01	0.11
(1,2970)	1:123:A:LYS:HE3	1:124:A:GLN:HB2	3	0.11	0.01	0.11
(1,2970)	1:123:A:LYS:HE3	1:124:A:GLN:HB3	3	0.11	0.01	0.11
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD11	2	0.48	0.01	0.48
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD12	2	0.48	0.01	0.48
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD13	2	0.48	0.01	0.48
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD21	2	0.48	0.01	0.48
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD22	2	0.48	0.01	0.48
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD23	2	0.48	0.01	0.48
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD11	2	0.16	0.05	0.16
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD12	2	0.16	0.05	0.16
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD13	2	0.16	0.05	0.16
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD21	2	0.16	0.05	0.16
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD22	2	0.16	0.05	0.16
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD23	2	0.16	0.05	0.16
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD11	2	0.16	0.05	0.16
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD12	2	0.16	0.05	0.16
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD13	2	0.16	0.05	0.16
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD21	2	0.16	0.05	0.16
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD22	2	0.16	0.05	0.16
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD23	2	0.16	0.05	0.16
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD11	2	0.14	0.02	0.14
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD12	2	0.14	0.02	0.14
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD13	2	0.14	0.02	0.14
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD21	2	0.14	0.02	0.14
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD22	2	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD23	2	0.14	0.02	0.14
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD11	2	0.14	0.02	0.14
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD12	2	0.14	0.02	0.14
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD13	2	0.14	0.02	0.14
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD21	2	0.14	0.02	0.14
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD22	2	0.14	0.02	0.14
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD23	2	0.14	0.02	0.14
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD11	2	0.13	0.02	0.13
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD12	2	0.13	0.02	0.13
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD13	2	0.13	0.02	0.13
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD21	2	0.13	0.02	0.13
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD22	2	0.13	0.02	0.13
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD23	2	0.13	0.02	0.13
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD11	2	0.13	0.02	0.13
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD12	2	0.13	0.02	0.13
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD13	2	0.13	0.02	0.13
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD21	2	0.13	0.02	0.13
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD22	2	0.13	0.02	0.13
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD23	2	0.13	0.02	0.13
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD11	2	0.12	0.02	0.12
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD12	2	0.12	0.02	0.12
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD13	2	0.12	0.02	0.12
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD21	2	0.12	0.02	0.12
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD22	2	0.12	0.02	0.12
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD23	2	0.12	0.02	0.12
(1,830)	1:93:A:ILE:HG21	1:98:A:GLN:H	2	0.12	0.01	0.12
(1,830)	1:93:A:ILE:HG22	1:98:A:GLN:H	2	0.12	0.01	0.12
(1,830)	1:93:A:ILE:HG23	1:98:A:GLN:H	2	0.12	0.01	0.12
(1,1623)	1:66:A:GLU:H	1:69:A:VAL:HG11	2	0.12	0.02	0.12
(1,1623)	1:66:A:GLU:H	1:69:A:VAL:HG12	2	0.12	0.02	0.12
(1,1623)	1:66:A:GLU:H	1:69:A:VAL:HG13	2	0.12	0.02	0.12
(1,3026)	1:134:A:LEU:HD11	1:137:A:LEU:H	2	0.12	0.02	0.12
(1,3026)	1:134:A:LEU:HD12	1:137:A:LEU:H	2	0.12	0.02	0.12
(1,3026)	1:134:A:LEU:HD13	1:137:A:LEU:H	2	0.12	0.02	0.12
(1,3026)	1:134:A:LEU:HD21	1:137:A:LEU:H	2	0.12	0.02	0.12
(1,3026)	1:134:A:LEU:HD22	1:137:A:LEU:H	2	0.12	0.02	0.12
(1,3026)	1:134:A:LEU:HD23	1:137:A:LEU:H	2	0.12	0.02	0.12
(1,2483)	1:59:A:LEU:HD11	1:62:A:THR:HG21	2	0.12	0.0	0.12
(1,2483)	1:59:A:LEU:HD11	1:62:A:THR:HG22	2	0.12	0.0	0.12
(1,2483)	1:59:A:LEU:HD11	1:62:A:THR:HG23	2	0.12	0.0	0.12
(1,2483)	1:59:A:LEU:HD12	1:62:A:THR:HG21	2	0.12	0.0	0.12
(1,2483)	1:59:A:LEU:HD12	1:62:A:THR:HG22	2	0.12	0.0	0.12

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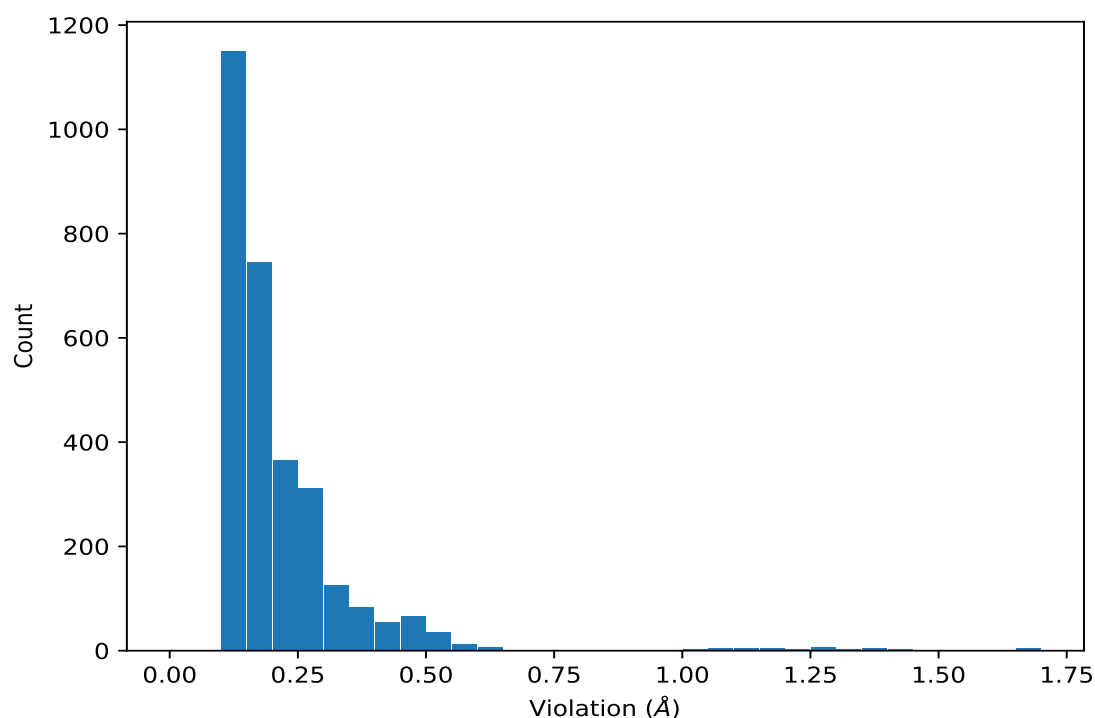
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2483)	1:59:A:LEU:HD12	1:62:A:THR:HG23	2	0.12	0.0	0.12
(1,2483)	1:59:A:LEU:HD13	1:62:A:THR:HG21	2	0.12	0.0	0.12
(1,2483)	1:59:A:LEU:HD13	1:62:A:THR:HG22	2	0.12	0.0	0.12
(1,2483)	1:59:A:LEU:HD13	1:62:A:THR:HG23	2	0.12	0.0	0.12
(1,2483)	1:59:A:LEU:HD21	1:62:A:THR:HG21	2	0.12	0.0	0.12
(1,2483)	1:59:A:LEU:HD21	1:62:A:THR:HG22	2	0.12	0.0	0.12
(1,2483)	1:59:A:LEU:HD21	1:62:A:THR:HG23	2	0.12	0.0	0.12
(1,2483)	1:59:A:LEU:HD22	1:62:A:THR:HG21	2	0.12	0.0	0.12
(1,2483)	1:59:A:LEU:HD22	1:62:A:THR:HG22	2	0.12	0.0	0.12
(1,2483)	1:59:A:LEU:HD22	1:62:A:THR:HG23	2	0.12	0.0	0.12
(1,2483)	1:59:A:LEU:HD23	1:62:A:THR:HG21	2	0.12	0.0	0.12
(1,2483)	1:59:A:LEU:HD23	1:62:A:THR:HG22	2	0.12	0.0	0.12
(1,2483)	1:59:A:LEU:HD23	1:62:A:THR:HG23	2	0.12	0.0	0.12
(1,190)	1:37:A:SER:HB2	1:38:A:LYS:HB2	2	0.11	0.01	0.11
(1,190)	1:37:A:SER:HB2	1:38:A:LYS:HB3	2	0.11	0.01	0.11
(1,190)	1:37:A:SER:HB3	1:38:A:LYS:HB2	2	0.11	0.01	0.11
(1,190)	1:37:A:SER:HB3	1:38:A:LYS:HB3	2	0.11	0.01	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	16	1.69
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	8	1.68
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	13	1.68
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	32	1.68
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	14	1.67
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	11	1.44
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	17	1.43
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	24	1.4
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	7	1.39
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	23	1.39
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	10	1.38
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	28	1.38
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	39	1.32
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	1	1.31
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	18	1.28
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	3	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	36	1.26
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	37	1.26
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	38	1.26
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	40	1.26
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	19	1.24
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	31	1.22
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	5	1.19
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	9	1.19
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	25	1.18
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	6	1.17
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	34	1.16
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	12	1.14
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	27	1.13
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	22	1.12
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	30	1.1
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	35	1.1
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	2	1.08
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	21	1.08
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	4	1.06
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	20	1.06
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	15	1.05
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	26	1.03
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	33	1.01
(1,717)	1:79:A:LEU:HG	1:82:A:ASN:HD21	29	0.93
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	28	0.62
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	28	0.62
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	28	0.62
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	28	0.62
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	28	0.62
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	28	0.62
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	23	0.57
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	23	0.57
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	23	0.57
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	23	0.57
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	23	0.57
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	23	0.57
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	17	0.55
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	17	0.55
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	17	0.55
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	17	0.55
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	17	0.55
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	17	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	40	0.53
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	40	0.53
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	40	0.53
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	40	0.53
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	40	0.53
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	40	0.53
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	37	0.5
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	37	0.5
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	37	0.5
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	37	0.5
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	37	0.5
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	37	0.5
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	37	0.5
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	37	0.5
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	37	0.5
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	37	0.5
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	37	0.5
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	37	0.5
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	35	0.5
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	35	0.5
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	35	0.5
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	35	0.5
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	35	0.5
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	35	0.5
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	35	0.5
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	35	0.5
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	35	0.5
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	35	0.5
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	35	0.5
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	35	0.5
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	39	0.5
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	39	0.5
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	39	0.5
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	39	0.5
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	39	0.5
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	39	0.5
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	40	0.49
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	40	0.49
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	40	0.49
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	40	0.49
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	40	0.49
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	40	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	40	0.49
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	40	0.49
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	40	0.49
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	40	0.49
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	40	0.49
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	40	0.49
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD11	40	0.49
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD12	40	0.49
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD13	40	0.49
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD21	40	0.49
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD22	40	0.49
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD23	40	0.49
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD11	29	0.48
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD12	29	0.48
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD13	29	0.48
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD21	29	0.48
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD22	29	0.48
(1,2253)	1:20:A:LEU:HA	1:20:A:LEU:HD23	29	0.48
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	30	0.47
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	30	0.47
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	30	0.47
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	30	0.47
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	30	0.47
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	30	0.47
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	30	0.47
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	30	0.47
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	30	0.47
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	30	0.47
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	30	0.47
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	30	0.47
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	25	0.47
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	25	0.47
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	25	0.47
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	25	0.47
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	25	0.47
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	25	0.47
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	32	0.47
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	32	0.47
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	32	0.47
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	32	0.47
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	32	0.47
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	32	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	3	0.45
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	3	0.45
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	3	0.45
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	3	0.45
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	3	0.45
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	3	0.45
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	11	0.45
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	11	0.45
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	11	0.45
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	11	0.45
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	11	0.45
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	11	0.45
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	16	0.45
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	16	0.45
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	16	0.45
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	16	0.45
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	16	0.45
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	16	0.45
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	14	0.44
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	14	0.44
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	14	0.44
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	14	0.44
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	14	0.44
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	14	0.44
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	29	0.43
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	29	0.43
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	29	0.43
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	29	0.43
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	29	0.43
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	29	0.43
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	29	0.43
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	29	0.43
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	29	0.43
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	29	0.43
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	29	0.43
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	29	0.43
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	13	0.43
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	13	0.43
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	13	0.43
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	13	0.43
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	13	0.43
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	13	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	18	0.43
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	18	0.43
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	18	0.43
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	18	0.43
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	18	0.43
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	18	0.43
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	24	0.43
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	24	0.43
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	24	0.43
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	24	0.43
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	24	0.43
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	24	0.43
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	8	0.41
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	8	0.41
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	8	0.41
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	8	0.41
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	8	0.41
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	8	0.41
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	9	0.41
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	9	0.41
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	9	0.41
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	9	0.41
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	9	0.41
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	9	0.41
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	38	0.4
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	38	0.4
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	38	0.4
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	38	0.4
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	38	0.4
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	38	0.4
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	19	0.38
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	19	0.38
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	19	0.38
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	19	0.38
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	19	0.38
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	19	0.38
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	1	0.37
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	1	0.37
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	1	0.37
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	1	0.37
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	1	0.37
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	1	0.37
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	1	0.37
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	1	0.37
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	1	0.37
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	1	0.37
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	1	0.37
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	31	0.37
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	31	0.37
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	31	0.37
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	31	0.37
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	31	0.37
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	31	0.37
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	36	0.37
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	36	0.37
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	36	0.37
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	36	0.37
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	36	0.37
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	36	0.37
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	12	0.36
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	12	0.36
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	12	0.36
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	12	0.36
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	12	0.36
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	12	0.36
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	2	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	2	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	2	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	2	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	2	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	2	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	2	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	2	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	2	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	2	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	2	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	2	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	28	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	28	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	28	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	28	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	28	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	28	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	28	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	28	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	28	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	28	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	28	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	28	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	36	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	36	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	36	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	36	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	36	0.35
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	36	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	36	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	36	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	36	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	36	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	36	0.35
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	36	0.35
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	5	0.35
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	5	0.35
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	5	0.35
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	5	0.35
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	5	0.35
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	5	0.35
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	21	0.35
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	21	0.35
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	21	0.35
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	21	0.35
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	21	0.35
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	21	0.35
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG2	23	0.34
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG3	23	0.34
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG2	23	0.34
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG3	23	0.34
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG2	23	0.34
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG3	23	0.34
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG2	23	0.34
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG3	23	0.34
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG2	23	0.34
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG3	23	0.34
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG2	23	0.34
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG3	23	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	10	0.34
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	10	0.34
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	10	0.34
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	10	0.34
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	10	0.34
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	10	0.34
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	1	0.33
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	1	0.33
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	1	0.33
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	1	0.33
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	1	0.33
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	1	0.33
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	35	0.33
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	35	0.33
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	35	0.33
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	35	0.33
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	35	0.33
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	35	0.33
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG2	29	0.32
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG3	29	0.32
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG2	29	0.32
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG3	29	0.32
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG2	29	0.32
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG3	29	0.32
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG2	29	0.32
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG3	29	0.32
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG2	29	0.32
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG3	29	0.32
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG2	29	0.32
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG3	29	0.32
(1,2742)	1:96:A:LEU:HD11	1:97:A:GLN:HA	1	0.32
(1,2742)	1:96:A:LEU:HD12	1:97:A:GLN:HA	1	0.32
(1,2742)	1:96:A:LEU:HD13	1:97:A:GLN:HA	1	0.32
(1,2742)	1:96:A:LEU:HD21	1:97:A:GLN:HA	1	0.32
(1,2742)	1:96:A:LEU:HD22	1:97:A:GLN:HA	1	0.32
(1,2742)	1:96:A:LEU:HD23	1:97:A:GLN:HA	1	0.32
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	6	0.32
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	6	0.32
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	6	0.32
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	6	0.32
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	6	0.32
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	7	0.32
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	7	0.32
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	7	0.32
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	7	0.32
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	7	0.32
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	7	0.32
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	30	0.32
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	30	0.32
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	30	0.32
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	30	0.32
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	30	0.32
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	30	0.32
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	37	0.32
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	37	0.32
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	37	0.32
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	37	0.32
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	37	0.32
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	37	0.32
(1,2742)	1:96:A:LEU:HD11	1:97:A:GLN:HA	31	0.31
(1,2742)	1:96:A:LEU:HD12	1:97:A:GLN:HA	31	0.31
(1,2742)	1:96:A:LEU:HD13	1:97:A:GLN:HA	31	0.31
(1,2742)	1:96:A:LEU:HD21	1:97:A:GLN:HA	31	0.31
(1,2742)	1:96:A:LEU:HD22	1:97:A:GLN:HA	31	0.31
(1,2742)	1:96:A:LEU:HD23	1:97:A:GLN:HA	31	0.31
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	34	0.31
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	34	0.31
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	34	0.31
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	34	0.31
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	34	0.31
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	34	0.31
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	21	0.3
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	21	0.3
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	21	0.3
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	21	0.3
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	21	0.3
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	21	0.3
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	21	0.3
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	21	0.3
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	21	0.3
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	21	0.3
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	21	0.3
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	21	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	31	0.3
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	31	0.3
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	31	0.3
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	31	0.3
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	31	0.3
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	31	0.3
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	23	0.3
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	23	0.3
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	23	0.3
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	23	0.3
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	23	0.3
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	23	0.3
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	23	0.3
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	23	0.3
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	23	0.3
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	23	0.3
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	23	0.3
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	23	0.3
(1,2742)	1:96:A:LEU:HD11	1:97:A:GLN:HA	36	0.3
(1,2742)	1:96:A:LEU:HD12	1:97:A:GLN:HA	36	0.3
(1,2742)	1:96:A:LEU:HD13	1:97:A:GLN:HA	36	0.3
(1,2742)	1:96:A:LEU:HD21	1:97:A:GLN:HA	36	0.3
(1,2742)	1:96:A:LEU:HD22	1:97:A:GLN:HA	36	0.3
(1,2742)	1:96:A:LEU:HD23	1:97:A:GLN:HA	36	0.3
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD11	39	0.3
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD12	39	0.3
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD13	39	0.3
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD21	39	0.3
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD22	39	0.3
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD23	39	0.3
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG2	39	0.29
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG3	39	0.29
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG2	39	0.29
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG3	39	0.29
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG2	39	0.29
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG3	39	0.29
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG2	39	0.29
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG3	39	0.29
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG2	39	0.29
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG3	39	0.29
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG2	39	0.29
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG3	39	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	40	0.29
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	40	0.29
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	40	0.29
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	40	0.29
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	40	0.29
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	40	0.29
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	40	0.29
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	40	0.29
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	40	0.29
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	40	0.29
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	40	0.29
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	40	0.29
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	31	0.29
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	31	0.29
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	31	0.29
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	31	0.29
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	31	0.29
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	31	0.29
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	31	0.29
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	31	0.29
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	31	0.29
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	31	0.29
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	31	0.29
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	31	0.29
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	2	0.29
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	2	0.29
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	2	0.29
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	2	0.29
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	2	0.29
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	2	0.29
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	14	0.28
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	14	0.28
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	14	0.28
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	14	0.28
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	14	0.28
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	14	0.28
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	27	0.28
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	27	0.28
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	27	0.28
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	27	0.28
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	27	0.28
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	27	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	4	0.28
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	4	0.28
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	4	0.28
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	4	0.28
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	4	0.28
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	4	0.28
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	20	0.28
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	20	0.28
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	20	0.28
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	20	0.28
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	20	0.28
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	20	0.28
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD11	27	0.28
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD12	27	0.28
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD13	27	0.28
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD21	27	0.28
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD22	27	0.28
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD23	27	0.28
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD11	27	0.28
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD12	27	0.28
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD13	27	0.28
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD21	27	0.28
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD22	27	0.28
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD23	27	0.28
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD11	27	0.28
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD12	27	0.28
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD13	27	0.28
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD21	27	0.28
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD22	27	0.28
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD23	27	0.28
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG2	5	0.27
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG3	5	0.27
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG2	5	0.27
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG3	5	0.27
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG2	5	0.27
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG3	5	0.27
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG2	5	0.27
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG3	5	0.27
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG2	5	0.27
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG3	5	0.27
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG2	5	0.27
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG3	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	30	0.27
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	30	0.27
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	30	0.27
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	30	0.27
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	30	0.27
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	30	0.27
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	30	0.27
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	30	0.27
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	30	0.27
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	30	0.27
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	30	0.27
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	30	0.27
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	35	0.27
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	35	0.27
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	35	0.27
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	35	0.27
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	35	0.27
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	35	0.27
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	35	0.27
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	35	0.27
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	35	0.27
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	35	0.27
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	35	0.27
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	35	0.27
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	9	0.27
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	9	0.27
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	9	0.27
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	9	0.27
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	9	0.27
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	9	0.27
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	24	0.27
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	24	0.27
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	24	0.27
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	24	0.27
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	24	0.27
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	24	0.27
(1,2742)	1:96:A:LEU:HD11	1:97:A:GLN:HA	37	0.27
(1,2742)	1:96:A:LEU:HD12	1:97:A:GLN:HA	37	0.27
(1,2742)	1:96:A:LEU:HD13	1:97:A:GLN:HA	37	0.27
(1,2742)	1:96:A:LEU:HD21	1:97:A:GLN:HA	37	0.27
(1,2742)	1:96:A:LEU:HD22	1:97:A:GLN:HA	37	0.27
(1,2742)	1:96:A:LEU:HD23	1:97:A:GLN:HA	37	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	27	0.27
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	27	0.27
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	27	0.27
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	27	0.27
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	27	0.27
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	27	0.27
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG2	38	0.26
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG3	38	0.26
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG2	38	0.26
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG3	38	0.26
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG2	38	0.26
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG3	38	0.26
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG2	38	0.26
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG3	38	0.26
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG2	38	0.26
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG3	38	0.26
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG2	38	0.26
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG3	38	0.26
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	31	0.26
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	31	0.26
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	31	0.26
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	31	0.26
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	31	0.26
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	31	0.26
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	31	0.26
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	31	0.26
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	31	0.26
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	31	0.26
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	31	0.26
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	31	0.26
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	35	0.26
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	35	0.26
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	35	0.26
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	35	0.26
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	35	0.26
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	35	0.26
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG2	14	0.25
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG3	14	0.25
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG2	14	0.25
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG3	14	0.25
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG2	14	0.25
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG3	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG2	14	0.25
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG3	14	0.25
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG2	14	0.25
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG3	14	0.25
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG2	14	0.25
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG3	14	0.25
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG2	19	0.25
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG3	19	0.25
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG2	19	0.25
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG3	19	0.25
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG2	19	0.25
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG3	19	0.25
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG2	19	0.25
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG3	19	0.25
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG2	19	0.25
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG3	19	0.25
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG2	19	0.25
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG3	19	0.25
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	2	0.25
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	2	0.25
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	2	0.25
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	2	0.25
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	2	0.25
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	2	0.25
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	2	0.25
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	2	0.25
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	2	0.25
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	2	0.25
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	2	0.25
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	2	0.25
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	27	0.25
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	27	0.25
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	27	0.25
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	27	0.25
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	27	0.25
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	27	0.25
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	27	0.25
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	27	0.25
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	27	0.25
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	27	0.25
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	27	0.25
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	27	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	36	0.25
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	36	0.25
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	36	0.25
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	36	0.25
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	36	0.25
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	36	0.25
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	36	0.25
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	36	0.25
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	36	0.25
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	36	0.25
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	36	0.25
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	36	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	2	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	2	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	2	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	2	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	2	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	2	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	21	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	21	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	21	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	21	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	21	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	21	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	26	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	26	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	26	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	26	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	26	0.25
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	26	0.25
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	24	0.25
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	24	0.25
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	24	0.25
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	24	0.25
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	24	0.25
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	24	0.25
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	24	0.25
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	24	0.25
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	24	0.25
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	24	0.25
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	24	0.25
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	24	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD21	40	0.25
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD22	40	0.25
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD23	40	0.25
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD21	40	0.25
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD22	40	0.25
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD23	40	0.25
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	22	0.25
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	22	0.25
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	22	0.25
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	22	0.25
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	22	0.25
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	22	0.25
(1,2485)	1:59:A:LEU:HD11	1:68:A:LEU:HD11	19	0.25
(1,2485)	1:59:A:LEU:HD11	1:68:A:LEU:HD12	19	0.25
(1,2485)	1:59:A:LEU:HD11	1:68:A:LEU:HD13	19	0.25
(1,2485)	1:59:A:LEU:HD11	1:68:A:LEU:HD21	19	0.25
(1,2485)	1:59:A:LEU:HD11	1:68:A:LEU:HD22	19	0.25
(1,2485)	1:59:A:LEU:HD11	1:68:A:LEU:HD23	19	0.25
(1,2485)	1:59:A:LEU:HD12	1:68:A:LEU:HD11	19	0.25
(1,2485)	1:59:A:LEU:HD12	1:68:A:LEU:HD12	19	0.25
(1,2485)	1:59:A:LEU:HD12	1:68:A:LEU:HD13	19	0.25
(1,2485)	1:59:A:LEU:HD12	1:68:A:LEU:HD21	19	0.25
(1,2485)	1:59:A:LEU:HD12	1:68:A:LEU:HD22	19	0.25
(1,2485)	1:59:A:LEU:HD12	1:68:A:LEU:HD23	19	0.25
(1,2485)	1:59:A:LEU:HD13	1:68:A:LEU:HD11	19	0.25
(1,2485)	1:59:A:LEU:HD13	1:68:A:LEU:HD12	19	0.25
(1,2485)	1:59:A:LEU:HD13	1:68:A:LEU:HD13	19	0.25
(1,2485)	1:59:A:LEU:HD13	1:68:A:LEU:HD21	19	0.25
(1,2485)	1:59:A:LEU:HD13	1:68:A:LEU:HD22	19	0.25
(1,2485)	1:59:A:LEU:HD13	1:68:A:LEU:HD23	19	0.25
(1,2485)	1:59:A:LEU:HD21	1:68:A:LEU:HD11	19	0.25
(1,2485)	1:59:A:LEU:HD21	1:68:A:LEU:HD12	19	0.25
(1,2485)	1:59:A:LEU:HD21	1:68:A:LEU:HD13	19	0.25
(1,2485)	1:59:A:LEU:HD21	1:68:A:LEU:HD21	19	0.25
(1,2485)	1:59:A:LEU:HD21	1:68:A:LEU:HD22	19	0.25
(1,2485)	1:59:A:LEU:HD21	1:68:A:LEU:HD23	19	0.25
(1,2485)	1:59:A:LEU:HD22	1:68:A:LEU:HD11	19	0.25
(1,2485)	1:59:A:LEU:HD22	1:68:A:LEU:HD12	19	0.25
(1,2485)	1:59:A:LEU:HD22	1:68:A:LEU:HD13	19	0.25
(1,2485)	1:59:A:LEU:HD22	1:68:A:LEU:HD21	19	0.25
(1,2485)	1:59:A:LEU:HD22	1:68:A:LEU:HD22	19	0.25
(1,2485)	1:59:A:LEU:HD22	1:68:A:LEU:HD23	19	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2485)	1:59:A:LEU:HD23	1:68:A:LEU:HD11	19	0.25
(1,2485)	1:59:A:LEU:HD23	1:68:A:LEU:HD12	19	0.25
(1,2485)	1:59:A:LEU:HD23	1:68:A:LEU:HD13	19	0.25
(1,2485)	1:59:A:LEU:HD23	1:68:A:LEU:HD21	19	0.25
(1,2485)	1:59:A:LEU:HD23	1:68:A:LEU:HD22	19	0.25
(1,2485)	1:59:A:LEU:HD23	1:68:A:LEU:HD23	19	0.25
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	17	0.24
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	17	0.24
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	17	0.24
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	17	0.24
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	17	0.24
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	17	0.24
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	17	0.24
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	17	0.24
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	17	0.24
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	17	0.24
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	17	0.24
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	17	0.24
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	25	0.24
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	25	0.24
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	25	0.24
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	25	0.24
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	25	0.24
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	25	0.24
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	25	0.24
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	25	0.24
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	25	0.24
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	25	0.24
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	25	0.24
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	25	0.24
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	37	0.24
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	37	0.24
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	37	0.24
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	37	0.24
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	37	0.24
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	37	0.24
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	19	0.24
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	19	0.24
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	19	0.24
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	19	0.24
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	19	0.24
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	19	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	19	0.24
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	19	0.24
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	19	0.24
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	19	0.24
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	19	0.24
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	19	0.24
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD11	5	0.24
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD12	5	0.24
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD13	5	0.24
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD21	5	0.24
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD22	5	0.24
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD23	5	0.24
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD11	5	0.24
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD12	5	0.24
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD13	5	0.24
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD21	5	0.24
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD22	5	0.24
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD23	5	0.24
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD11	5	0.24
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD12	5	0.24
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD13	5	0.24
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD21	5	0.24
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD22	5	0.24
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD23	5	0.24
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD11	5	0.24
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD12	5	0.24
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD13	5	0.24
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD21	5	0.24
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD22	5	0.24
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD23	5	0.24
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD11	5	0.24
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD12	5	0.24
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD13	5	0.24
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD21	5	0.24
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD22	5	0.24
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD23	5	0.24
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD11	5	0.24
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD12	5	0.24
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD13	5	0.24
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD21	5	0.24
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD22	5	0.24
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD23	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	40	0.24
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	40	0.24
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	40	0.24
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	40	0.24
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	40	0.24
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	40	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD11	10	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD12	10	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD13	10	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD21	10	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD22	10	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD23	10	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD11	10	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD12	10	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD13	10	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD21	10	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD22	10	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD23	10	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD11	10	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD12	10	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD13	10	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD21	10	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD22	10	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD23	10	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD11	25	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD12	25	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD13	25	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD21	25	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD22	25	0.24
(1,2356)	1:39:A:ILE:HD11	1:59:A:LEU:HD23	25	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD11	25	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD12	25	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD13	25	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD21	25	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD22	25	0.24
(1,2356)	1:39:A:ILE:HD12	1:59:A:LEU:HD23	25	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD11	25	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD12	25	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD13	25	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD21	25	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD22	25	0.24
(1,2356)	1:39:A:ILE:HD13	1:59:A:LEU:HD23	25	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG2	7	0.23
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG3	7	0.23
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG2	7	0.23
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG3	7	0.23
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG2	7	0.23
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG3	7	0.23
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG2	7	0.23
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG3	7	0.23
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG2	7	0.23
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG3	7	0.23
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG2	7	0.23
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG3	7	0.23
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	1	0.23
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	1	0.23
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	1	0.23
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	1	0.23
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	1	0.23
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	1	0.23
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	1	0.23
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	1	0.23
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	1	0.23
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	1	0.23
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	1	0.23
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	1	0.23
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	28	0.23
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	28	0.23
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	28	0.23
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	28	0.23
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	28	0.23
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	28	0.23
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	28	0.23
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	28	0.23
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	28	0.23
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	28	0.23
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	28	0.23
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	28	0.23
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	17	0.23
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	17	0.23
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	17	0.23
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	17	0.23
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	17	0.23
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD11	5	0.23
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD12	5	0.23
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD13	5	0.23
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD21	5	0.23
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD22	5	0.23
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD23	5	0.23
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG2	4	0.22
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG3	4	0.22
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG2	4	0.22
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG3	4	0.22
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG2	4	0.22
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG3	4	0.22
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG2	4	0.22
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG3	4	0.22
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG2	4	0.22
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG3	4	0.22
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG2	4	0.22
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG3	4	0.22
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG2	16	0.22
(1,3077)	1:142:A:VAL:HG11	1:146:A:MET:HG3	16	0.22
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG2	16	0.22
(1,3077)	1:142:A:VAL:HG12	1:146:A:MET:HG3	16	0.22
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG2	16	0.22
(1,3077)	1:142:A:VAL:HG13	1:146:A:MET:HG3	16	0.22
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG2	16	0.22
(1,3077)	1:142:A:VAL:HG21	1:146:A:MET:HG3	16	0.22
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG2	16	0.22
(1,3077)	1:142:A:VAL:HG22	1:146:A:MET:HG3	16	0.22
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG2	16	0.22
(1,3077)	1:142:A:VAL:HG23	1:146:A:MET:HG3	16	0.22
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	25	0.22
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	25	0.22
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	25	0.22
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	25	0.22
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	25	0.22
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	25	0.22
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	4	0.22
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	4	0.22
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	4	0.22
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	4	0.22
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	4	0.22
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	4	0.22
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	4	0.22
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	4	0.22
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	4	0.22
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	4	0.22
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	4	0.22
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	5	0.22
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	5	0.22
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	5	0.22
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	5	0.22
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	5	0.22
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	5	0.22
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	5	0.22
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	5	0.22
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	5	0.22
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	5	0.22
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	5	0.22
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	5	0.22
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	14	0.22
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	14	0.22
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	14	0.22
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	14	0.22
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	14	0.22
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	14	0.22
(1,2742)	1:96:A:LEU:HD11	1:97:A:GLN:HA	24	0.22
(1,2742)	1:96:A:LEU:HD12	1:97:A:GLN:HA	24	0.22
(1,2742)	1:96:A:LEU:HD13	1:97:A:GLN:HA	24	0.22
(1,2742)	1:96:A:LEU:HD21	1:97:A:GLN:HA	24	0.22
(1,2742)	1:96:A:LEU:HD22	1:97:A:GLN:HA	24	0.22
(1,2742)	1:96:A:LEU:HD23	1:97:A:GLN:HA	24	0.22
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	12	0.21
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	12	0.21
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	12	0.21
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	12	0.21
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	12	0.21
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	12	0.21
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	12	0.21
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	12	0.21
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	12	0.21
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	12	0.21
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	12	0.21
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	22	0.21
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	22	0.21
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	22	0.21
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	22	0.21
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	22	0.21
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	22	0.21
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	22	0.21
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	22	0.21
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	22	0.21
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	22	0.21
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	22	0.21
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	22	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	4	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	4	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	4	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	4	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	4	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	4	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	30	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	30	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	30	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	30	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	30	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	30	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	36	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	36	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	36	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	36	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	36	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	36	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	39	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	39	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	39	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	39	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	39	0.21
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	39	0.21
(1,2936)	1:120:A:LYS:H	1:122:A:VAL:HG11	22	0.21
(1,2936)	1:120:A:LYS:H	1:122:A:VAL:HG12	22	0.21
(1,2936)	1:120:A:LYS:H	1:122:A:VAL:HG13	22	0.21
(1,2936)	1:120:A:LYS:H	1:122:A:VAL:HG21	22	0.21
(1,2936)	1:120:A:LYS:H	1:122:A:VAL:HG22	22	0.21
(1,2936)	1:120:A:LYS:H	1:122:A:VAL:HG23	22	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD11	26	0.21
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD12	26	0.21
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD13	26	0.21
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD21	26	0.21
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD22	26	0.21
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD23	26	0.21
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG21	21	0.21
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG22	21	0.21
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG23	21	0.21
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	9	0.2
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	9	0.2
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	9	0.2
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	9	0.2
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	9	0.2
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	9	0.2
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	9	0.2
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	9	0.2
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	9	0.2
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	9	0.2
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	9	0.2
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	9	0.2
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	26	0.2
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	26	0.2
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	26	0.2
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	26	0.2
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	26	0.2
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	26	0.2
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	26	0.2
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	26	0.2
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	26	0.2
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	26	0.2
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	26	0.2
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	26	0.2
(1,2742)	1:96:A:LEU:HD11	1:97:A:GLN:HA	33	0.2
(1,2742)	1:96:A:LEU:HD12	1:97:A:GLN:HA	33	0.2
(1,2742)	1:96:A:LEU:HD13	1:97:A:GLN:HA	33	0.2
(1,2742)	1:96:A:LEU:HD21	1:97:A:GLN:HA	33	0.2
(1,2742)	1:96:A:LEU:HD22	1:97:A:GLN:HA	33	0.2
(1,2742)	1:96:A:LEU:HD23	1:97:A:GLN:HA	33	0.2
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	29	0.2
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	29	0.2
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	29	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	29	0.2
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	29	0.2
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	29	0.2
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD11	29	0.2
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD12	29	0.2
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD13	29	0.2
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD21	29	0.2
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD22	29	0.2
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD23	29	0.2
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD11	29	0.2
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD12	29	0.2
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD13	29	0.2
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD21	29	0.2
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD22	29	0.2
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD23	29	0.2
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD11	29	0.2
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD12	29	0.2
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD13	29	0.2
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD21	29	0.2
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD22	29	0.2
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD23	29	0.2
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD11	40	0.2
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD12	40	0.2
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD13	40	0.2
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD21	40	0.2
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD22	40	0.2
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD23	40	0.2
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD11	40	0.2
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD12	40	0.2
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD13	40	0.2
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD21	40	0.2
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD22	40	0.2
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD23	40	0.2
(1,816)	1:91:A:ASN:HD22	1:93:A:ILE:HD11	39	0.2
(1,816)	1:91:A:ASN:HD22	1:93:A:ILE:HD12	39	0.2
(1,816)	1:91:A:ASN:HD22	1:93:A:ILE:HD13	39	0.2
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	3	0.19
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	3	0.19
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	3	0.19
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	3	0.19
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	3	0.19
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	3	0.19
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	3	0.19
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	3	0.19
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	3	0.19
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	3	0.19
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	3	0.19
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	24	0.19
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	24	0.19
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	24	0.19
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	24	0.19
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	24	0.19
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	24	0.19
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	24	0.19
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	24	0.19
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	24	0.19
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	24	0.19
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	24	0.19
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	24	0.19
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	12	0.19
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	12	0.19
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	12	0.19
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	12	0.19
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	12	0.19
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	12	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	7	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	7	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	7	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	7	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	7	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	7	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	7	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	7	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	7	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	7	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	7	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	7	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	20	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	20	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	20	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	20	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	20	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	20	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	20	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	20	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	20	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	20	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	20	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	22	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	22	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	22	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	22	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	22	0.19
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	22	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	22	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	22	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	22	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	22	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	22	0.19
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	22	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	21	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	21	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	21	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	21	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	21	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	21	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	23	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	23	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	23	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	23	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	23	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	23	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	28	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	28	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	28	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	28	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	28	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	28	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	40	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	40	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	40	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	40	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	40	0.19
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	40	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD21	14	0.19
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD22	14	0.19
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD23	14	0.19
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD21	14	0.19
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD22	14	0.19
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD23	14	0.19
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD21	39	0.19
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD22	39	0.19
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD23	39	0.19
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD21	39	0.19
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD22	39	0.19
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD23	39	0.19
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	15	0.19
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	15	0.19
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	15	0.19
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	15	0.19
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	15	0.19
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	15	0.19
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	26	0.19
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	26	0.19
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	26	0.19
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	26	0.19
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	26	0.19
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	26	0.19
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	40	0.19
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	40	0.19
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	40	0.19
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	40	0.19
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	40	0.19
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	40	0.19
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG21	14	0.19
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG22	14	0.19
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG23	14	0.19
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	6	0.18
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	6	0.18
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	6	0.18
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	6	0.18
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	6	0.18
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	6	0.18
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	6	0.18
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	6	0.18
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	6	0.18
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	6	0.18
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	6	0.18
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	11	0.18
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	11	0.18
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	11	0.18
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	11	0.18
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	11	0.18
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	11	0.18
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	11	0.18
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	11	0.18
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	11	0.18
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	11	0.18
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	11	0.18
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	11	0.18
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	13	0.18
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	13	0.18
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	13	0.18
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	13	0.18
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	13	0.18
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	13	0.18
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	13	0.18
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	13	0.18
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	13	0.18
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	13	0.18
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	13	0.18
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	13	0.18
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	15	0.18
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	15	0.18
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	15	0.18
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	15	0.18
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	15	0.18
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	15	0.18
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	15	0.18
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	15	0.18
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	15	0.18
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	15	0.18
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	15	0.18
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	15	0.18
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	28	0.18
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	28	0.18
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	28	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	28	0.18
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	28	0.18
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	28	0.18
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	33	0.18
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	33	0.18
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	33	0.18
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	33	0.18
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	33	0.18
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	33	0.18
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	33	0.18
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	33	0.18
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	33	0.18
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	33	0.18
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	33	0.18
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	33	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	1	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	1	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	1	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	1	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	1	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	1	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	24	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	24	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	24	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	24	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	24	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	24	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	30	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	30	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	30	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	30	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	30	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	30	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	31	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	31	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	31	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	31	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	31	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	31	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	35	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	35	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	35	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	35	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	35	0.18
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	35	0.18
(1,2829)	1:104:A:GLN:HE21	1:140:A:VAL:HG11	20	0.18
(1,2829)	1:104:A:GLN:HE21	1:140:A:VAL:HG12	20	0.18
(1,2829)	1:104:A:GLN:HE21	1:140:A:VAL:HG13	20	0.18
(1,2829)	1:104:A:GLN:HE21	1:140:A:VAL:HG21	20	0.18
(1,2829)	1:104:A:GLN:HE21	1:140:A:VAL:HG22	20	0.18
(1,2829)	1:104:A:GLN:HE21	1:140:A:VAL:HG23	20	0.18
(1,2829)	1:104:A:GLN:HE22	1:140:A:VAL:HG11	20	0.18
(1,2829)	1:104:A:GLN:HE22	1:140:A:VAL:HG12	20	0.18
(1,2829)	1:104:A:GLN:HE22	1:140:A:VAL:HG13	20	0.18
(1,2829)	1:104:A:GLN:HE22	1:140:A:VAL:HG21	20	0.18
(1,2829)	1:104:A:GLN:HE22	1:140:A:VAL:HG22	20	0.18
(1,2829)	1:104:A:GLN:HE22	1:140:A:VAL:HG23	20	0.18
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	21	0.18
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	21	0.18
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	21	0.18
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	21	0.18
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	21	0.18
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	21	0.18
(1,2742)	1:96:A:LEU:HD11	1:97:A:GLN:HA	8	0.18
(1,2742)	1:96:A:LEU:HD12	1:97:A:GLN:HA	8	0.18
(1,2742)	1:96:A:LEU:HD13	1:97:A:GLN:HA	8	0.18
(1,2742)	1:96:A:LEU:HD21	1:97:A:GLN:HA	8	0.18
(1,2742)	1:96:A:LEU:HD22	1:97:A:GLN:HA	8	0.18
(1,2742)	1:96:A:LEU:HD23	1:97:A:GLN:HA	8	0.18
(1,2742)	1:96:A:LEU:HD11	1:97:A:GLN:HA	38	0.18
(1,2742)	1:96:A:LEU:HD12	1:97:A:GLN:HA	38	0.18
(1,2742)	1:96:A:LEU:HD13	1:97:A:GLN:HA	38	0.18
(1,2742)	1:96:A:LEU:HD21	1:97:A:GLN:HA	38	0.18
(1,2742)	1:96:A:LEU:HD22	1:97:A:GLN:HA	38	0.18
(1,2742)	1:96:A:LEU:HD23	1:97:A:GLN:HA	38	0.18
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	17	0.18
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	17	0.18
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	17	0.18
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	17	0.18
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	17	0.18
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	17	0.18
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	25	0.18
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	25	0.18
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	25	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	25	0.18
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	25	0.18
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	25	0.18
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	21	0.18
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	21	0.18
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	21	0.18
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD11	14	0.18
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD12	14	0.18
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD13	14	0.18
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	10	0.17
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	10	0.17
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	10	0.17
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	10	0.17
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	10	0.17
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	10	0.17
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	10	0.17
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	10	0.17
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	10	0.17
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	10	0.17
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	10	0.17
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	10	0.17
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	20	0.17
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	20	0.17
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	20	0.17
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	20	0.17
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	20	0.17
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	20	0.17
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	20	0.17
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	20	0.17
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	20	0.17
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	20	0.17
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	20	0.17
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	20	0.17
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	33	0.17
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	33	0.17
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	33	0.17
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	33	0.17
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	33	0.17
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	33	0.17
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	33	0.17
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	33	0.17
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	33	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	33	0.17
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	33	0.17
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	33	0.17
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	3	0.17
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	3	0.17
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	3	0.17
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	3	0.17
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	3	0.17
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	3	0.17
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	23	0.17
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	23	0.17
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	23	0.17
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	23	0.17
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	23	0.17
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	23	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	26	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	26	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	26	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	26	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	26	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	26	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	26	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	26	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	26	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	26	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	26	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	26	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	32	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	32	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	32	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	32	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	32	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	32	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	32	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	32	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	32	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	32	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	32	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	32	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	38	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	38	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	38	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	38	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	38	0.17
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	38	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	38	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	38	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	38	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	38	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	38	0.17
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	38	0.17
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	17	0.17
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	17	0.17
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	17	0.17
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	17	0.17
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	17	0.17
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	17	0.17
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	29	0.17
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	29	0.17
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	29	0.17
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	29	0.17
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	29	0.17
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	29	0.17
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD11	3	0.17
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD12	3	0.17
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD13	3	0.17
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD21	3	0.17
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD22	3	0.17
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD23	3	0.17
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD11	3	0.17
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD12	3	0.17
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD13	3	0.17
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD21	3	0.17
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD22	3	0.17
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD23	3	0.17
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD11	3	0.17
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD12	3	0.17
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD13	3	0.17
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD21	3	0.17
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD22	3	0.17
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD23	3	0.17
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD11	3	0.17
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD12	3	0.17
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD13	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD21	3	0.17
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD22	3	0.17
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD23	3	0.17
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD11	3	0.17
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD12	3	0.17
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD13	3	0.17
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD21	3	0.17
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD22	3	0.17
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD23	3	0.17
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD11	3	0.17
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD12	3	0.17
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD13	3	0.17
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD21	3	0.17
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD22	3	0.17
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD23	3	0.17
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD11	2	0.17
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD12	2	0.17
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD13	2	0.17
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD21	2	0.17
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD22	2	0.17
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD23	2	0.17
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD11	2	0.17
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD12	2	0.17
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD13	2	0.17
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD21	2	0.17
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD22	2	0.17
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD23	2	0.17
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD11	2	0.17
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD12	2	0.17
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD13	2	0.17
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD21	2	0.17
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD22	2	0.17
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD23	2	0.17
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	2	0.17
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	2	0.17
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	2	0.17
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	2	0.17
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	2	0.17
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	2	0.17
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	11	0.17
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	11	0.17
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	11	0.17
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	11	0.17
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	11	0.17
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	14	0.17
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	14	0.17
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	14	0.17
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	14	0.17
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	14	0.17
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	14	0.17
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	21	0.17
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	21	0.17
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	21	0.17
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	21	0.17
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	21	0.17
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	21	0.17
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	14	0.17
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	14	0.17
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	14	0.17
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	39	0.17
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	39	0.17
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	39	0.17
(1,127)	1:26:A:ARG:HA	1:26:A:ARG:HD2	21	0.17
(1,127)	1:26:A:ARG:HA	1:26:A:ARG:HD3	21	0.17
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	8	0.16
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	8	0.16
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	8	0.16
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	8	0.16
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	8	0.16
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	8	0.16
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	8	0.16
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	8	0.16
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	8	0.16
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	8	0.16
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	8	0.16
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	8	0.16
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	6	0.16
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	6	0.16
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	6	0.16
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	6	0.16
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	6	0.16
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	6	0.16
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	27	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	27	0.16
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	27	0.16
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	27	0.16
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	27	0.16
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	27	0.16
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	29	0.16
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	29	0.16
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	29	0.16
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	29	0.16
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	29	0.16
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	29	0.16
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	30	0.16
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	30	0.16
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	30	0.16
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	30	0.16
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	30	0.16
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	30	0.16
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD11	37	0.16
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD12	37	0.16
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD13	37	0.16
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD21	37	0.16
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD22	37	0.16
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD23	37	0.16
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD11	37	0.16
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD12	37	0.16
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD13	37	0.16
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD21	37	0.16
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD22	37	0.16
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD23	37	0.16
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD11	37	0.16
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD12	37	0.16
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD13	37	0.16
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD21	37	0.16
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD22	37	0.16
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD23	37	0.16
(1,2492)	1:59:A:LEU:HD11	1:102:A:THR:HG21	1	0.16
(1,2492)	1:59:A:LEU:HD11	1:102:A:THR:HG22	1	0.16
(1,2492)	1:59:A:LEU:HD11	1:102:A:THR:HG23	1	0.16
(1,2492)	1:59:A:LEU:HD12	1:102:A:THR:HG21	1	0.16
(1,2492)	1:59:A:LEU:HD12	1:102:A:THR:HG22	1	0.16
(1,2492)	1:59:A:LEU:HD12	1:102:A:THR:HG23	1	0.16
(1,2492)	1:59:A:LEU:HD13	1:102:A:THR:HG21	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2492)	1:59:A:LEU:HD13	1:102:A:THR:HG22	1	0.16
(1,2492)	1:59:A:LEU:HD13	1:102:A:THR:HG23	1	0.16
(1,2492)	1:59:A:LEU:HD21	1:102:A:THR:HG21	1	0.16
(1,2492)	1:59:A:LEU:HD21	1:102:A:THR:HG22	1	0.16
(1,2492)	1:59:A:LEU:HD21	1:102:A:THR:HG23	1	0.16
(1,2492)	1:59:A:LEU:HD22	1:102:A:THR:HG21	1	0.16
(1,2492)	1:59:A:LEU:HD22	1:102:A:THR:HG22	1	0.16
(1,2492)	1:59:A:LEU:HD22	1:102:A:THR:HG23	1	0.16
(1,2492)	1:59:A:LEU:HD23	1:102:A:THR:HG21	1	0.16
(1,2492)	1:59:A:LEU:HD23	1:102:A:THR:HG22	1	0.16
(1,2492)	1:59:A:LEU:HD23	1:102:A:THR:HG23	1	0.16
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	23	0.16
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	23	0.16
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	23	0.16
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	23	0.16
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	23	0.16
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	23	0.16
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	36	0.16
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	36	0.16
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	36	0.16
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	36	0.16
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	36	0.16
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	36	0.16
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	30	0.16
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	30	0.16
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	30	0.16
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	35	0.16
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	35	0.16
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	35	0.16
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD11	23	0.16
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD12	23	0.16
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD13	23	0.16
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD11	25	0.16
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD12	25	0.16
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD13	25	0.16
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD11	39	0.16
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD12	39	0.16
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD13	39	0.16
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	34	0.15
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	34	0.15
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	34	0.15
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	34	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	34	0.15
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	34	0.15
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	34	0.15
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	34	0.15
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	34	0.15
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	34	0.15
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	34	0.15
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	34	0.15
(1,3032)	1:136:A:LYS:H	1:136:A:LYS:HG2	21	0.15
(1,3032)	1:136:A:LYS:H	1:136:A:LYS:HG3	21	0.15
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD11	37	0.15
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD12	37	0.15
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD13	37	0.15
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD21	37	0.15
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD22	37	0.15
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD23	37	0.15
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD11	37	0.15
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD12	37	0.15
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD13	37	0.15
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD21	37	0.15
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD22	37	0.15
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD23	37	0.15
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	4	0.15
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	4	0.15
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	4	0.15
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	4	0.15
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	4	0.15
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	4	0.15
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	33	0.15
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	33	0.15
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	33	0.15
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	33	0.15
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	33	0.15
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	33	0.15
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD11	26	0.15
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD12	26	0.15
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD13	26	0.15
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD21	26	0.15
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD22	26	0.15
(1,2809)	1:103:A:LEU:HD11	1:108:A:LEU:HD23	26	0.15
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD11	26	0.15
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD12	26	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD13	26	0.15
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD21	26	0.15
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD22	26	0.15
(1,2809)	1:103:A:LEU:HD12	1:108:A:LEU:HD23	26	0.15
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD11	26	0.15
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD12	26	0.15
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD13	26	0.15
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD21	26	0.15
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD22	26	0.15
(1,2809)	1:103:A:LEU:HD13	1:108:A:LEU:HD23	26	0.15
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD11	26	0.15
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD12	26	0.15
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD13	26	0.15
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD21	26	0.15
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD22	26	0.15
(1,2809)	1:103:A:LEU:HD21	1:108:A:LEU:HD23	26	0.15
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD11	26	0.15
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD12	26	0.15
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD13	26	0.15
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD21	26	0.15
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD22	26	0.15
(1,2809)	1:103:A:LEU:HD22	1:108:A:LEU:HD23	26	0.15
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD11	26	0.15
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD12	26	0.15
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD13	26	0.15
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD21	26	0.15
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD22	26	0.15
(1,2809)	1:103:A:LEU:HD23	1:108:A:LEU:HD23	26	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	4	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	4	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	4	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	4	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	4	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	4	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	14	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	14	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	14	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	14	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	14	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	14	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	17	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	17	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	17	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	17	0.15
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	17	0.15
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD21	3	0.15
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD22	3	0.15
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD23	3	0.15
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD21	3	0.15
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD22	3	0.15
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD23	3	0.15
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD11	31	0.15
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD12	31	0.15
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD13	31	0.15
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD21	31	0.15
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD22	31	0.15
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD23	31	0.15
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD11	31	0.15
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD12	31	0.15
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD13	31	0.15
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD21	31	0.15
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD22	31	0.15
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD23	31	0.15
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD11	14	0.15
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD12	14	0.15
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD13	14	0.15
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD21	14	0.15
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD22	14	0.15
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD23	14	0.15
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD11	14	0.15
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD12	14	0.15
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD13	14	0.15
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD21	14	0.15
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD22	14	0.15
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD23	14	0.15
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD11	14	0.15
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD12	14	0.15
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD13	14	0.15
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD21	14	0.15
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD22	14	0.15
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD23	14	0.15
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD11	23	0.15
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD12	23	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD13	23	0.15
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD21	23	0.15
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD22	23	0.15
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD23	23	0.15
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD11	23	0.15
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD12	23	0.15
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD13	23	0.15
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD21	23	0.15
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD22	23	0.15
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD23	23	0.15
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD11	23	0.15
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD12	23	0.15
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD13	23	0.15
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD21	23	0.15
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD22	23	0.15
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD23	23	0.15
(1,2374)	1:42:A:LEU:HD11	1:55:A:TYR:HD1	31	0.15
(1,2374)	1:42:A:LEU:HD11	1:55:A:TYR:HD2	31	0.15
(1,2374)	1:42:A:LEU:HD12	1:55:A:TYR:HD1	31	0.15
(1,2374)	1:42:A:LEU:HD12	1:55:A:TYR:HD2	31	0.15
(1,2374)	1:42:A:LEU:HD13	1:55:A:TYR:HD1	31	0.15
(1,2374)	1:42:A:LEU:HD13	1:55:A:TYR:HD2	31	0.15
(1,2374)	1:42:A:LEU:HD21	1:55:A:TYR:HD1	31	0.15
(1,2374)	1:42:A:LEU:HD21	1:55:A:TYR:HD2	31	0.15
(1,2374)	1:42:A:LEU:HD22	1:55:A:TYR:HD1	31	0.15
(1,2374)	1:42:A:LEU:HD22	1:55:A:TYR:HD2	31	0.15
(1,2374)	1:42:A:LEU:HD23	1:55:A:TYR:HD1	31	0.15
(1,2374)	1:42:A:LEU:HD23	1:55:A:TYR:HD2	31	0.15
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	1	0.15
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	1	0.15
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	1	0.15
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	1	0.15
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	1	0.15
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	1	0.15
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	4	0.15
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	4	0.15
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	4	0.15
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	4	0.15
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	4	0.15
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	4	0.15
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	30	0.15
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	30	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	30	0.15
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	30	0.15
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	30	0.15
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	30	0.15
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD11	21	0.15
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD12	21	0.15
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD13	21	0.15
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD21	21	0.15
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD22	21	0.15
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD23	21	0.15
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	23	0.15
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	23	0.15
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	23	0.15
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	25	0.15
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	25	0.15
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	25	0.15
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	28	0.15
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	28	0.15
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	28	0.15
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	29	0.15
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	29	0.15
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	29	0.15
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD11	12	0.15
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD12	12	0.15
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD13	12	0.15
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	18	0.14
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	18	0.14
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	18	0.14
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	18	0.14
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	18	0.14
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	18	0.14
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	18	0.14
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	18	0.14
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	18	0.14
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	18	0.14
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	18	0.14
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	18	0.14
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB2	32	0.14
(1,3071)	1:142:A:VAL:HG11	1:143:A:SER:HB3	32	0.14
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB2	32	0.14
(1,3071)	1:142:A:VAL:HG12	1:143:A:SER:HB3	32	0.14
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB2	32	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3071)	1:142:A:VAL:HG13	1:143:A:SER:HB3	32	0.14
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB2	32	0.14
(1,3071)	1:142:A:VAL:HG21	1:143:A:SER:HB3	32	0.14
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB2	32	0.14
(1,3071)	1:142:A:VAL:HG22	1:143:A:SER:HB3	32	0.14
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB2	32	0.14
(1,3071)	1:142:A:VAL:HG23	1:143:A:SER:HB3	32	0.14
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	8	0.14
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	8	0.14
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	8	0.14
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	8	0.14
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	8	0.14
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	8	0.14
(1,2991)	1:127:A:LYS:HE2	1:142:A:VAL:HG11	35	0.14
(1,2991)	1:127:A:LYS:HE2	1:142:A:VAL:HG12	35	0.14
(1,2991)	1:127:A:LYS:HE2	1:142:A:VAL:HG13	35	0.14
(1,2991)	1:127:A:LYS:HE2	1:142:A:VAL:HG21	35	0.14
(1,2991)	1:127:A:LYS:HE2	1:142:A:VAL:HG22	35	0.14
(1,2991)	1:127:A:LYS:HE2	1:142:A:VAL:HG23	35	0.14
(1,2991)	1:127:A:LYS:HE3	1:142:A:VAL:HG11	35	0.14
(1,2991)	1:127:A:LYS:HE3	1:142:A:VAL:HG12	35	0.14
(1,2991)	1:127:A:LYS:HE3	1:142:A:VAL:HG13	35	0.14
(1,2991)	1:127:A:LYS:HE3	1:142:A:VAL:HG21	35	0.14
(1,2991)	1:127:A:LYS:HE3	1:142:A:VAL:HG22	35	0.14
(1,2991)	1:127:A:LYS:HE3	1:142:A:VAL:HG23	35	0.14
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	10	0.14
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	10	0.14
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	10	0.14
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	10	0.14
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	10	0.14
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	10	0.14
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	10	0.14
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	10	0.14
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	10	0.14
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	10	0.14
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	10	0.14
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	10	0.14
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD11	34	0.14
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD12	34	0.14
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD13	34	0.14
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD21	34	0.14
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD22	34	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2929)	1:117:A:ASN:HD21	1:121:A:LEU:HD23	34	0.14
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD11	34	0.14
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD12	34	0.14
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD13	34	0.14
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD21	34	0.14
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD22	34	0.14
(1,2929)	1:117:A:ASN:HD22	1:121:A:LEU:HD23	34	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	9	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	9	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	9	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	9	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	9	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	9	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	11	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	11	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	11	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	11	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	11	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	11	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	18	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	18	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	18	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	18	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	18	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	18	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	20	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	20	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	20	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	20	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	20	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	20	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	25	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	25	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	25	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	25	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	25	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	25	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	36	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	36	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	36	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	36	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	36	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	36	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	37	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	37	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	37	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	37	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	37	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	37	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	38	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	38	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	38	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	38	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	38	0.14
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	38	0.14
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	31	0.14
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	31	0.14
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	31	0.14
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	31	0.14
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	31	0.14
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	31	0.14
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	35	0.14
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	35	0.14
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	35	0.14
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	35	0.14
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	35	0.14
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	35	0.14
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD21	17	0.14
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD22	17	0.14
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD23	17	0.14
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD21	17	0.14
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD22	17	0.14
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD23	17	0.14
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD11	14	0.14
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD12	14	0.14
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD13	14	0.14
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD21	14	0.14
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD22	14	0.14
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD23	14	0.14
(1,2662)	1:84:A:LEU:HD11	1:97:A:GLN:H	14	0.14
(1,2662)	1:84:A:LEU:HD12	1:97:A:GLN:H	14	0.14
(1,2662)	1:84:A:LEU:HD13	1:97:A:GLN:H	14	0.14
(1,2662)	1:84:A:LEU:HD21	1:97:A:GLN:H	14	0.14
(1,2662)	1:84:A:LEU:HD22	1:97:A:GLN:H	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2662)	1:84:A:LEU:HD23	1:97:A:GLN:H	14	0.14
(1,2662)	1:84:A:LEU:HD11	1:97:A:GLN:H	40	0.14
(1,2662)	1:84:A:LEU:HD12	1:97:A:GLN:H	40	0.14
(1,2662)	1:84:A:LEU:HD13	1:97:A:GLN:H	40	0.14
(1,2662)	1:84:A:LEU:HD21	1:97:A:GLN:H	40	0.14
(1,2662)	1:84:A:LEU:HD22	1:97:A:GLN:H	40	0.14
(1,2662)	1:84:A:LEU:HD23	1:97:A:GLN:H	40	0.14
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD11	37	0.14
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD12	37	0.14
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD13	37	0.14
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD21	37	0.14
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD22	37	0.14
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD23	37	0.14
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD11	4	0.14
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD12	4	0.14
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD13	4	0.14
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD21	4	0.14
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD22	4	0.14
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD23	4	0.14
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD11	4	0.14
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD12	4	0.14
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD13	4	0.14
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD21	4	0.14
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD22	4	0.14
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD23	4	0.14
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD11	4	0.14
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD12	4	0.14
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD13	4	0.14
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD21	4	0.14
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD22	4	0.14
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD23	4	0.14
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD11	27	0.14
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD12	27	0.14
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD13	27	0.14
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD21	27	0.14
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD22	27	0.14
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD23	27	0.14
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD11	27	0.14
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD12	27	0.14
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD13	27	0.14
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD21	27	0.14
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD22	27	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD23	27	0.14
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD11	27	0.14
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD12	27	0.14
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD13	27	0.14
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD21	27	0.14
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD22	27	0.14
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD23	27	0.14
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD11	14	0.14
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD12	14	0.14
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD13	14	0.14
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD21	14	0.14
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD22	14	0.14
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD23	14	0.14
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	12	0.14
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	12	0.14
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	12	0.14
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	12	0.14
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	12	0.14
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	12	0.14
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	29	0.14
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	29	0.14
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	29	0.14
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	29	0.14
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	29	0.14
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	29	0.14
(1,1264)	1:147:A:ALA:HB1	1:151:A:SER:HB2	9	0.14
(1,1264)	1:147:A:ALA:HB1	1:151:A:SER:HB3	9	0.14
(1,1264)	1:147:A:ALA:HB2	1:151:A:SER:HB2	9	0.14
(1,1264)	1:147:A:ALA:HB2	1:151:A:SER:HB3	9	0.14
(1,1264)	1:147:A:ALA:HB3	1:151:A:SER:HB2	9	0.14
(1,1264)	1:147:A:ALA:HB3	1:151:A:SER:HB3	9	0.14
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	1	0.14
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	1	0.14
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	1	0.14
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	2	0.14
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	2	0.14
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	2	0.14
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	4	0.14
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	4	0.14
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	4	0.14
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	31	0.14
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	31	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	31	0.14
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG21	40	0.14
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG22	40	0.14
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG23	40	0.14
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD11	37	0.14
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD12	37	0.14
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD13	37	0.14
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD11	38	0.14
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD12	38	0.14
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD13	38	0.14
(2,2)	1:88:A:LYS:HG3	1:96:A:LEU:HD21	21	0.13
(2,2)	1:88:A:LYS:HG3	1:96:A:LEU:HD22	21	0.13
(2,2)	1:88:A:LYS:HG3	1:96:A:LEU:HD23	21	0.13
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	6	0.13
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	6	0.13
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	6	0.13
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	6	0.13
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	6	0.13
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	6	0.13
(1,3026)	1:134:A:LEU:HD11	1:137:A:LEU:H	37	0.13
(1,3026)	1:134:A:LEU:HD12	1:137:A:LEU:H	37	0.13
(1,3026)	1:134:A:LEU:HD13	1:137:A:LEU:H	37	0.13
(1,3026)	1:134:A:LEU:HD21	1:137:A:LEU:H	37	0.13
(1,3026)	1:134:A:LEU:HD22	1:137:A:LEU:H	37	0.13
(1,3026)	1:134:A:LEU:HD23	1:137:A:LEU:H	37	0.13
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	12	0.13
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	12	0.13
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	12	0.13
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	12	0.13
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	12	0.13
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	12	0.13
(1,2874)	1:110:A:VAL:HG11	1:148:A:VAL:H	29	0.13
(1,2874)	1:110:A:VAL:HG12	1:148:A:VAL:H	29	0.13
(1,2874)	1:110:A:VAL:HG13	1:148:A:VAL:H	29	0.13
(1,2874)	1:110:A:VAL:HG21	1:148:A:VAL:H	29	0.13
(1,2874)	1:110:A:VAL:HG22	1:148:A:VAL:H	29	0.13
(1,2874)	1:110:A:VAL:HG23	1:148:A:VAL:H	29	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	23	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	23	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	23	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	23	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	23	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	23	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	25	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	25	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	25	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	25	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	25	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	25	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	39	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	39	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	39	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	39	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	39	0.13
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	39	0.13
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD21	18	0.13
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD22	18	0.13
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD23	18	0.13
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD21	18	0.13
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD22	18	0.13
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD23	18	0.13
(1,2599)	1:72:A:ILE:HA	1:80:A:LEU:HD11	28	0.13
(1,2599)	1:72:A:ILE:HA	1:80:A:LEU:HD12	28	0.13
(1,2599)	1:72:A:ILE:HA	1:80:A:LEU:HD13	28	0.13
(1,2599)	1:72:A:ILE:HA	1:80:A:LEU:HD21	28	0.13
(1,2599)	1:72:A:ILE:HA	1:80:A:LEU:HD22	28	0.13
(1,2599)	1:72:A:ILE:HA	1:80:A:LEU:HD23	28	0.13
(1,2565)	1:68:A:LEU:HD11	1:107:A:PRO:HD2	29	0.13
(1,2565)	1:68:A:LEU:HD12	1:107:A:PRO:HD2	29	0.13
(1,2565)	1:68:A:LEU:HD13	1:107:A:PRO:HD2	29	0.13
(1,2565)	1:68:A:LEU:HD21	1:107:A:PRO:HD2	29	0.13
(1,2565)	1:68:A:LEU:HD22	1:107:A:PRO:HD2	29	0.13
(1,2565)	1:68:A:LEU:HD23	1:107:A:PRO:HD2	29	0.13
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	3	0.13
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	3	0.13
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	3	0.13
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	3	0.13
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	3	0.13
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	3	0.13
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	5	0.13
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	5	0.13
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	5	0.13
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	5	0.13
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	5	0.13
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	9	0.13
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	9	0.13
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	9	0.13
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	9	0.13
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	9	0.13
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	9	0.13
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	10	0.13
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	10	0.13
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	10	0.13
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	10	0.13
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	10	0.13
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	10	0.13
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	15	0.13
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	15	0.13
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	15	0.13
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	15	0.13
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	15	0.13
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	15	0.13
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	24	0.13
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	24	0.13
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	24	0.13
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	24	0.13
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	24	0.13
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	24	0.13
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	27	0.13
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	27	0.13
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	27	0.13
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	27	0.13
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	27	0.13
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	27	0.13
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	28	0.13
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	28	0.13
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	28	0.13
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	28	0.13
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	28	0.13
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	28	0.13
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	31	0.13
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	31	0.13
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	31	0.13
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	31	0.13
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	31	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	31	0.13
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	35	0.13
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	35	0.13
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	35	0.13
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	35	0.13
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	35	0.13
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	35	0.13
(1,2246)	1:17:A:LEU:HD11	1:55:A:TYR:HD1	28	0.13
(1,2246)	1:17:A:LEU:HD11	1:55:A:TYR:HD2	28	0.13
(1,2246)	1:17:A:LEU:HD12	1:55:A:TYR:HD1	28	0.13
(1,2246)	1:17:A:LEU:HD12	1:55:A:TYR:HD2	28	0.13
(1,2246)	1:17:A:LEU:HD13	1:55:A:TYR:HD1	28	0.13
(1,2246)	1:17:A:LEU:HD13	1:55:A:TYR:HD2	28	0.13
(1,2246)	1:17:A:LEU:HD21	1:55:A:TYR:HD1	28	0.13
(1,2246)	1:17:A:LEU:HD21	1:55:A:TYR:HD2	28	0.13
(1,2246)	1:17:A:LEU:HD22	1:55:A:TYR:HD1	28	0.13
(1,2246)	1:17:A:LEU:HD22	1:55:A:TYR:HD2	28	0.13
(1,2246)	1:17:A:LEU:HD23	1:55:A:TYR:HD1	28	0.13
(1,2246)	1:17:A:LEU:HD23	1:55:A:TYR:HD2	28	0.13
(1,1623)	1:66:A:GLU:H	1:69:A:VAL:HG11	40	0.13
(1,1623)	1:66:A:GLU:H	1:69:A:VAL:HG12	40	0.13
(1,1623)	1:66:A:GLU:H	1:69:A:VAL:HG13	40	0.13
(1,830)	1:93:A:ILE:HG21	1:98:A:GLN:H	21	0.13
(1,830)	1:93:A:ILE:HG22	1:98:A:GLN:H	21	0.13
(1,830)	1:93:A:ILE:HG23	1:98:A:GLN:H	21	0.13
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	12	0.13
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	12	0.13
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	12	0.13
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	16	0.13
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	16	0.13
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	16	0.13
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	19	0.13
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	19	0.13
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	19	0.13
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	27	0.13
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	27	0.13
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	27	0.13
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	36	0.13
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	36	0.13
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	36	0.13
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	37	0.13
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	37	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	37	0.13
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG21	30	0.13
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG22	30	0.13
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG23	30	0.13
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG21	36	0.13
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG22	36	0.13
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG23	36	0.13
(1,704)	1:78:A:LYS:HA	1:78:A:LYS:HD2	40	0.13
(1,704)	1:78:A:LYS:HA	1:78:A:LYS:HD3	40	0.13
(1,524)	1:62:A:THR:HG21	1:67:A:ILE:HA	2	0.13
(1,524)	1:62:A:THR:HG22	1:67:A:ILE:HA	2	0.13
(1,524)	1:62:A:THR:HG23	1:67:A:ILE:HA	2	0.13
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD11	13	0.13
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD12	13	0.13
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD13	13	0.13
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD11	15	0.13
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD12	15	0.13
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD13	15	0.13
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD11	34	0.13
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD12	34	0.13
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD13	34	0.13
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	15	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	15	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	15	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	15	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	15	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	15	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	18	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	18	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	18	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	18	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	18	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	18	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD11	38	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD12	38	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD13	38	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD21	38	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD22	38	0.12
(1,3035)	1:137:A:LEU:H	1:137:A:LEU:HD23	38	0.12
(1,2970)	1:123:A:LYS:HE2	1:124:A:GLN:HB2	29	0.12
(1,2970)	1:123:A:LYS:HE2	1:124:A:GLN:HB3	29	0.12
(1,2970)	1:123:A:LYS:HE3	1:124:A:GLN:HB2	29	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2970)	1:123:A:LYS:HE3	1:124:A:GLN:HB3	29	0.12
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD11	11	0.12
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD12	11	0.12
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD13	11	0.12
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD21	11	0.12
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD22	11	0.12
(1,2928)	1:117:A:ASN:HB2	1:121:A:LEU:HD23	11	0.12
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD11	11	0.12
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD12	11	0.12
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD13	11	0.12
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD21	11	0.12
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD22	11	0.12
(1,2928)	1:117:A:ASN:HB3	1:121:A:LEU:HD23	11	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	7	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	7	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	7	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	7	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	7	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	7	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	8	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	8	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	8	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	8	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	8	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	8	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	15	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	15	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	15	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	15	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	15	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	15	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	39	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	39	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	39	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	39	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	39	0.12
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	39	0.12
(1,2855)	1:109:A:THR:HA	1:110:A:VAL:HG11	26	0.12
(1,2855)	1:109:A:THR:HA	1:110:A:VAL:HG12	26	0.12
(1,2855)	1:109:A:THR:HA	1:110:A:VAL:HG13	26	0.12
(1,2855)	1:109:A:THR:HA	1:110:A:VAL:HG21	26	0.12
(1,2855)	1:109:A:THR:HA	1:110:A:VAL:HG22	26	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2855)	1:109:A:THR:HA	1:110:A:VAL:HG23	26	0.12
(1,2800)	1:103:A:LEU:H	1:108:A:LEU:HD11	2	0.12
(1,2800)	1:103:A:LEU:H	1:108:A:LEU:HD12	2	0.12
(1,2800)	1:103:A:LEU:H	1:108:A:LEU:HD13	2	0.12
(1,2800)	1:103:A:LEU:H	1:108:A:LEU:HD21	2	0.12
(1,2800)	1:103:A:LEU:H	1:108:A:LEU:HD22	2	0.12
(1,2800)	1:103:A:LEU:H	1:108:A:LEU:HD23	2	0.12
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	5	0.12
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	5	0.12
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	5	0.12
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	5	0.12
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	5	0.12
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	5	0.12
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	12	0.12
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	12	0.12
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	12	0.12
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	12	0.12
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	12	0.12
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	12	0.12
(1,2742)	1:96:A:LEU:HD11	1:97:A:GLN:HA	34	0.12
(1,2742)	1:96:A:LEU:HD12	1:97:A:GLN:HA	34	0.12
(1,2742)	1:96:A:LEU:HD13	1:97:A:GLN:HA	34	0.12
(1,2742)	1:96:A:LEU:HD21	1:97:A:GLN:HA	34	0.12
(1,2742)	1:96:A:LEU:HD22	1:97:A:GLN:HA	34	0.12
(1,2742)	1:96:A:LEU:HD23	1:97:A:GLN:HA	34	0.12
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD11	14	0.12
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD12	14	0.12
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD13	14	0.12
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD21	14	0.12
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD22	14	0.12
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD23	14	0.12
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD11	14	0.12
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD12	14	0.12
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD13	14	0.12
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD21	14	0.12
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD22	14	0.12
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD23	14	0.12
(1,2662)	1:84:A:LEU:HD11	1:97:A:GLN:H	13	0.12
(1,2662)	1:84:A:LEU:HD12	1:97:A:GLN:H	13	0.12
(1,2662)	1:84:A:LEU:HD13	1:97:A:GLN:H	13	0.12
(1,2662)	1:84:A:LEU:HD21	1:97:A:GLN:H	13	0.12
(1,2662)	1:84:A:LEU:HD22	1:97:A:GLN:H	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2662)	1:84:A:LEU:HD23	1:97:A:GLN:H	13	0.12
(1,2662)	1:84:A:LEU:HD11	1:97:A:GLN:H	17	0.12
(1,2662)	1:84:A:LEU:HD12	1:97:A:GLN:H	17	0.12
(1,2662)	1:84:A:LEU:HD13	1:97:A:GLN:H	17	0.12
(1,2662)	1:84:A:LEU:HD21	1:97:A:GLN:H	17	0.12
(1,2662)	1:84:A:LEU:HD22	1:97:A:GLN:H	17	0.12
(1,2662)	1:84:A:LEU:HD23	1:97:A:GLN:H	17	0.12
(1,2662)	1:84:A:LEU:HD11	1:97:A:GLN:H	27	0.12
(1,2662)	1:84:A:LEU:HD12	1:97:A:GLN:H	27	0.12
(1,2662)	1:84:A:LEU:HD13	1:97:A:GLN:H	27	0.12
(1,2662)	1:84:A:LEU:HD21	1:97:A:GLN:H	27	0.12
(1,2662)	1:84:A:LEU:HD22	1:97:A:GLN:H	27	0.12
(1,2662)	1:84:A:LEU:HD23	1:97:A:GLN:H	27	0.12
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD11	21	0.12
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD12	21	0.12
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD13	21	0.12
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD21	21	0.12
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD22	21	0.12
(1,2529)	1:62:A:THR:HG21	1:68:A:LEU:HD23	21	0.12
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD11	21	0.12
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD12	21	0.12
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD13	21	0.12
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD21	21	0.12
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD22	21	0.12
(1,2529)	1:62:A:THR:HG22	1:68:A:LEU:HD23	21	0.12
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD11	21	0.12
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD12	21	0.12
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD13	21	0.12
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD21	21	0.12
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD22	21	0.12
(1,2529)	1:62:A:THR:HG23	1:68:A:LEU:HD23	21	0.12
(1,2483)	1:59:A:LEU:HD11	1:62:A:THR:HG21	19	0.12
(1,2483)	1:59:A:LEU:HD11	1:62:A:THR:HG22	19	0.12
(1,2483)	1:59:A:LEU:HD11	1:62:A:THR:HG23	19	0.12
(1,2483)	1:59:A:LEU:HD12	1:62:A:THR:HG21	19	0.12
(1,2483)	1:59:A:LEU:HD12	1:62:A:THR:HG22	19	0.12
(1,2483)	1:59:A:LEU:HD12	1:62:A:THR:HG23	19	0.12
(1,2483)	1:59:A:LEU:HD13	1:62:A:THR:HG21	19	0.12
(1,2483)	1:59:A:LEU:HD13	1:62:A:THR:HG22	19	0.12
(1,2483)	1:59:A:LEU:HD13	1:62:A:THR:HG23	19	0.12
(1,2483)	1:59:A:LEU:HD21	1:62:A:THR:HG21	19	0.12
(1,2483)	1:59:A:LEU:HD21	1:62:A:THR:HG22	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2483)	1:59:A:LEU:HD21	1:62:A:THR:HG23	19	0.12
(1,2483)	1:59:A:LEU:HD22	1:62:A:THR:HG21	19	0.12
(1,2483)	1:59:A:LEU:HD22	1:62:A:THR:HG22	19	0.12
(1,2483)	1:59:A:LEU:HD22	1:62:A:THR:HG23	19	0.12
(1,2483)	1:59:A:LEU:HD23	1:62:A:THR:HG21	19	0.12
(1,2483)	1:59:A:LEU:HD23	1:62:A:THR:HG22	19	0.12
(1,2483)	1:59:A:LEU:HD23	1:62:A:THR:HG23	19	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD11	17	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD12	17	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD13	17	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD21	17	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD22	17	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD23	17	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD11	17	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD12	17	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD13	17	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD21	17	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD22	17	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD23	17	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD11	17	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD12	17	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD13	17	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD21	17	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD22	17	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD23	17	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD11	39	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD12	39	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD13	39	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD21	39	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD22	39	0.12
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD23	39	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD11	39	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD12	39	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD13	39	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD21	39	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD22	39	0.12
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD23	39	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD11	39	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD12	39	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD13	39	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD21	39	0.12
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD22	39	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD23	39	0.12
(1,2374)	1:42:A:LEU:HD11	1:55:A:TYR:HD1	11	0.12
(1,2374)	1:42:A:LEU:HD11	1:55:A:TYR:HD2	11	0.12
(1,2374)	1:42:A:LEU:HD12	1:55:A:TYR:HD1	11	0.12
(1,2374)	1:42:A:LEU:HD12	1:55:A:TYR:HD2	11	0.12
(1,2374)	1:42:A:LEU:HD13	1:55:A:TYR:HD1	11	0.12
(1,2374)	1:42:A:LEU:HD13	1:55:A:TYR:HD2	11	0.12
(1,2374)	1:42:A:LEU:HD21	1:55:A:TYR:HD1	11	0.12
(1,2374)	1:42:A:LEU:HD21	1:55:A:TYR:HD2	11	0.12
(1,2374)	1:42:A:LEU:HD22	1:55:A:TYR:HD1	11	0.12
(1,2374)	1:42:A:LEU:HD22	1:55:A:TYR:HD2	11	0.12
(1,2374)	1:42:A:LEU:HD23	1:55:A:TYR:HD1	11	0.12
(1,2374)	1:42:A:LEU:HD23	1:55:A:TYR:HD2	11	0.12
(1,2374)	1:42:A:LEU:HD11	1:55:A:TYR:HD1	30	0.12
(1,2374)	1:42:A:LEU:HD11	1:55:A:TYR:HD2	30	0.12
(1,2374)	1:42:A:LEU:HD12	1:55:A:TYR:HD1	30	0.12
(1,2374)	1:42:A:LEU:HD12	1:55:A:TYR:HD2	30	0.12
(1,2374)	1:42:A:LEU:HD13	1:55:A:TYR:HD1	30	0.12
(1,2374)	1:42:A:LEU:HD13	1:55:A:TYR:HD2	30	0.12
(1,2374)	1:42:A:LEU:HD21	1:55:A:TYR:HD1	30	0.12
(1,2374)	1:42:A:LEU:HD21	1:55:A:TYR:HD2	30	0.12
(1,2374)	1:42:A:LEU:HD22	1:55:A:TYR:HD1	30	0.12
(1,2374)	1:42:A:LEU:HD22	1:55:A:TYR:HD2	30	0.12
(1,2374)	1:42:A:LEU:HD23	1:55:A:TYR:HD1	30	0.12
(1,2374)	1:42:A:LEU:HD23	1:55:A:TYR:HD2	30	0.12
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	13	0.12
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	13	0.12
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	13	0.12
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	13	0.12
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	13	0.12
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	13	0.12
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	16	0.12
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	16	0.12
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	16	0.12
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	16	0.12
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	16	0.12
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	16	0.12
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	22	0.12
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	22	0.12
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	22	0.12
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	22	0.12
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	22	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	22	0.12
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	39	0.12
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	39	0.12
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	39	0.12
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	39	0.12
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	39	0.12
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	39	0.12
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	5	0.12
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	5	0.12
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	5	0.12
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	26	0.12
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	26	0.12
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	26	0.12
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG21	2	0.12
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG22	2	0.12
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG23	2	0.12
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD11	32	0.12
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD12	32	0.12
(1,244)	1:11:A:ILE:HB	1:11:A:ILE:HD13	32	0.12
(1,190)	1:37:A:SER:HB2	1:38:A:LYS:HB2	14	0.12
(1,190)	1:37:A:SER:HB2	1:38:A:LYS:HB3	14	0.12
(1,190)	1:37:A:SER:HB3	1:38:A:LYS:HB2	14	0.12
(1,190)	1:37:A:SER:HB3	1:38:A:LYS:HB3	14	0.12
(1,2970)	1:123:A:LYS:HE2	1:124:A:GLN:HB2	27	0.11
(1,2970)	1:123:A:LYS:HE2	1:124:A:GLN:HB3	27	0.11
(1,2970)	1:123:A:LYS:HE3	1:124:A:GLN:HB2	27	0.11
(1,2970)	1:123:A:LYS:HE3	1:124:A:GLN:HB3	27	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	10	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	10	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	10	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	10	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	10	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	10	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	19	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	19	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	19	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	19	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	19	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	19	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	22	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	22	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	22	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	22	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	22	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	22	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	26	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	26	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	26	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	26	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	26	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	26	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	32	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	32	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	32	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	32	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	32	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	32	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	34	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	34	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	34	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	34	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	34	0.11
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	34	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	2	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	2	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	2	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	2	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	2	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	2	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	9	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	9	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	9	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	9	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	9	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	9	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	11	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	11	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	11	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	11	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	11	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	11	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	16	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	16	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	16	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	16	0.11
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	16	0.11
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD11	22	0.11
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD12	22	0.11
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD13	22	0.11
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD21	22	0.11
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD22	22	0.11
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD23	22	0.11
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD11	22	0.11
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD12	22	0.11
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD13	22	0.11
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD21	22	0.11
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD22	22	0.11
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD23	22	0.11
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD21	11	0.11
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD22	11	0.11
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD23	11	0.11
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD21	11	0.11
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD22	11	0.11
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD23	11	0.11
(1,2691)	1:88:A:LYS:H	1:88:A:LYS:HG2	40	0.11
(1,2691)	1:88:A:LYS:H	1:88:A:LYS:HG3	40	0.11
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD11	24	0.11
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD12	24	0.11
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD13	24	0.11
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD21	24	0.11
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD22	24	0.11
(1,2690)	1:87:A:SER:HB2	1:96:A:LEU:HD23	24	0.11
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD11	24	0.11
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD12	24	0.11
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD13	24	0.11
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD21	24	0.11
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD22	24	0.11
(1,2690)	1:87:A:SER:HB3	1:96:A:LEU:HD23	24	0.11
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD11	25	0.11
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD12	25	0.11
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD13	25	0.11
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD21	25	0.11
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD22	25	0.11
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD23	25	0.11
(1,2662)	1:84:A:LEU:HD11	1:97:A:GLN:H	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2662)	1:84:A:LEU:HD12	1:97:A:GLN:H	11	0.11
(1,2662)	1:84:A:LEU:HD13	1:97:A:GLN:H	11	0.11
(1,2662)	1:84:A:LEU:HD21	1:97:A:GLN:H	11	0.11
(1,2662)	1:84:A:LEU:HD22	1:97:A:GLN:H	11	0.11
(1,2662)	1:84:A:LEU:HD23	1:97:A:GLN:H	11	0.11
(1,2662)	1:84:A:LEU:HD11	1:97:A:GLN:H	12	0.11
(1,2662)	1:84:A:LEU:HD12	1:97:A:GLN:H	12	0.11
(1,2662)	1:84:A:LEU:HD13	1:97:A:GLN:H	12	0.11
(1,2662)	1:84:A:LEU:HD21	1:97:A:GLN:H	12	0.11
(1,2662)	1:84:A:LEU:HD22	1:97:A:GLN:H	12	0.11
(1,2662)	1:84:A:LEU:HD23	1:97:A:GLN:H	12	0.11
(1,2662)	1:84:A:LEU:HD11	1:97:A:GLN:H	16	0.11
(1,2662)	1:84:A:LEU:HD12	1:97:A:GLN:H	16	0.11
(1,2662)	1:84:A:LEU:HD13	1:97:A:GLN:H	16	0.11
(1,2662)	1:84:A:LEU:HD21	1:97:A:GLN:H	16	0.11
(1,2662)	1:84:A:LEU:HD22	1:97:A:GLN:H	16	0.11
(1,2662)	1:84:A:LEU:HD23	1:97:A:GLN:H	16	0.11
(1,2662)	1:84:A:LEU:HD11	1:97:A:GLN:H	21	0.11
(1,2662)	1:84:A:LEU:HD12	1:97:A:GLN:H	21	0.11
(1,2662)	1:84:A:LEU:HD13	1:97:A:GLN:H	21	0.11
(1,2662)	1:84:A:LEU:HD21	1:97:A:GLN:H	21	0.11
(1,2662)	1:84:A:LEU:HD22	1:97:A:GLN:H	21	0.11
(1,2662)	1:84:A:LEU:HD23	1:97:A:GLN:H	21	0.11
(1,2662)	1:84:A:LEU:HD11	1:97:A:GLN:H	25	0.11
(1,2662)	1:84:A:LEU:HD12	1:97:A:GLN:H	25	0.11
(1,2662)	1:84:A:LEU:HD13	1:97:A:GLN:H	25	0.11
(1,2662)	1:84:A:LEU:HD21	1:97:A:GLN:H	25	0.11
(1,2662)	1:84:A:LEU:HD22	1:97:A:GLN:H	25	0.11
(1,2662)	1:84:A:LEU:HD23	1:97:A:GLN:H	25	0.11
(1,2623)	1:79:A:LEU:HD11	1:82:A:ASN:HD21	33	0.11
(1,2623)	1:79:A:LEU:HD12	1:82:A:ASN:HD21	33	0.11
(1,2623)	1:79:A:LEU:HD13	1:82:A:ASN:HD21	33	0.11
(1,2623)	1:79:A:LEU:HD21	1:82:A:ASN:HD21	33	0.11
(1,2623)	1:79:A:LEU:HD22	1:82:A:ASN:HD21	33	0.11
(1,2623)	1:79:A:LEU:HD23	1:82:A:ASN:HD21	33	0.11
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD11	27	0.11
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD12	27	0.11
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD13	27	0.11
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD21	27	0.11
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD22	27	0.11
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD23	27	0.11
(1,2565)	1:68:A:LEU:HD11	1:107:A:PRO:HD2	40	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2565)	1:68:A:LEU:HD12	1:107:A:PRO:HD2	40	0.11
(1,2565)	1:68:A:LEU:HD13	1:107:A:PRO:HD2	40	0.11
(1,2565)	1:68:A:LEU:HD21	1:107:A:PRO:HD2	40	0.11
(1,2565)	1:68:A:LEU:HD22	1:107:A:PRO:HD2	40	0.11
(1,2565)	1:68:A:LEU:HD23	1:107:A:PRO:HD2	40	0.11
(1,2483)	1:59:A:LEU:HD11	1:62:A:THR:HG21	33	0.11
(1,2483)	1:59:A:LEU:HD11	1:62:A:THR:HG22	33	0.11
(1,2483)	1:59:A:LEU:HD11	1:62:A:THR:HG23	33	0.11
(1,2483)	1:59:A:LEU:HD12	1:62:A:THR:HG21	33	0.11
(1,2483)	1:59:A:LEU:HD12	1:62:A:THR:HG22	33	0.11
(1,2483)	1:59:A:LEU:HD12	1:62:A:THR:HG23	33	0.11
(1,2483)	1:59:A:LEU:HD13	1:62:A:THR:HG21	33	0.11
(1,2483)	1:59:A:LEU:HD13	1:62:A:THR:HG22	33	0.11
(1,2483)	1:59:A:LEU:HD13	1:62:A:THR:HG23	33	0.11
(1,2483)	1:59:A:LEU:HD21	1:62:A:THR:HG21	33	0.11
(1,2483)	1:59:A:LEU:HD21	1:62:A:THR:HG22	33	0.11
(1,2483)	1:59:A:LEU:HD21	1:62:A:THR:HG23	33	0.11
(1,2483)	1:59:A:LEU:HD22	1:62:A:THR:HG21	33	0.11
(1,2483)	1:59:A:LEU:HD22	1:62:A:THR:HG22	33	0.11
(1,2483)	1:59:A:LEU:HD22	1:62:A:THR:HG23	33	0.11
(1,2483)	1:59:A:LEU:HD23	1:62:A:THR:HG21	33	0.11
(1,2483)	1:59:A:LEU:HD23	1:62:A:THR:HG22	33	0.11
(1,2483)	1:59:A:LEU:HD23	1:62:A:THR:HG23	33	0.11
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD11	35	0.11
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD12	35	0.11
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD13	35	0.11
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD21	35	0.11
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD22	35	0.11
(1,2435)	1:53:A:CYS:HB2	1:95:A:LEU:HD23	35	0.11
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD11	35	0.11
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD12	35	0.11
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD13	35	0.11
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD21	35	0.11
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD22	35	0.11
(1,2435)	1:53:A:CYS:HB3	1:95:A:LEU:HD23	35	0.11
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD11	36	0.11
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD12	36	0.11
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD13	36	0.11
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD21	36	0.11
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD22	36	0.11
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD23	36	0.11
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD11	36	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD12	36	0.11
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD13	36	0.11
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD21	36	0.11
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD22	36	0.11
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD23	36	0.11
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD11	36	0.11
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD12	36	0.11
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD13	36	0.11
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD21	36	0.11
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD22	36	0.11
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD23	36	0.11
(1,2374)	1:42:A:LEU:HD11	1:55:A:TYR:HD1	17	0.11
(1,2374)	1:42:A:LEU:HD11	1:55:A:TYR:HD2	17	0.11
(1,2374)	1:42:A:LEU:HD12	1:55:A:TYR:HD1	17	0.11
(1,2374)	1:42:A:LEU:HD12	1:55:A:TYR:HD2	17	0.11
(1,2374)	1:42:A:LEU:HD13	1:55:A:TYR:HD1	17	0.11
(1,2374)	1:42:A:LEU:HD13	1:55:A:TYR:HD2	17	0.11
(1,2374)	1:42:A:LEU:HD21	1:55:A:TYR:HD1	17	0.11
(1,2374)	1:42:A:LEU:HD21	1:55:A:TYR:HD2	17	0.11
(1,2374)	1:42:A:LEU:HD22	1:55:A:TYR:HD1	17	0.11
(1,2374)	1:42:A:LEU:HD22	1:55:A:TYR:HD2	17	0.11
(1,2374)	1:42:A:LEU:HD23	1:55:A:TYR:HD1	17	0.11
(1,2374)	1:42:A:LEU:HD23	1:55:A:TYR:HD2	17	0.11
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	7	0.11
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	7	0.11
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	7	0.11
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	7	0.11
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	7	0.11
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	7	0.11
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	8	0.11
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	8	0.11
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	8	0.11
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	8	0.11
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	8	0.11
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	8	0.11
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	26	0.11
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	26	0.11
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	26	0.11
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	26	0.11
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	26	0.11
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	26	0.11
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	37	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	37	0.11
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	37	0.11
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	37	0.11
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	37	0.11
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	37	0.11
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	38	0.11
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	38	0.11
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	38	0.11
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	38	0.11
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	38	0.11
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	38	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD11	14	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD12	14	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD13	14	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD21	14	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD22	14	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD23	14	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD11	35	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD12	35	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD13	35	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD21	35	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD22	35	0.11
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD23	35	0.11
(1,2017)	1:123:A:LYS:H	1:123:A:LYS:HB2	35	0.11
(1,1319)	1:117:A:ASN:HB2	1:120:A:LYS:HB2	21	0.11
(1,1319)	1:117:A:ASN:HB2	1:120:A:LYS:HB3	21	0.11
(1,1264)	1:147:A:ALA:HB1	1:151:A:SER:HB2	19	0.11
(1,1264)	1:147:A:ALA:HB1	1:151:A:SER:HB3	19	0.11
(1,1264)	1:147:A:ALA:HB2	1:151:A:SER:HB2	19	0.11
(1,1264)	1:147:A:ALA:HB2	1:151:A:SER:HB3	19	0.11
(1,1264)	1:147:A:ALA:HB3	1:151:A:SER:HB2	19	0.11
(1,1264)	1:147:A:ALA:HB3	1:151:A:SER:HB3	19	0.11
(1,1264)	1:147:A:ALA:HB1	1:151:A:SER:HB2	23	0.11
(1,1264)	1:147:A:ALA:HB1	1:151:A:SER:HB3	23	0.11
(1,1264)	1:147:A:ALA:HB2	1:151:A:SER:HB2	23	0.11
(1,1264)	1:147:A:ALA:HB2	1:151:A:SER:HB3	23	0.11
(1,1264)	1:147:A:ALA:HB3	1:151:A:SER:HB2	23	0.11
(1,1264)	1:147:A:ALA:HB3	1:151:A:SER:HB3	23	0.11
(1,848)	1:17:A:LEU:HD11	1:55:A:TYR:HD1	36	0.11
(1,848)	1:17:A:LEU:HD11	1:55:A:TYR:HD2	36	0.11
(1,848)	1:17:A:LEU:HD12	1:55:A:TYR:HD1	36	0.11
(1,848)	1:17:A:LEU:HD12	1:55:A:TYR:HD2	36	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:17:A:LEU:HD13	1:55:A:TYR:HD1	36	0.11
(1,848)	1:17:A:LEU:HD13	1:55:A:TYR:HD2	36	0.11
(1,830)	1:93:A:ILE:HG21	1:98:A:GLN:H	14	0.11
(1,830)	1:93:A:ILE:HG22	1:98:A:GLN:H	14	0.11
(1,830)	1:93:A:ILE:HG23	1:98:A:GLN:H	14	0.11
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	6	0.11
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	6	0.11
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	6	0.11
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	7	0.11
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	7	0.11
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	7	0.11
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	9	0.11
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	9	0.11
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	9	0.11
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	15	0.11
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	15	0.11
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	15	0.11
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	20	0.11
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	20	0.11
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	20	0.11
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG21	13	0.11
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG22	13	0.11
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG23	13	0.11
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG21	17	0.11
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG22	17	0.11
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG23	17	0.11
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG21	27	0.11
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG22	27	0.11
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG23	27	0.11
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG21	37	0.11
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG22	37	0.11
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG23	37	0.11
(1,685)	1:77:A:TYR:HD1	1:108:A:LEU:HD11	27	0.11
(1,685)	1:77:A:TYR:HD1	1:108:A:LEU:HD12	27	0.11
(1,685)	1:77:A:TYR:HD1	1:108:A:LEU:HD13	27	0.11
(1,685)	1:77:A:TYR:HD2	1:108:A:LEU:HD11	27	0.11
(1,685)	1:77:A:TYR:HD2	1:108:A:LEU:HD12	27	0.11
(1,685)	1:77:A:TYR:HD2	1:108:A:LEU:HD13	27	0.11
(1,641)	1:72:A:ILE:HG21	1:75:A:GLY:HA2	40	0.11
(1,641)	1:72:A:ILE:HG22	1:75:A:GLY:HA2	40	0.11
(1,641)	1:72:A:ILE:HG23	1:75:A:GLY:HA2	40	0.11
(1,524)	1:62:A:THR:HG21	1:67:A:ILE:HA	29	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,524)	1:62:A:THR:HG22	1:67:A:ILE:HA	29	0.11
(1,524)	1:62:A:THR:HG23	1:67:A:ILE:HA	29	0.11
(1,112)	1:24:A:LEU:HD11	1:30:A:VAL:H	30	0.11
(1,112)	1:24:A:LEU:HD12	1:30:A:VAL:H	30	0.11
(1,112)	1:24:A:LEU:HD13	1:30:A:VAL:H	30	0.11
(1,3026)	1:134:A:LEU:HD11	1:137:A:LEU:H	31	0.1
(1,3026)	1:134:A:LEU:HD12	1:137:A:LEU:H	31	0.1
(1,3026)	1:134:A:LEU:HD13	1:137:A:LEU:H	31	0.1
(1,3026)	1:134:A:LEU:HD21	1:137:A:LEU:H	31	0.1
(1,3026)	1:134:A:LEU:HD22	1:137:A:LEU:H	31	0.1
(1,3026)	1:134:A:LEU:HD23	1:137:A:LEU:H	31	0.1
(1,2970)	1:123:A:LYS:HE2	1:124:A:GLN:HB2	36	0.1
(1,2970)	1:123:A:LYS:HE2	1:124:A:GLN:HB3	36	0.1
(1,2970)	1:123:A:LYS:HE3	1:124:A:GLN:HB2	36	0.1
(1,2970)	1:123:A:LYS:HE3	1:124:A:GLN:HB3	36	0.1
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	2	0.1
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	2	0.1
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	2	0.1
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	2	0.1
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	2	0.1
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	2	0.1
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD11	16	0.1
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD12	16	0.1
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD13	16	0.1
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD21	16	0.1
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD22	16	0.1
(1,2878)	1:112:A:HIS:H	1:113:A:LEU:HD23	16	0.1
(1,2868)	1:110:A:VAL:HG11	1:112:A:HIS:H	2	0.1
(1,2868)	1:110:A:VAL:HG12	1:112:A:HIS:H	2	0.1
(1,2868)	1:110:A:VAL:HG13	1:112:A:HIS:H	2	0.1
(1,2868)	1:110:A:VAL:HG21	1:112:A:HIS:H	2	0.1
(1,2868)	1:110:A:VAL:HG22	1:112:A:HIS:H	2	0.1
(1,2868)	1:110:A:VAL:HG23	1:112:A:HIS:H	2	0.1
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	19	0.1
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	19	0.1
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	19	0.1
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	19	0.1
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	19	0.1
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	19	0.1
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD11	27	0.1
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD12	27	0.1
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD13	27	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD21	27	0.1
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD22	27	0.1
(1,2797)	1:102:A:THR:HG1	1:103:A:LEU:HD23	27	0.1
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD11	33	0.1
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD12	33	0.1
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD13	33	0.1
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD21	33	0.1
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD22	33	0.1
(1,2716)	1:92:A:ASN:HD21	1:95:A:LEU:HD23	33	0.1
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD11	33	0.1
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD12	33	0.1
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD13	33	0.1
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD21	33	0.1
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD22	33	0.1
(1,2716)	1:92:A:ASN:HD22	1:95:A:LEU:HD23	33	0.1
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD21	4	0.1
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD22	4	0.1
(1,2701)	1:88:A:LYS:HD2	1:125:A:LEU:HD23	4	0.1
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD21	4	0.1
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD22	4	0.1
(1,2701)	1:88:A:LYS:HD3	1:125:A:LEU:HD23	4	0.1
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD11	39	0.1
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD12	39	0.1
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD13	39	0.1
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD21	39	0.1
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD22	39	0.1
(1,2680)	1:86:A:TYR:H	1:96:A:LEU:HD23	39	0.1
(1,2662)	1:84:A:LEU:HD11	1:97:A:GLN:H	22	0.1
(1,2662)	1:84:A:LEU:HD12	1:97:A:GLN:H	22	0.1
(1,2662)	1:84:A:LEU:HD13	1:97:A:GLN:H	22	0.1
(1,2662)	1:84:A:LEU:HD21	1:97:A:GLN:H	22	0.1
(1,2662)	1:84:A:LEU:HD22	1:97:A:GLN:H	22	0.1
(1,2662)	1:84:A:LEU:HD23	1:97:A:GLN:H	22	0.1
(1,2662)	1:84:A:LEU:HD11	1:97:A:GLN:H	30	0.1
(1,2662)	1:84:A:LEU:HD12	1:97:A:GLN:H	30	0.1
(1,2662)	1:84:A:LEU:HD13	1:97:A:GLN:H	30	0.1
(1,2662)	1:84:A:LEU:HD21	1:97:A:GLN:H	30	0.1
(1,2662)	1:84:A:LEU:HD22	1:97:A:GLN:H	30	0.1
(1,2662)	1:84:A:LEU:HD23	1:97:A:GLN:H	30	0.1
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD11	33	0.1
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD12	33	0.1
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD13	33	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD21	33	0.1
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD22	33	0.1
(1,2608)	1:77:A:TYR:HB3	1:108:A:LEU:HD23	33	0.1
(1,2565)	1:68:A:LEU:HD11	1:107:A:PRO:HD2	4	0.1
(1,2565)	1:68:A:LEU:HD12	1:107:A:PRO:HD2	4	0.1
(1,2565)	1:68:A:LEU:HD13	1:107:A:PRO:HD2	4	0.1
(1,2565)	1:68:A:LEU:HD21	1:107:A:PRO:HD2	4	0.1
(1,2565)	1:68:A:LEU:HD22	1:107:A:PRO:HD2	4	0.1
(1,2565)	1:68:A:LEU:HD23	1:107:A:PRO:HD2	4	0.1
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD11	30	0.1
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD12	30	0.1
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD13	30	0.1
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD21	30	0.1
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD22	30	0.1
(1,2387)	1:43:A:MET:HE1	1:59:A:LEU:HD23	30	0.1
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD11	30	0.1
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD12	30	0.1
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD13	30	0.1
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD21	30	0.1
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD22	30	0.1
(1,2387)	1:43:A:MET:HE2	1:59:A:LEU:HD23	30	0.1
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD11	30	0.1
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD12	30	0.1
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD13	30	0.1
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD21	30	0.1
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD22	30	0.1
(1,2387)	1:43:A:MET:HE3	1:59:A:LEU:HD23	30	0.1
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD11	12	0.1
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD12	12	0.1
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD13	12	0.1
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD21	12	0.1
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD22	12	0.1
(1,2384)	1:43:A:MET:HG2	1:79:A:LEU:HD23	12	0.1
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	18	0.1
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	18	0.1
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	18	0.1
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	18	0.1
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	18	0.1
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	18	0.1
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	20	0.1
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	20	0.1
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	20	0.1
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	20	0.1
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	20	0.1
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	33	0.1
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	33	0.1
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	33	0.1
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	33	0.1
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	33	0.1
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	33	0.1
(1,2371)	1:42:A:LEU:HD11	1:43:A:MET:H	34	0.1
(1,2371)	1:42:A:LEU:HD12	1:43:A:MET:H	34	0.1
(1,2371)	1:42:A:LEU:HD13	1:43:A:MET:H	34	0.1
(1,2371)	1:42:A:LEU:HD21	1:43:A:MET:H	34	0.1
(1,2371)	1:42:A:LEU:HD22	1:43:A:MET:H	34	0.1
(1,2371)	1:42:A:LEU:HD23	1:43:A:MET:H	34	0.1
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD11	39	0.1
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD12	39	0.1
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD13	39	0.1
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD21	39	0.1
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD22	39	0.1
(1,2366)	1:41:A:SER:H	1:42:A:LEU:HD23	39	0.1
(1,1623)	1:66:A:GLU:H	1:69:A:VAL:HG11	30	0.1
(1,1623)	1:66:A:GLU:H	1:69:A:VAL:HG12	30	0.1
(1,1623)	1:66:A:GLU:H	1:69:A:VAL:HG13	30	0.1
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	3	0.1
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	3	0.1
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	3	0.1
(1,811)	1:93:A:ILE:HD11	1:94:A:PRO:HD2	22	0.1
(1,811)	1:93:A:ILE:HD12	1:94:A:PRO:HD2	22	0.1
(1,811)	1:93:A:ILE:HD13	1:94:A:PRO:HD2	22	0.1
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG21	23	0.1
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG22	23	0.1
(1,797)	1:87:A:SER:HA	1:89:A:THR:HG23	23	0.1
(1,524)	1:62:A:THR:HG21	1:67:A:ILE:HA	21	0.1
(1,524)	1:62:A:THR:HG22	1:67:A:ILE:HA	21	0.1
(1,524)	1:62:A:THR:HG23	1:67:A:ILE:HA	21	0.1
(1,190)	1:37:A:SER:HB2	1:38:A:LYS:HB2	16	0.1
(1,190)	1:37:A:SER:HB2	1:38:A:LYS:HB3	16	0.1
(1,190)	1:37:A:SER:HB3	1:38:A:LYS:HB2	16	0.1
(1,190)	1:37:A:SER:HB3	1:38:A:LYS:HB3	16	0.1

10 Dihedral-angle violation analysis [i](#)

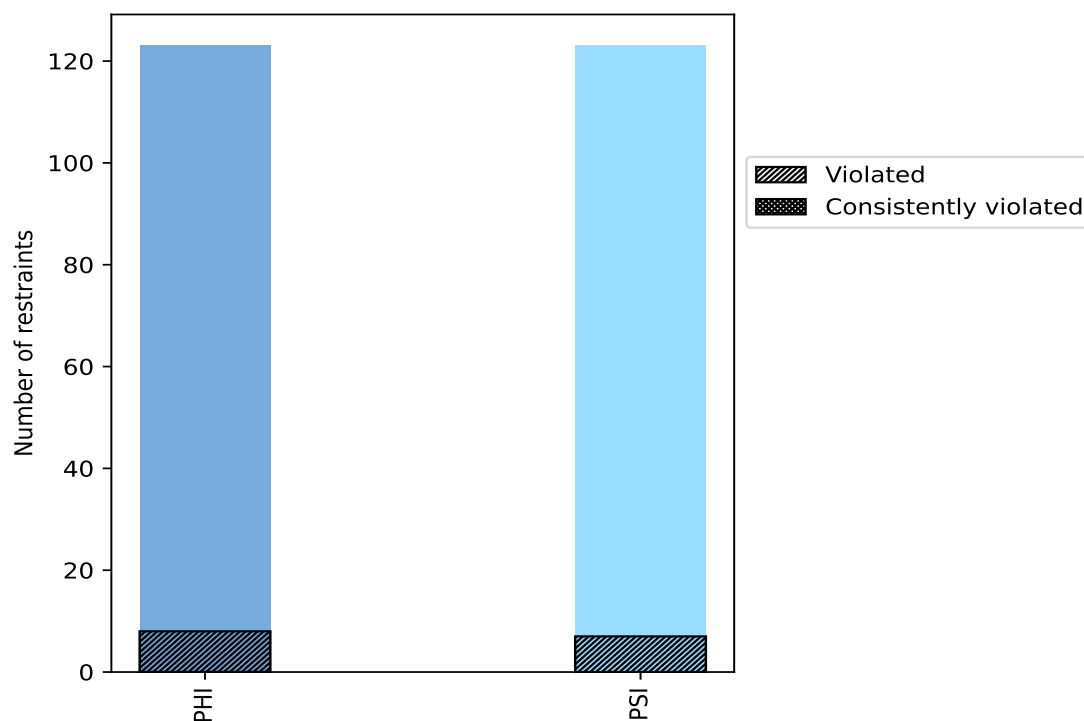
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	123	50.0	8	6.5	3.3	0	0.0	0.0
PSI	123	50.0	7	5.7	2.8	0	0.0	0.0
Total	246	100.0	15	6.1	6.1	0	0.0	0.0

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

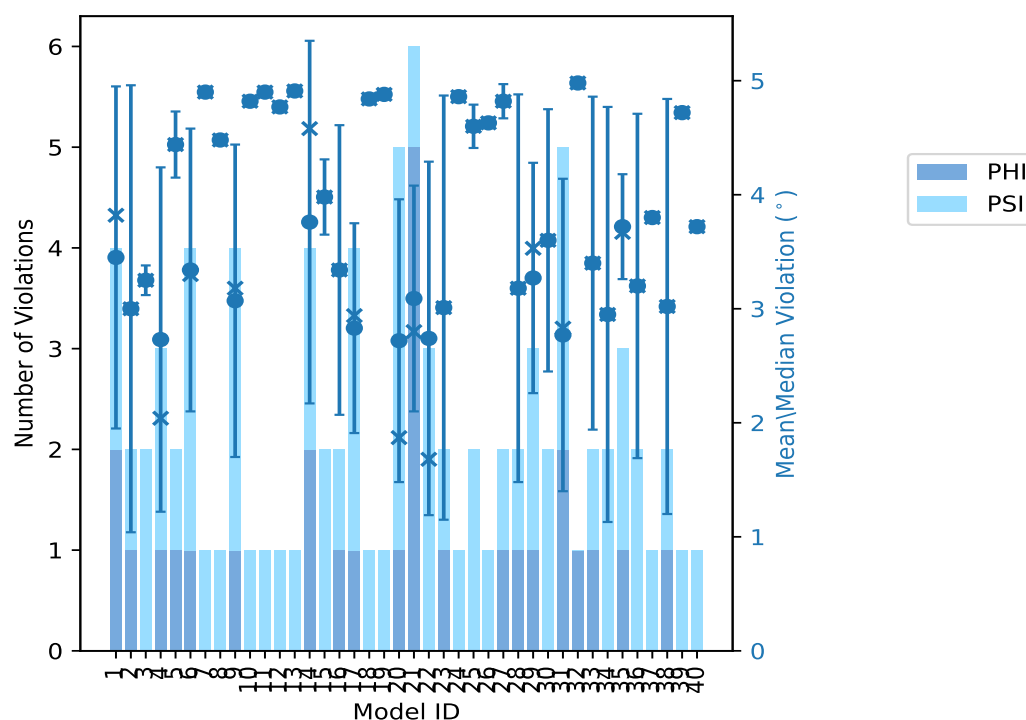
Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	2	2	4	3.45	5.01	1.5	3.82
2	1	1	2	3.0	4.96	1.96	3.0
3	0	2	2	3.25	3.38	0.13	3.25
4	1	2	3	2.73	4.83	1.51	2.04
5	1	1	2	4.44	4.73	0.29	4.44
6	1	3	4	3.34	4.87	1.24	3.3
7	0	1	1	4.9	4.9	0.0	4.9
8	0	1	1	4.48	4.48	0.0	4.48
9	1	3	4	3.07	4.77	1.37	3.18
10	0	1	1	4.82	4.82	0.0	4.82
11	0	1	1	4.9	4.9	0.0	4.9
12	0	1	1	4.77	4.77	0.0	4.77
13	0	1	1	4.91	4.91	0.0	4.91
14	2	2	4	3.76	4.85	1.59	4.58
15	0	2	2	3.98	4.31	0.33	3.98
16	1	1	2	3.34	4.61	1.27	3.34
17	1	3	4	2.83	3.75	0.92	2.94
18	0	1	1	4.84	4.84	0.0	4.84
19	0	1	1	4.88	4.88	0.0	4.88
20	1	4	5	2.72	4.94	1.24	1.87
21	5	1	6	3.09	5.02	0.99	2.8
22	0	3	3	2.74	4.93	1.55	1.68
23	1	1	2	3.01	4.88	1.86	3.01
24	0	1	1	4.86	4.86	0.0	4.86
25	0	2	2	4.6	4.79	0.19	4.6
26	0	1	1	4.63	4.63	0.0	4.63
27	1	1	2	4.82	4.97	0.15	4.82
28	1	1	2	3.18	4.87	1.7	3.18
29	1	2	3	3.27	4.35	1.01	3.53
30	0	2	2	3.6	4.76	1.15	3.6
31	2	3	5	2.77	4.95	1.37	2.83
32	1	0	1	4.98	4.98	0.0	4.98
33	1	1	2	3.4	4.86	1.46	3.4
34	0	2	2	2.95	4.77	1.82	2.95
35	1	2	3	3.72	4.3	0.46	3.67
36	0	2	2	3.2	4.71	1.51	3.2
37	0	1	1	3.8	3.8	0.0	3.8
38	1	1	2	3.02	4.83	1.82	3.02

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Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
39	0	1	1	4.72	4.72	0.0	4.72
40	0	1	1	3.72	3.72	0.0	3.72

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
5	1	6	1	2.5
1	0	1	2	5.0
0	2	2	3	7.5
0	0	0	4	10.0

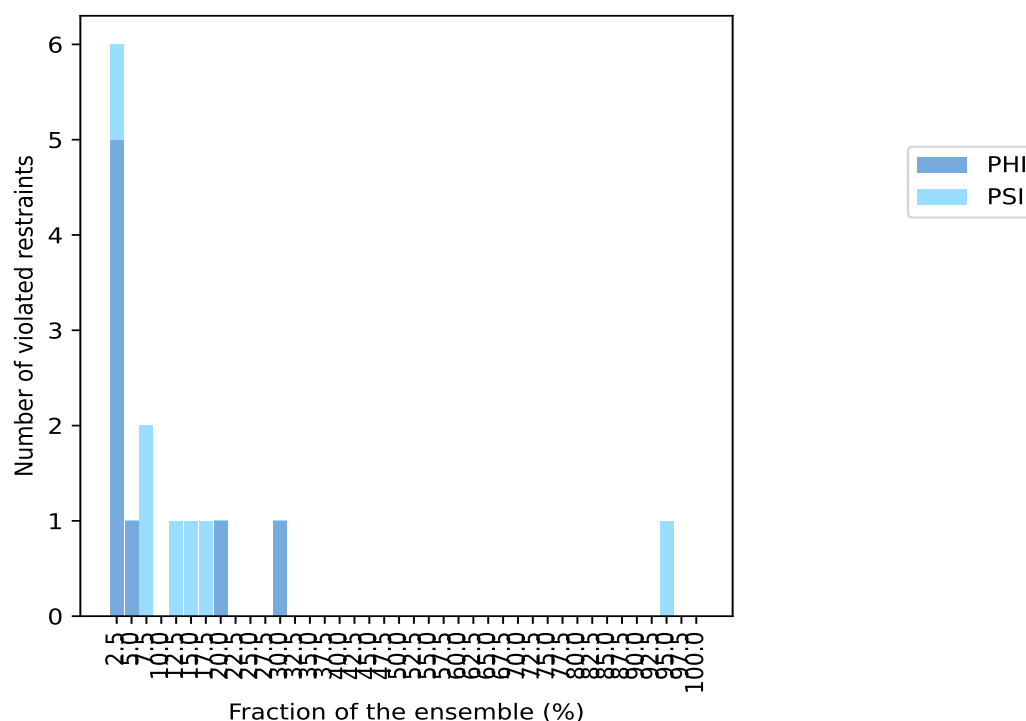
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	1	1	5	12.5
0	1	1	6	15.0
0	1	1	7	17.5
1	0	1	8	20.0
0	0	0	9	22.5
0	0	0	10	25.0
0	0	0	11	27.5
1	0	1	12	30.0
0	0	0	13	32.5
0	0	0	14	35.0
0	0	0	15	37.5
0	0	0	16	40.0
0	0	0	17	42.5
0	0	0	18	45.0
0	0	0	19	47.5
0	0	0	20	50.0
0	0	0	21	52.5
0	0	0	22	55.0
0	0	0	23	57.5
0	0	0	24	60.0
0	0	0	25	62.5
0	0	0	26	65.0
0	0	0	27	67.5
0	0	0	28	70.0
0	0	0	29	72.5
0	0	0	30	75.0
0	0	0	31	77.5
0	0	0	32	80.0
0	0	0	33	82.5
0	0	0	34	85.0
0	0	0	35	87.5
0	0	0	36	90.0
0	0	0	37	92.5
0	1	1	38	95.0
0	0	0	39	97.5
0	0	0	40	100.0

¹ Number of models with violations

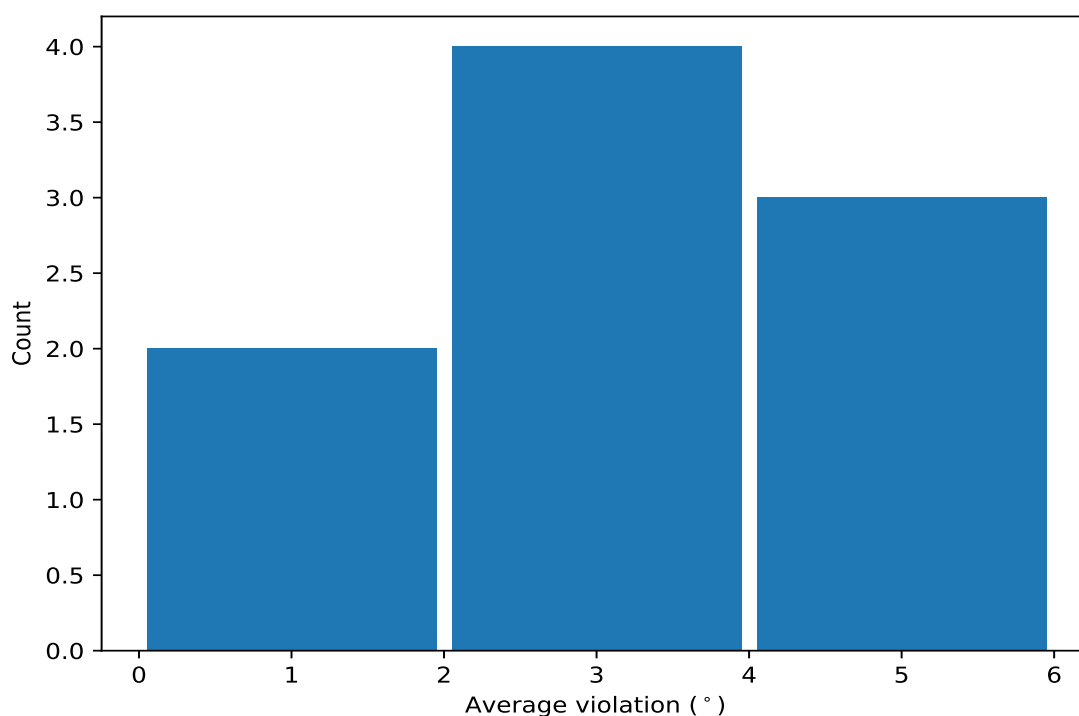
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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



10.4.2 Table: Most violated dihedral-angle 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.

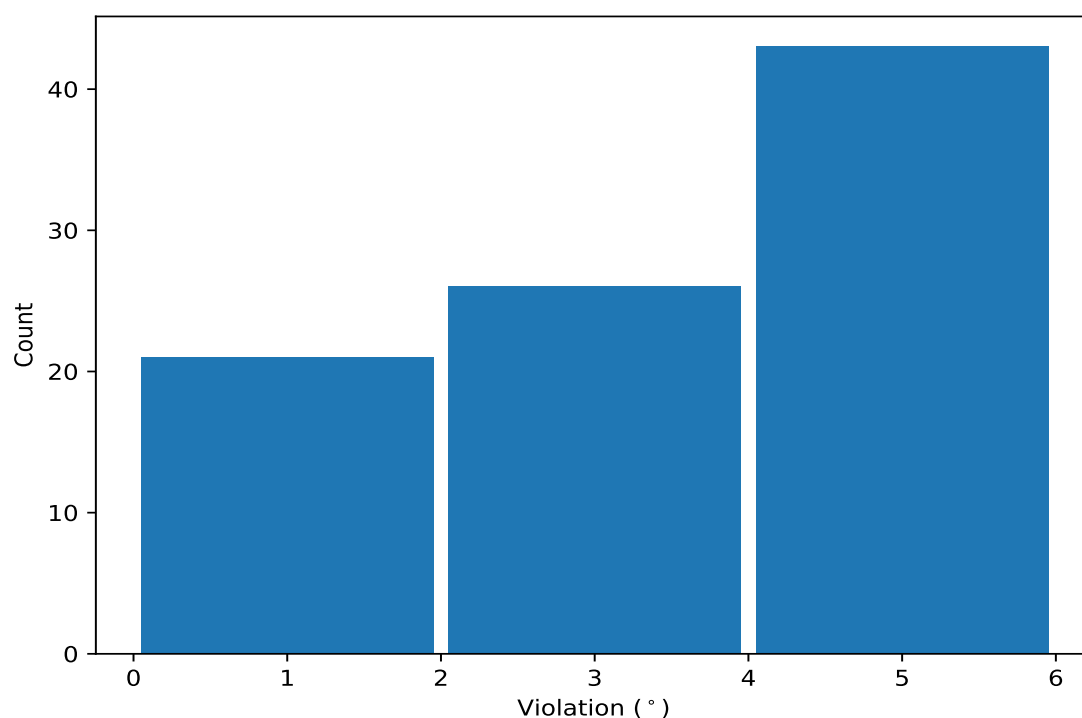
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	38	4.57	0.49	4.78
(1,207)	1:131:A:ASP:C	1:132:A:GLU:N	1:132:A:GLU:CA	1:132:A:GLU:C	12	2.23	1.04	2.04
(1,43)	1:33:A:VAL:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	8	2.37	1.13	2.0
(1,40)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:VAL:N	7	3.22	1.17	3.42
(1,180)	1:116:A:ASN:N	1:116:A:ASN:CA	1:116:A:ASN:C	1:117:A:ASN:N	6	4.26	0.54	4.39
(1,186)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:LEU:N	5	1.55	0.39	1.68
(1,192)	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	1:124:A:GLN:N	3	2.84	0.89	3.24
(1,172)	1:112:A:HIS:N	1:112:A:HIS:CA	1:112:A:HIS:C	1:113:A:LEU:N	3	1.57	0.31	1.68
(1,209)	1:132:A:GLU:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	2	4.79	0.06	4.79

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	21	5.02
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	1	5.01
(1,67)	1:48:A:LYS:C	1:49:A:MET:N	1:49:A:MET:CA	1:49:A:MET:C	32	4.98
(1,207)	1:131:A:ASP:C	1:132:A:GLU:N	1:132:A:GLU:CA	1:132:A:GLU:C	27	4.97
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	2	4.96
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	31	4.95
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	20	4.94
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	22	4.93
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	13	4.91
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	7	4.9
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	11	4.9
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	19	4.88
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	23	4.88
(1,180)	1:116:A:ASN:N	1:116:A:ASN:CA	1:116:A:ASN:C	1:117:A:ASN:N	6	4.87
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	28	4.87
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	24	4.86
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	33	4.86
(1,209)	1:132:A:GLU:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	14	4.85
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	18	4.84
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	4	4.83
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	38	4.83

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	10	4.82
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	25	4.79
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	14	4.78
(1,180)	1:116:A:ASN:N	1:116:A:ASN:CA	1:116:A:ASN:C	1:117:A:ASN:N	9	4.77
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	12	4.77
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	34	4.77
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	30	4.76
(1,209)	1:132:A:GLU:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	5	4.73
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	39	4.72
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	36	4.71
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	27	4.68
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	26	4.63
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	16	4.61
(1,40)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:VAL:N	1	4.49
(1,180)	1:116:A:ASN:N	1:116:A:ASN:CA	1:116:A:ASN:C	1:117:A:ASN:N	8	4.48
(1,40)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:VAL:N	25	4.4
(1,43)	1:33:A:VAL:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	14	4.38
(1,40)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:VAL:N	29	4.35
(1,180)	1:116:A:ASN:N	1:116:A:ASN:CA	1:116:A:ASN:C	1:117:A:ASN:N	15	4.31
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	35	4.3
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	6	4.21
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	5	4.16
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	9	3.87
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	37	3.8
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	17	3.75
(1,180)	1:116:A:ASN:N	1:116:A:ASN:CA	1:116:A:ASN:C	1:117:A:ASN:N	17	3.72
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	40	3.72
(1,192)	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	1:124:A:GLN:N	35	3.67
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	15	3.65
(1,43)	1:33:A:VAL:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	21	3.62
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	29	3.53
(1,40)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:VAL:N	31	3.42
(1,180)	1:116:A:ASN:N	1:116:A:ASN:CA	1:116:A:ASN:C	1:117:A:ASN:N	3	3.38
(1,192)	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	1:124:A:GLN:N	20	3.24
(1,207)	1:131:A:ASP:C	1:132:A:GLU:N	1:132:A:GLU:CA	1:132:A:GLU:C	35	3.18
(1,43)	1:33:A:VAL:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	1	3.15
(1,132)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:LYS:N	3	3.12
(1,127)	1:84:A:LEU:C	1:85:A:THR:N	1:85:A:THR:CA	1:85:A:THR:C	21	2.84
(1,207)	1:131:A:ASP:C	1:132:A:GLU:N	1:132:A:GLU:CA	1:132:A:GLU:C	31	2.83
(1,131)	1:86:A:TYR:C	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	21	2.75
(1,207)	1:131:A:ASP:C	1:132:A:GLU:N	1:132:A:GLU:CA	1:132:A:GLU:C	9	2.49
(1,40)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:VAL:N	30	2.45
(1,207)	1:131:A:ASP:C	1:132:A:GLU:N	1:132:A:GLU:CA	1:132:A:GLU:C	6	2.39
(1,95)	1:66:A:GLU:C	1:67:A:ILE:N	1:67:A:ILE:CA	1:67:A:ILE:C	17	2.17
(1,7)	1:14:A:LYS:C	1:15:A:GLU:N	1:15:A:GLU:CA	1:15:A:GLU:C	21	2.17
(1,207)	1:131:A:ASP:C	1:132:A:GLU:N	1:132:A:GLU:CA	1:132:A:GLU:C	21	2.15
(1,43)	1:33:A:VAL:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	16	2.08
(1,186)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:LEU:N	4	2.04
(1,207)	1:131:A:ASP:C	1:132:A:GLU:N	1:132:A:GLU:CA	1:132:A:GLU:C	33	1.94
(1,43)	1:33:A:VAL:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	29	1.92
(1,172)	1:112:A:HIS:N	1:112:A:HIS:CA	1:112:A:HIS:C	1:113:A:LEU:N	6	1.89

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,207)	1:131:A:ASP:C	1:132:A:GLU:N	1:132:A:GLU:CA	1:132:A:GLU:C	20	1.87
(1,186)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:LEU:N	20	1.83
(1,40)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:VAL:N	20	1.71
(1,40)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:VAL:N	36	1.69
(1,186)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:LEU:N	22	1.68
(1,172)	1:112:A:HIS:N	1:112:A:HIS:CA	1:112:A:HIS:C	1:113:A:LEU:N	17	1.68
(1,192)	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	1:124:A:GLN:N	22	1.6
(1,207)	1:131:A:ASP:C	1:132:A:GLU:N	1:132:A:GLU:CA	1:132:A:GLU:C	28	1.48
(1,43)	1:33:A:VAL:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	31	1.47
(1,43)	1:33:A:VAL:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	4	1.32
(1,207)	1:131:A:ASP:C	1:132:A:GLU:N	1:132:A:GLU:CA	1:132:A:GLU:C	38	1.2
(1,186)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:LEU:N	31	1.18
(1,207)	1:131:A:ASP:C	1:132:A:GLU:N	1:132:A:GLU:CA	1:132:A:GLU:C	23	1.15
(1,172)	1:112:A:HIS:N	1:112:A:HIS:CA	1:112:A:HIS:C	1:113:A:LEU:N	9	1.15
(1,207)	1:131:A:ASP:C	1:132:A:GLU:N	1:132:A:GLU:CA	1:132:A:GLU:C	1	1.14
(1,126)	1:84:A:LEU:N	1:84:A:LEU:CA	1:84:A:LEU:C	1:85:A:THR:N	34	1.14
(1,186)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:LEU:N	14	1.03
(1,43)	1:33:A:VAL:C	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:C	2	1.03