



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 01:44 AM UTC

PDB ID : 5K5G / pdb_00005k5g
BMRB ID : 30099
Title : Structure of human islet amyloid polypeptide in complex with an engineered binding protein
Authors : Mirecka, E.A.; Feuerstein, S.; Gremer, L.; Schroeder, G.F.; Stoldt, M.; Willbold, D.; Hoyer, W.
Deposited on : 2016-05-23

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

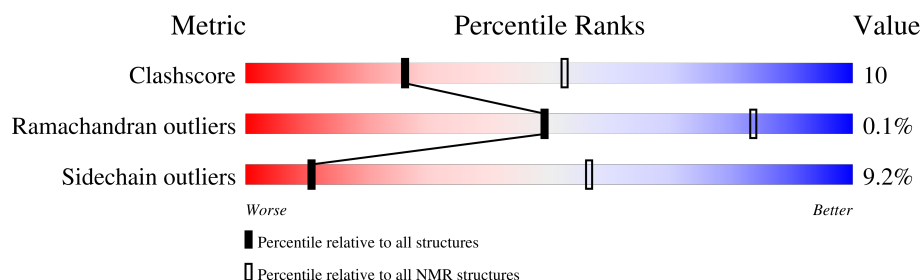
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 42%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	37	
2	B	69	
2	C	69	

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:12-A:28, B:15-B:56, C:13-C:56 (103)	0.62	3

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	3, 6, 8, 9
2	2, 5, 7
3	1, 4
Single-model clusters	10

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1622 atoms, of which 798 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Islet amyloid polypeptide.

Mol	Chain	Residues	Atoms					Trace
1	A	21	Total	C	H	N	O	0
			318	100	158	30	30	

- Molecule 2 is a protein called HI18.

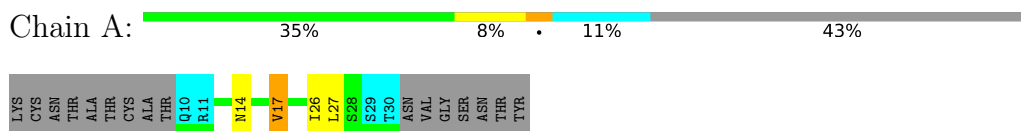
Mol	Chain	Residues	Atoms						Trace
2	B	44	Total	C	H	N	O	S	0
			652	207	320	57	67	1	
2	C	44	Total	C	H	N	O	S	0
			652	207	320	57	67	1	

4 Residue-property plots [i](#)

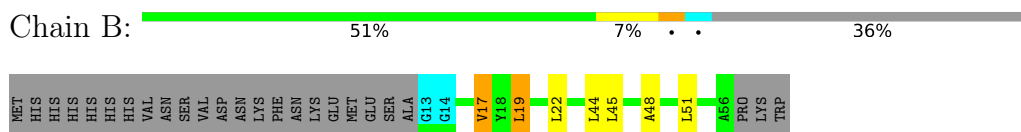
4.1 Average score per residue in the NMR ensemble

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

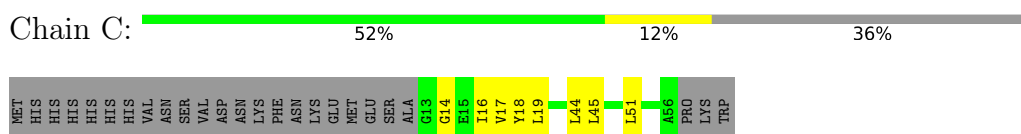
- Molecule 1: Islet amyloid polypeptide



- Molecule 2: HI18



- Molecule 2: HI18

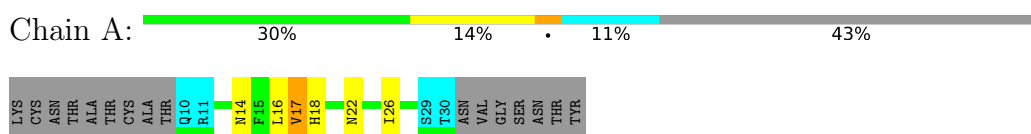


4.2 Scores per residue for each member of the ensemble

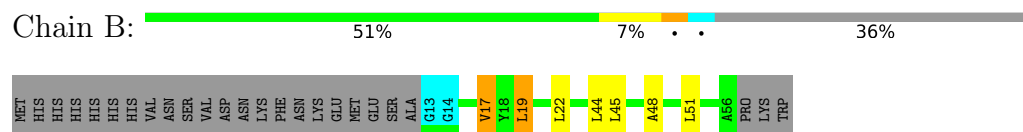
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

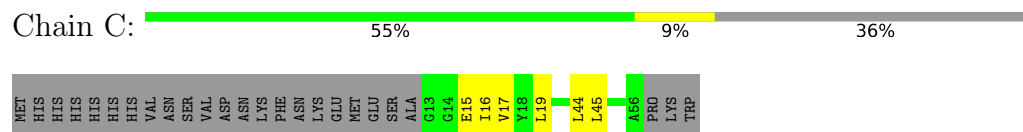
- Molecule 1: Islet amyloid polypeptide



- Molecule 2: HI18

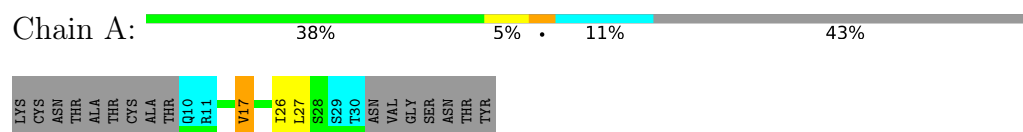


- Molecule 2: HI18

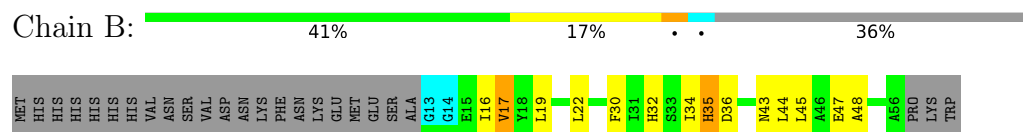


4.2.2 Score per residue for model 2

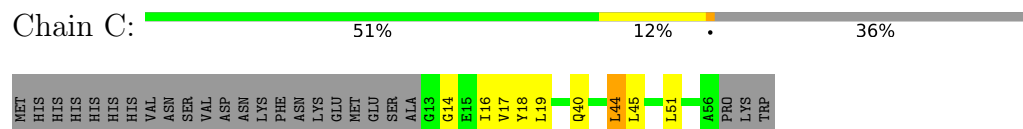
- Molecule 1: Islet amyloid polypeptide



- Molecule 2: HI18

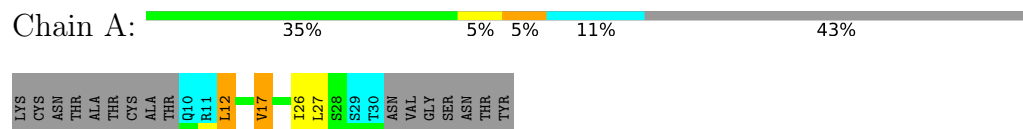


- Molecule 2: HI18



4.2.3 Score per residue for model 3 (medoid)

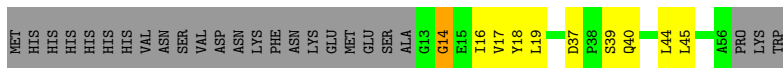
- Molecule 1: Islet amyloid polypeptide



- Molecule 2: HI18

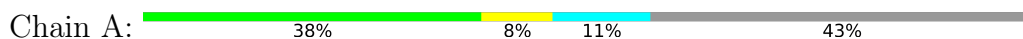


- Molecule 2: HI18



4.2.4 Score per residue for model 4

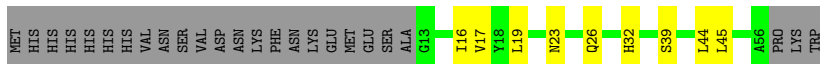
- Molecule 1: Islet amyloid polypeptide



- Molecule 2: HI18

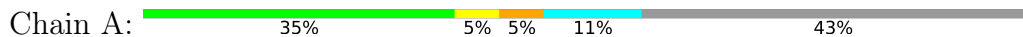


- Molecule 2: HI18

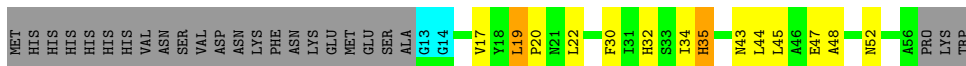


4.2.5 Score per residue for model 5

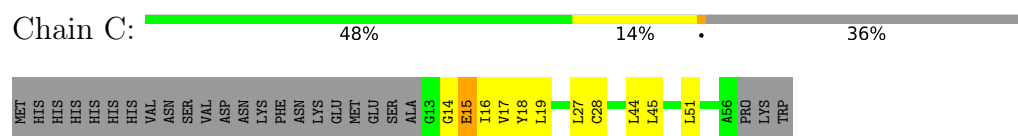
- Molecule 1: Islet amyloid polypeptide



- Molecule 2: HI18

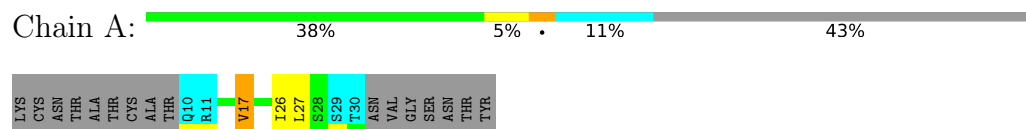


- Molecule 2: HI18

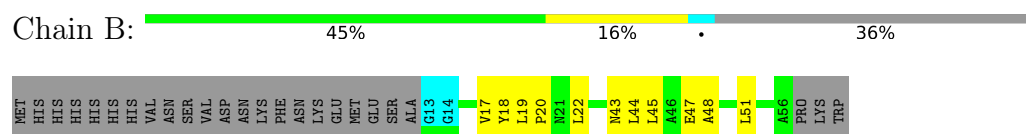


4.2.6 Score per residue for model 6

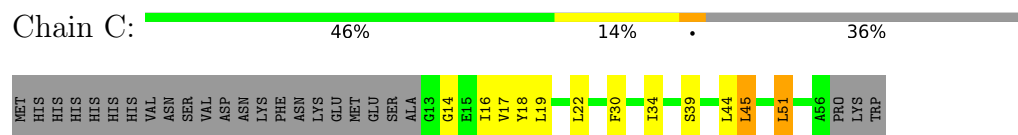
- Molecule 1: Islet amyloid polypeptide



- Molecule 2: HI18

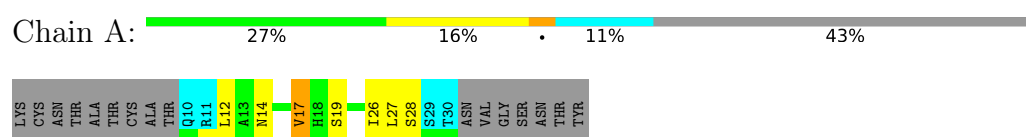


- Molecule 2: HI18

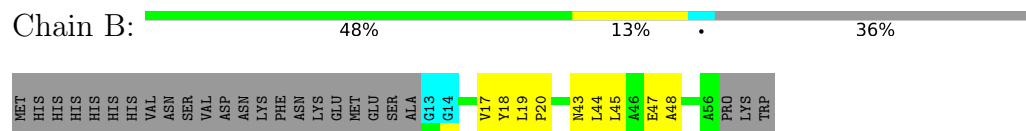


4.2.7 Score per residue for model 7

- Molecule 1: Islet amyloid polypeptide

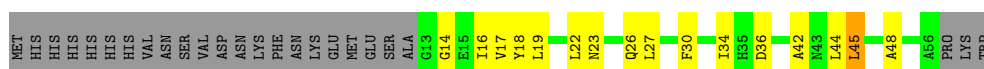


- Molecule 2: HI18



- Molecule 2: HI18



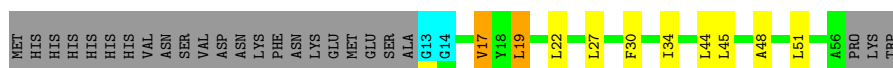


4.2.8 Score per residue for model 8

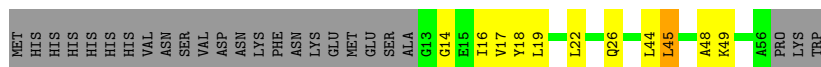
- Molecule 1: Islet amyloid polypeptide



- Molecule 2: HI18

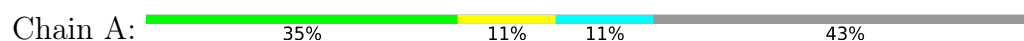


- Molecule 2: HI18

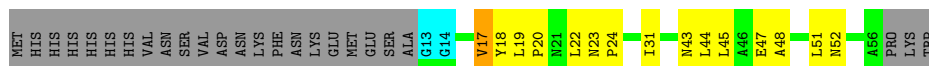


4.2.9 Score per residue for model 9

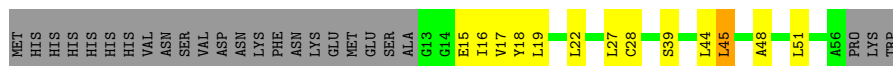
- Molecule 1: Islet amyloid polypeptide



- Molecule 2: HI18

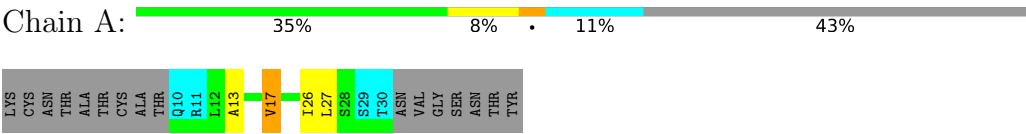


- Molecule 2: HI18

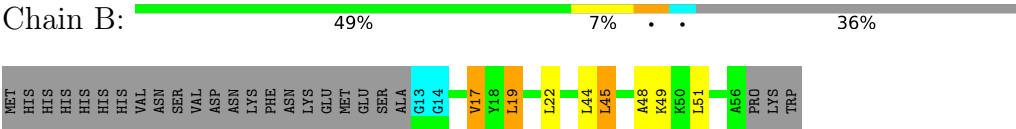


4.2.10 Score per residue for model 10

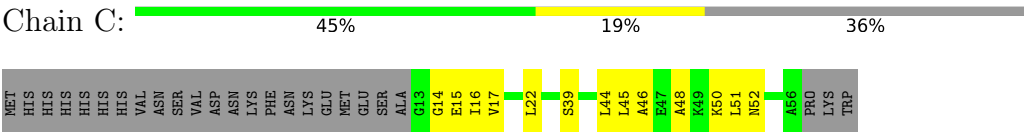
- Molecule 1: Islet amyloid polypeptide



- Molecule 2: HI18



- Molecule 2: HI18



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	1.21
ARIA	refinement	2.3.2
CcpNmr Analysis	structure solution	2.3
NMRPipe	structure solution	7.9
VnmrJ	structure solution	2.3A

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	3
Total number of shifts	1074
Number of shifts mapped to atoms	1074
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	42%

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	0.60±0.05	0±0/130 (0.0± 0.0%)	0.75±0.03	0±0/177 (0.0± 0.0%)
2	B	0.45±0.02	0±0/330 (0.0± 0.0%)	0.81±0.03	0±0/450 (0.0± 0.1%)
2	C	0.43±0.01	0±0/338 (0.0± 0.0%)	0.79±0.03	0±0/460 (0.0± 0.0%)
All	All	0.47	0/7980 (0.0%)	0.79	2/10870 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	35	HIS	CA-CB-CG	5.43	119.23	113.80	5	2

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	127	125	124	4±1
2	B	324	314	312	8±2
2	C	332	320	317	8±2
All	All	7830	7590	7530	155

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:19:LEU:HD13	2:B:48:ALA:HB1	0.83	1.49	8	3
2:B:32:HIS:HA	2:B:35:HIS:CE1	0.76	2.16	5	2
1:A:26:ILE:HD12	2:C:16:ILE:HG12	0.66	1.67	7	10
2:C:17:VAL:HG12	2:C:19:LEU:CD1	0.64	2.23	6	9
2:B:22:LEU:CD2	2:B:51:LEU:HB3	0.60	2.27	8	6
2:C:17:VAL:HG11	2:C:45:LEU:HB3	0.59	1.73	4	2
1:A:27:LEU:O	2:C:14:GLY:HA2	0.59	1.98	8	7
2:C:18:TYR:C	2:C:19:LEU:HD12	0.58	2.23	6	7
2:C:17:VAL:HG12	2:C:19:LEU:HD11	0.58	1.74	3	8
2:C:17:VAL:HG11	2:C:45:LEU:HD21	0.56	1.76	6	3
2:B:20:PRO:HD2	2:B:52:ASN:OD1	0.55	2.02	5	2
2:B:23:ASN:HB2	2:B:26:GLN:OE1	0.54	2.02	3	1
2:B:43:ASN:O	2:B:47:GLU:HG3	0.54	2.03	6	2
2:C:37:ASP:OD2	2:C:40:GLN:HG2	0.54	2.03	3	1
2:B:22:LEU:HD21	2:B:51:LEU:HB3	0.53	1.80	8	3
2:B:19:LEU:CD1	2:B:48:ALA:HB1	0.52	2.31	8	3
2:B:45:LEU:O	2:B:49:LYS:HG3	0.52	2.04	4	2
1:A:18:HIS:HB3	1:A:22:ASN:OD1	0.52	2.05	1	1
1:A:14:ASN:HB3	1:A:26:ILE:HG23	0.52	1.82	1	1
2:B:30:PHE:O	2:B:34:ILE:HG12	0.51	2.05	2	3
2:B:22:LEU:HD12	2:B:27:LEU:HD23	0.51	1.82	8	1
2:C:45:LEU:C	2:C:45:LEU:HD13	0.51	2.30	6	4
2:C:17:VAL:HG11	2:C:45:LEU:HD22	0.51	1.82	10	2
2:B:19:LEU:HD12	2:B:22:LEU:CD1	0.50	2.36	1	2
1:A:17:VAL:HG13	2:B:17:VAL:HG23	0.50	1.83	8	8
2:B:18:TYR:O	2:B:20:PRO:HD3	0.50	2.06	7	3
2:B:43:ASN:O	2:B:47:GLU:HG2	0.49	2.08	2	3
2:B:21:ASN:ND2	2:B:56:ALA:HA	0.49	2.23	4	1
1:A:16:LEU:HA	2:B:17:VAL:O	0.48	2.08	4	3
2:C:17:VAL:CG1	2:C:45:LEU:HD22	0.48	2.38	4	2
2:B:19:LEU:HG	2:B:48:ALA:HB1	0.48	1.83	2	6
2:C:15:GLU:H	2:C:15:GLU:CD	0.48	2.17	5	2
2:B:22:LEU:HD12	2:B:27:LEU:CD2	0.48	2.39	8	1
2:C:17:VAL:CG1	2:C:45:LEU:HD21	0.48	2.39	6	2
2:C:30:PHE:O	2:C:34:ILE:HG12	0.47	2.09	7	2
2:C:22:LEU:HD11	2:C:48:ALA:HB1	0.47	1.86	10	4
2:B:19:LEU:HB3	2:B:22:LEU:HG	0.46	1.86	2	6
2:B:48:ALA:HA	2:B:51:LEU:HB2	0.46	1.87	8	2
2:C:26:GLN:HA	2:C:26:GLN:OE1	0.45	2.11	8	1
2:C:23:ASN:HB2	2:C:26:GLN:OE1	0.45	2.12	7	1
2:B:19:LEU:N	2:B:19:LEU:HD22	0.44	2.27	4	3
1:A:17:VAL:CG1	2:B:17:VAL:HG23	0.44	2.42	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:27:LEU:HD12	2:C:28:CYS:N	0.44	2.28	5	2
2:B:35:HIS:CD2	2:B:36:ASP:HB2	0.43	2.48	2	1
2:B:23:ASN:OD1	2:B:24:PRO:HD2	0.43	2.14	9	1
1:A:13:ALA:HB2	1:A:27:LEU:HD23	0.43	1.89	10	1
2:B:19:LEU:HD12	2:B:22:LEU:HD11	0.42	1.91	1	1
2:C:40:GLN:O	2:C:44:LEU:HD22	0.42	2.14	2	1
2:C:22:LEU:HD13	2:C:27:LEU:HB3	0.42	1.92	7	1
1:A:17:VAL:O	2:B:16:ILE:HA	0.42	2.13	2	1
2:C:22:LEU:CD2	2:C:51:LEU:HB3	0.42	2.44	6	1
2:B:19:LEU:HD22	2:B:19:LEU:N	0.42	2.30	3	1
1:A:14:ASN:HD22	1:A:14:ASN:N	0.42	2.13	5	1
1:A:14:ASN:OD1	2:B:20:PRO:HB3	0.41	2.14	7	1
2:C:46:ALA:O	2:C:50:LYS:HG2	0.41	2.15	10	1
1:A:12:LEU:HD22	1:A:12:LEU:N	0.41	2.30	3	1
2:B:31:ILE:HG21	2:C:27:LEU:HD21	0.41	1.93	9	1
2:C:42:ALA:O	2:C:45:LEU:HB3	0.40	2.16	7	1
1:A:26:ILE:HG13	2:C:15:GLU:O	0.40	2.15	9	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	17/37 (46%)	14±0 (84±3%)	3±0 (16±3%)	0±0 (0±0%)	100	100
2	B	41/69 (59%)	40±1 (97±2%)	1±1 (3±2%)	0±0 (0±0%)	100	100
2	C	42/69 (61%)	40±1 (95±2%)	2±1 (5±2%)	0±0 (0±1%)	44	80
All	All	1000/1750 (57%)	936 (94%)	63 (6%)	1 (0%)	49	83

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
2	C	14	GLY	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	14/31 (45%)	13±0 (90±3%)	1±0 (10±3%)	9	54
2	B	36/60 (60%)	33±1 (91±2%)	3±1 (9±2%)	11	57
2	C	36/60 (60%)	33±0 (91±1%)	3±0 (9±1%)	11	56
All	All	860/1510 (57%)	781 (91%)	79 (9%)	11	56

All 19 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	17	VAL	10
2	B	44	LEU	10
2	B	45	LEU	10
2	C	44	LEU	10
2	C	45	LEU	8
2	B	17	VAL	6
2	B	19	LEU	5
2	C	51	LEU	5
1	A	14	ASN	3
2	C	15	GLU	2
2	C	39	SER	2
1	A	12	LEU	1
2	C	23	ASN	1
2	C	26	GLN	1
2	C	32	HIS	1
2	C	36	ASP	1
2	C	49	LYS	1
2	B	52	ASN	1
2	C	52	ASN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no 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 42% for the well-defined parts and 43% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	222
Number of shifts mapped to atoms	222
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

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

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 13%, i.e. 178 atoms were assigned a chemical shift out of a possible 1345. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	78/506 (15%)	32/203 (16%)	30/206 (15%)	16/97 (16%)
Sidechain	95/741 (13%)	65/485 (13%)	29/235 (12%)	1/21 (5%)
Aromatic	5/98 (5%)	5/48 (10%)	0/40 (0%)	0/10 (0%)
Overall	178/1345 (13%)	102/736 (14%)	59/481 (12%)	17/128 (13%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 16%, i.e. 222 atoms were assigned a chemical shift out of a possible 1414. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	96/538 (18%)	40/217 (18%)	36/218 (17%)	20/103 (19%)
Sidechain	121/778 (16%)	83/508 (16%)	37/245 (15%)	1/25 (4%)
Aromatic	5/98 (5%)	5/48 (10%)	0/40 (0%)	0/10 (0%)
Overall	222/1414 (16%)	128/773 (17%)	73/503 (15%)	21/138 (15%)

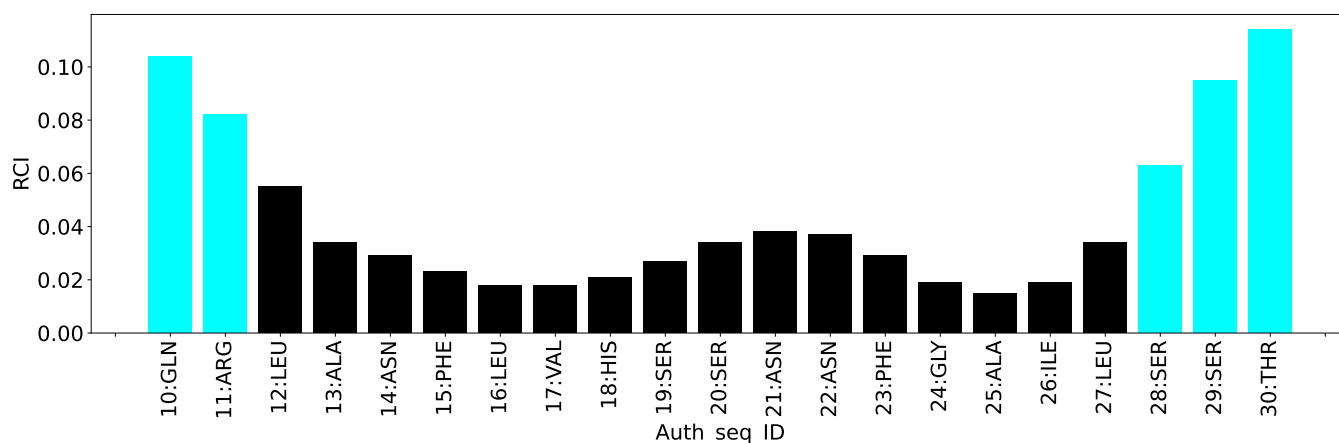
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 Bookkeeping [i](#)

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	424
Number of shifts mapped to atoms	424
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	41	-0.24 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	40	0.45 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	38	-0.13 ± 0.29	None needed (< 0.5 ppm)

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 32%, i.e. 424 atoms were assigned a chemical shift out of a possible 1345. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	158/506 (31%)	79/203 (39%)	41/206 (20%)	38/97 (39%)
Sidechain	260/741 (35%)	178/485 (37%)	82/235 (35%)	0/21 (0%)
Aromatic	6/98 (6%)	6/48 (12%)	0/40 (0%)	0/10 (0%)
Overall	424/1345 (32%)	263/736 (36%)	123/481 (26%)	38/128 (30%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 30%, i.e. 424 atoms were assigned a chemical shift out of a possible 1414. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	158/538 (29%)	79/217 (36%)	41/218 (19%)	38/103 (37%)
Sidechain	260/778 (33%)	178/508 (35%)	82/245 (33%)	0/25 (0%)
Aromatic	6/98 (6%)	6/48 (12%)	0/40 (0%)	0/10 (0%)
Overall	424/1414 (30%)	263/773 (34%)	123/503 (24%)	38/138 (28%)

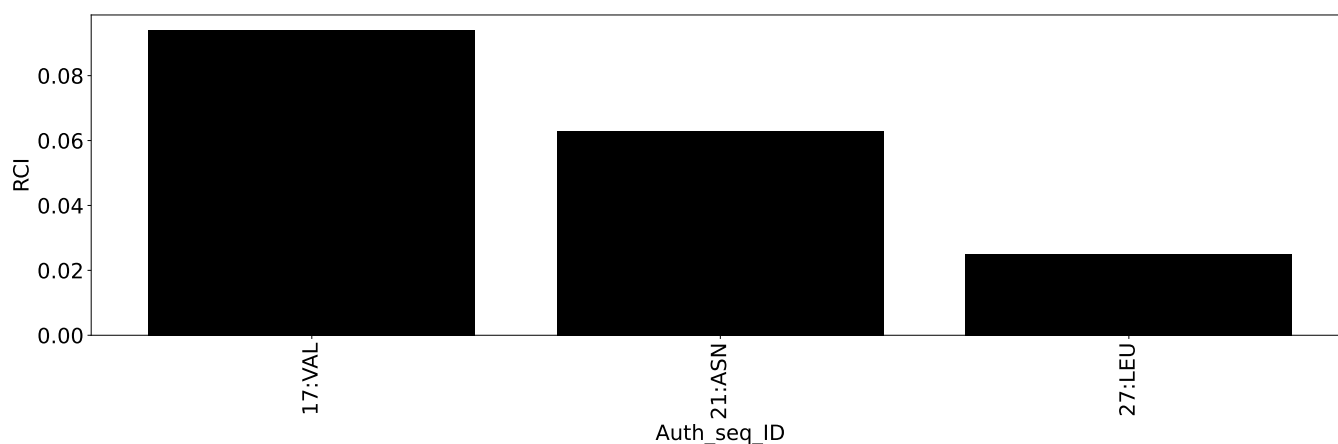
7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

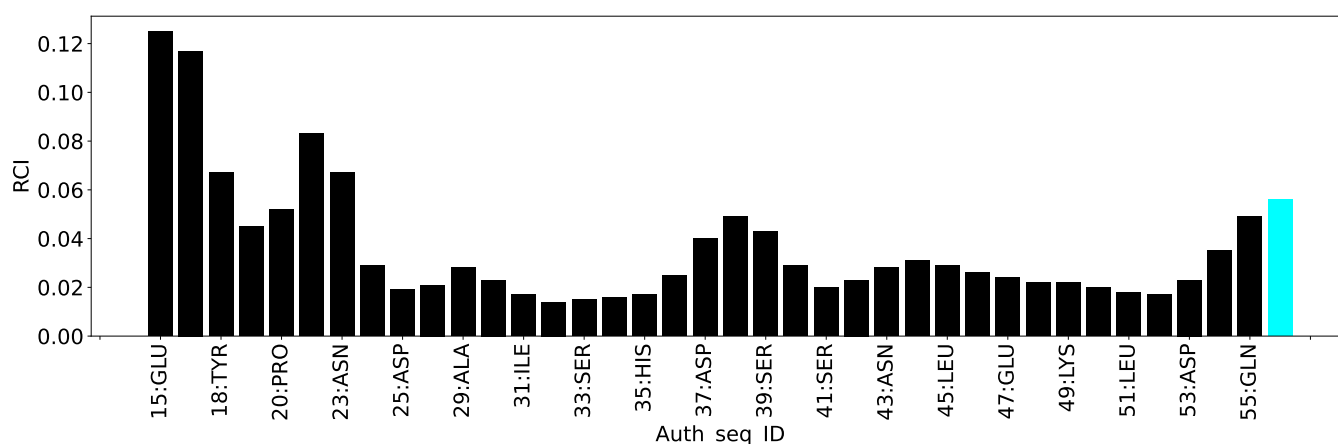
7.2.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



7.3 Chemical shift list 3

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_3*

7.3.1 Bookkeeping [i](#)

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	428
Number of shifts mapped to atoms	428
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.3.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	42	-0.26 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	40	0.45 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	39	-0.30 ± 0.29	None needed (< 0.5 ppm)

7.3.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 32%, i.e. 424 atoms were assigned a chemical shift out of a possible 1345. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	158/506 (31%)	79/203 (39%)	41/206 (20%)	38/97 (39%)
Sidechain	260/741 (35%)	178/485 (37%)	82/235 (35%)	0/21 (0%)
Aromatic	6/98 (6%)	6/48 (12%)	0/40 (0%)	0/10 (0%)
Overall	424/1345 (32%)	263/736 (36%)	123/481 (26%)	38/128 (30%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 30%, i.e. 428 atoms were assigned a chemical shift out of a possible 1414. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	162/538 (30%)	81/217 (37%)	42/218 (19%)	39/103 (38%)

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	Total	¹H	¹³C	¹⁵N
Sidechain	260/778 (33%)	178/508 (35%)	82/245 (33%)	0/25 (0%)
Aromatic	6/98 (6%)	6/48 (12%)	0/40 (0%)	0/10 (0%)
Overall	428/1414 (30%)	265/773 (34%)	124/503 (25%)	39/138 (28%)

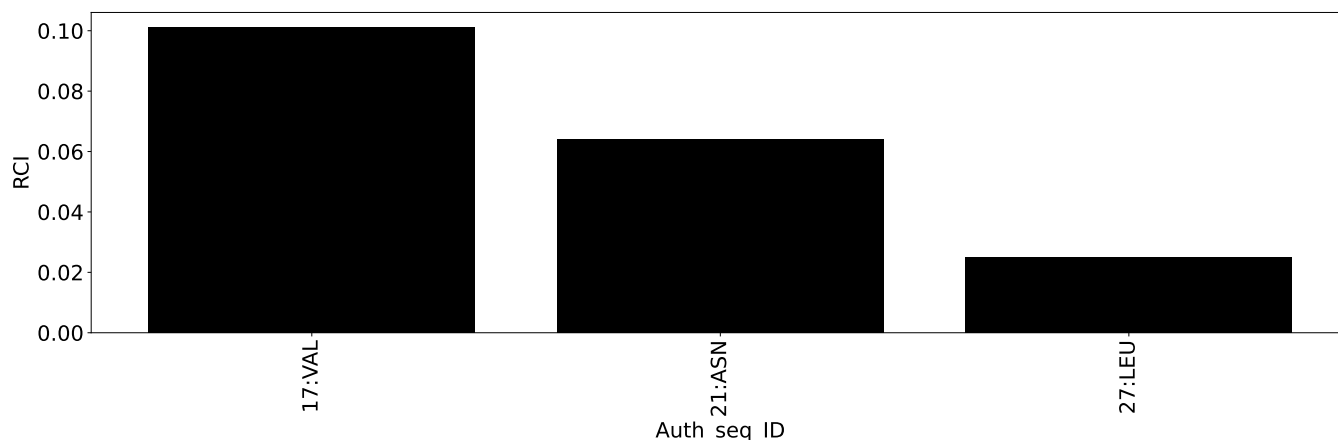
7.3.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

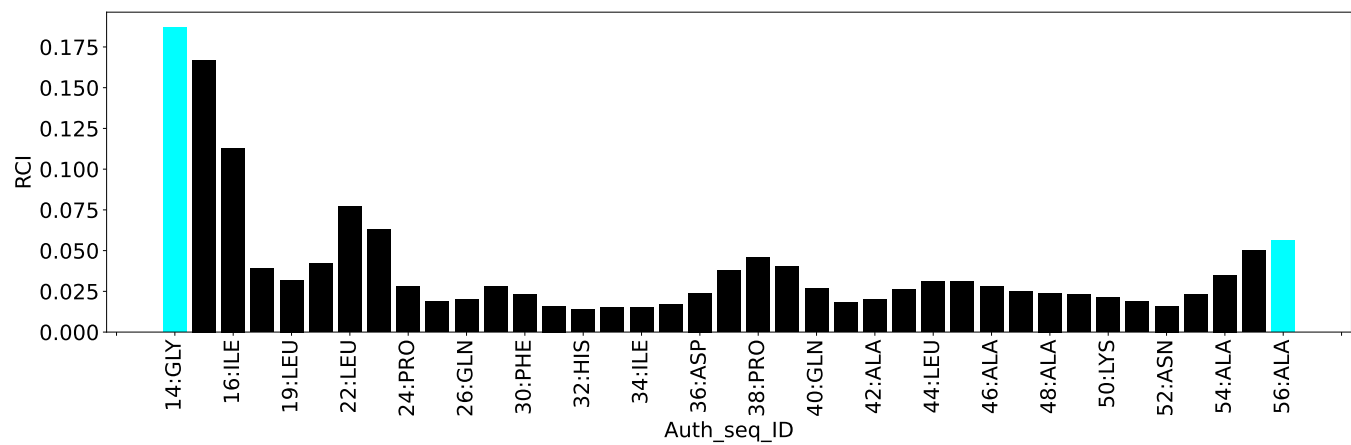
7.3.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



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	1939
Intra-residue ($ i-j =0$)	930
Sequential ($ i-j =1$)	480
Medium range ($ i-j >1$ and $ i-j <5$)	221
Long range ($ i-j \geq 5$)	163
Inter-chain	145
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	186
Number of unmapped restraints	0
Number of restraints per residue	12.1
Number of long range restraints per residue ¹	0.9

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	33.5	0.2
0.2-0.5 (Medium)	48.5	0.5
>0.5 (Large)	81.9	3.36

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)	11.2	9.57
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

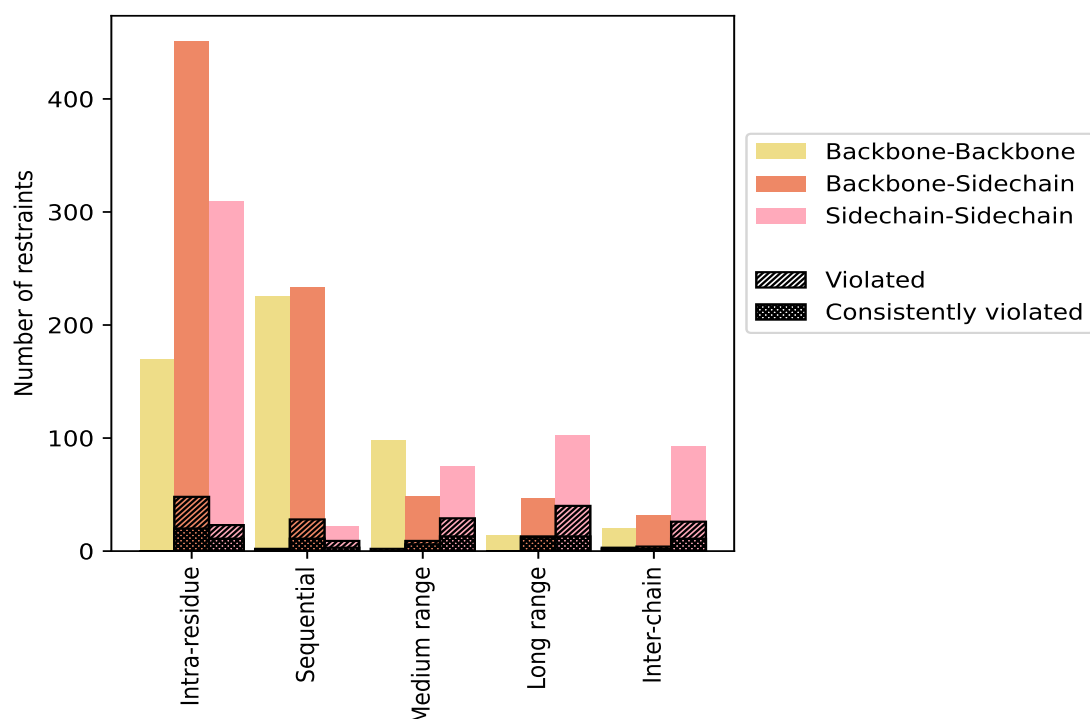
9.1 Summary of distance violations ⓘ

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)	930	48.0	71	7.6	3.7	31	3.3	1.6
Backbone-Backbone	170	8.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	451	23.3	48	10.6	2.5	20	4.4	1.0
Sidechain-Sidechain	309	15.9	23	7.4	1.2	11	3.6	0.6
Sequential (i-j =1)	480	24.8	39	8.1	2.0	15	3.1	0.8
Backbone-Backbone	225	11.6	2	0.9	0.1	1	0.4	0.1
Backbone-Sidechain	233	12.0	28	12.0	1.4	11	4.7	0.6
Sidechain-Sidechain	22	1.1	9	40.9	0.5	3	13.6	0.2
Medium range (i-j >1 & i-j <5)	221	11.4	40	18.1	2.1	19	8.6	1.0
Backbone-Backbone	98	5.1	2	2.0	0.1	0	0.0	0.0
Backbone-Sidechain	48	2.5	9	18.8	0.5	6	12.5	0.3
Sidechain-Sidechain	75	3.9	29	38.7	1.5	13	17.3	0.7
Long range (i-j ≥5)	163	8.4	53	32.5	2.7	25	15.3	1.3
Backbone-Backbone	14	0.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	47	2.4	13	27.7	0.7	12	25.5	0.6
Sidechain-Sidechain	102	5.3	40	39.2	2.1	13	12.7	0.7
Inter-chain	145	7.5	33	22.8	1.7	15	10.3	0.8
Backbone-Backbone	20	1.0	3	15.0	0.2	2	10.0	0.1
Backbone-Sidechain	32	1.7	4	12.5	0.2	2	6.2	0.1
Sidechain-Sidechain	93	4.8	26	28.0	1.3	11	11.8	0.6
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	1939	100.0	236	12.2	12.2	105	5.4	5.4
Backbone-Backbone	527	27.2	7	1.3	0.4	3	0.6	0.2
Backbone-Sidechain	811	41.8	102	12.6	5.3	51	6.3	2.6
Sidechain-Sidechain	601	31.0	127	21.1	6.5	51	8.5	2.6

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

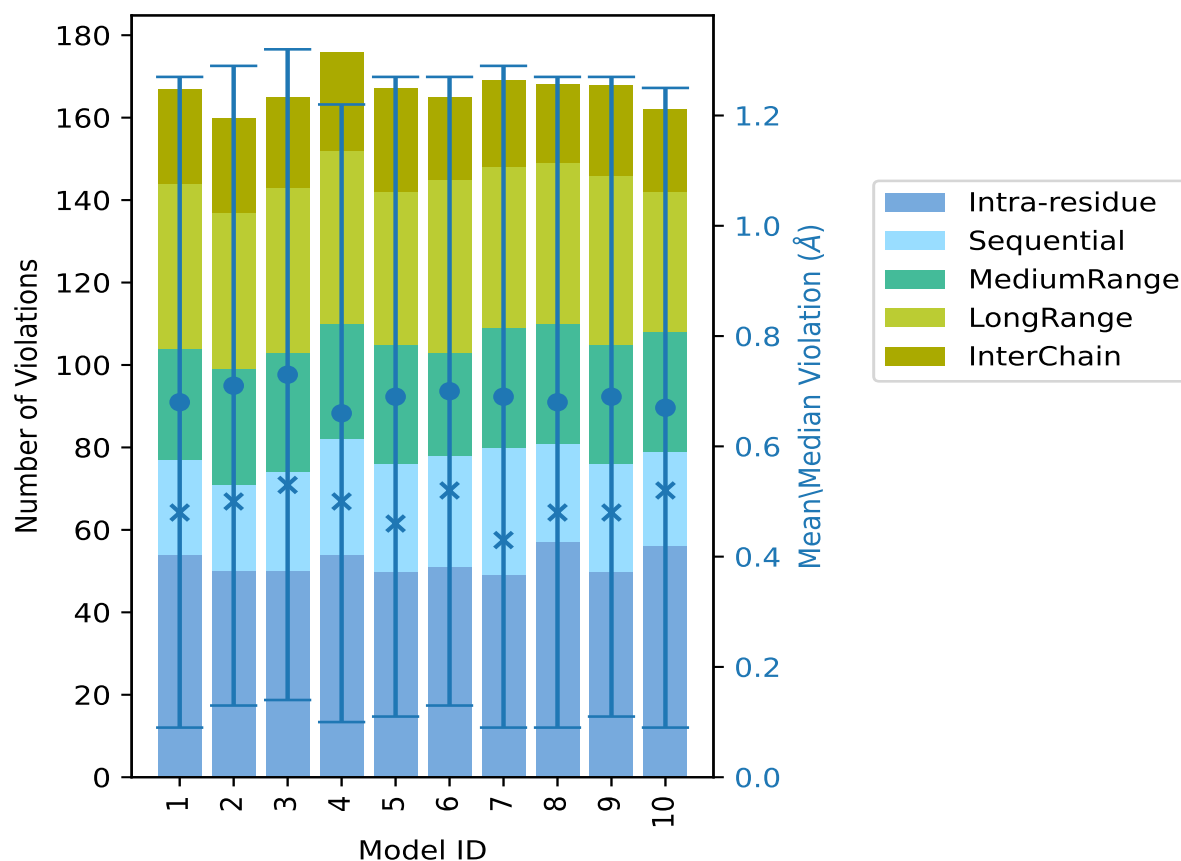
9.2 Distance violation statistics for each model [i](#)

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	54	23	27	40	23	167	0.68	3.22	0.59	0.48
2	50	21	28	38	23	160	0.71	2.64	0.58	0.5
3	50	24	29	40	22	165	0.73	2.67	0.59	0.53
4	54	28	28	42	24	176	0.66	2.84	0.56	0.5
5	50	26	29	37	25	167	0.69	2.87	0.58	0.46
6	51	27	25	42	20	165	0.7	2.75	0.57	0.52
7	49	31	29	39	21	169	0.69	2.87	0.6	0.43
8	57	24	29	39	19	168	0.68	3.36	0.59	0.48
9	50	26	29	41	22	168	0.69	2.65	0.58	0.48
10	56	23	29	34	20	162	0.67	3.24	0.58	0.52

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, 1703(IR:859, SQ:441, MR:181, LR:110, IC:112) 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	6	6	4	5	26	1	10.0
4	2	1	3	3	13	2	20.0
6	4	4	2	1	17	3	30.0

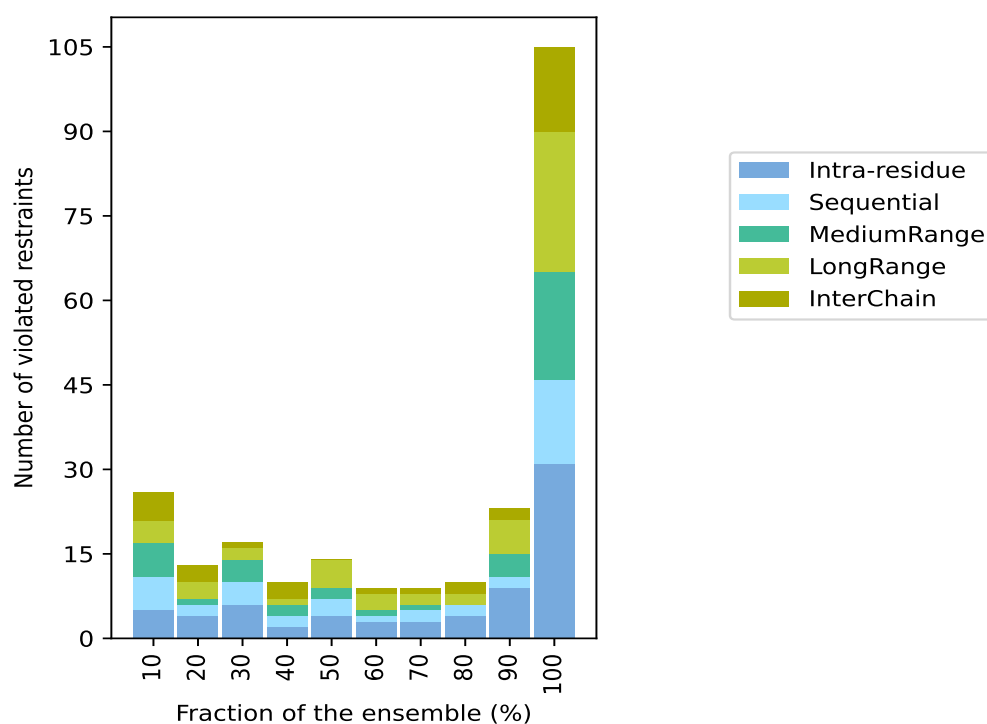
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
2	2	2	1	3	10	4	40.0
4	3	2	5	0	14	5	50.0
3	1	1	3	1	9	6	60.0
3	2	1	2	1	9	7	70.0
4	2	0	2	2	10	8	80.0
9	2	4	6	2	23	9	90.0
31	15	19	25	15	105	10	100.0

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](#)

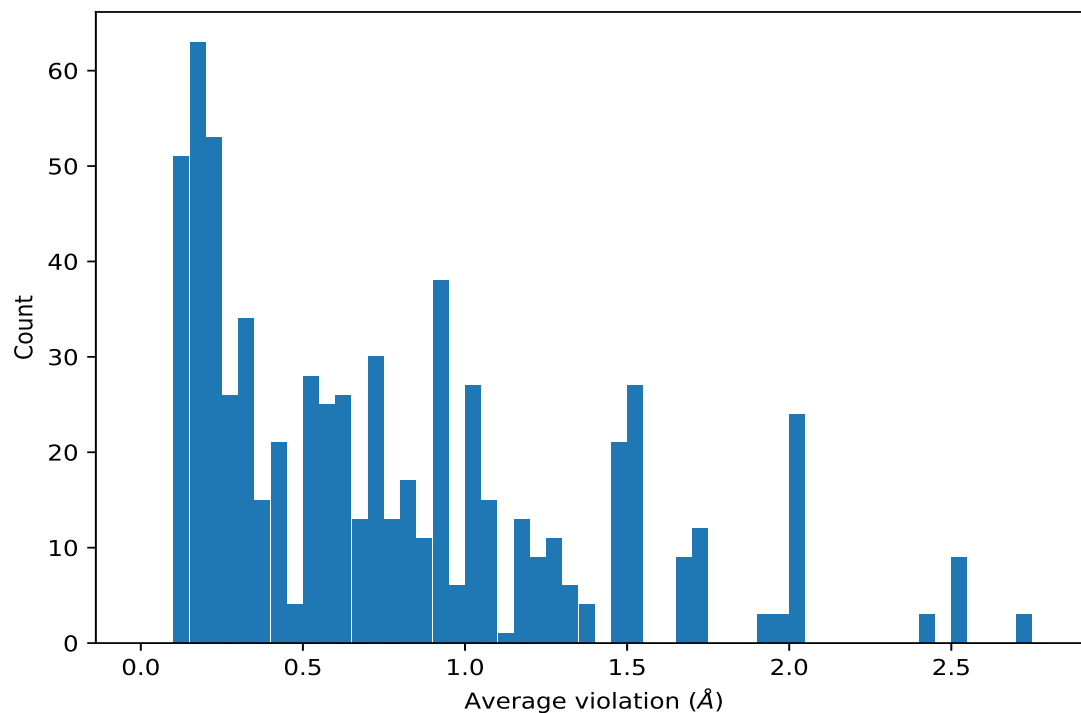


9.4 Most violated distance restraints in the ensemble [i](#)

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)
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD11	10	2.73	0.15	2.79
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD12	10	2.73	0.15	2.79
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD13	10	2.73	0.15	2.79
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD21	10	2.52	0.34	2.64
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD22	10	2.52	0.34	2.64
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD23	10	2.52	0.34	2.64
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD21	10	2.52	0.34	2.64
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD22	10	2.52	0.34	2.64
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD23	10	2.52	0.34	2.64
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD21	10	2.52	0.34	2.64
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD22	10	2.52	0.34	2.64
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD23	10	2.52	0.34	2.64
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD11	10	2.43	0.07	2.46
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD12	10	2.43	0.07	2.46
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD13	10	2.43	0.07	2.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG11	10	2.03	0.82	1.62
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG12	10	2.03	0.82	1.62
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG13	10	2.03	0.82	1.62
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG11	10	2.03	0.82	1.62
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG12	10	2.03	0.82	1.62
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG13	10	2.03	0.82	1.62
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG11	10	2.03	0.82	1.62
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG12	10	2.03	0.82	1.62
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG13	10	2.03	0.82	1.62
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	10	2.03	0.05	2.01
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	10	2.03	0.05	2.01
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	10	2.03	0.05	2.01
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	10	2.03	0.05	2.01
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	10	2.03	0.05	2.01
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	10	2.03	0.05	2.01
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	10	2.03	0.05	2.01
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	10	2.03	0.05	2.01
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	10	2.03	0.05	2.01
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG2	10	2.02	0.17	2.04
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG3	10	2.02	0.17	2.04
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG2	10	2.02	0.17	2.04
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG3	10	2.02	0.17	2.04
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG2	10	2.02	0.17	2.04
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG3	10	2.02	0.17	2.04
(1,399)	1:27:A:LEU:HD11	1:12:A:LEU:HA	10	1.98	0.12	1.94
(1,399)	1:27:A:LEU:HD12	1:12:A:LEU:HA	10	1.98	0.12	1.94
(1,399)	1:27:A:LEU:HD13	1:12:A:LEU:HA	10	1.98	0.12	1.94
(1,1436)	2:19:B:LEU:HD21	2:52:B:ASN:H	10	1.94	0.45	2.13
(1,1436)	2:19:B:LEU:HD22	2:52:B:ASN:H	10	1.94	0.45	2.13
(1,1436)	2:19:B:LEU:HD23	2:52:B:ASN:H	10	1.94	0.45	2.13
(1,1930)	2:19:C:LEU:HD11	2:48:C:ALA:HA	10	1.73	0.44	1.88
(1,1930)	2:19:C:LEU:HD12	2:48:C:ALA:HA	10	1.73	0.44	1.88
(1,1930)	2:19:C:LEU:HD13	2:48:C:ALA:HA	10	1.73	0.44	1.88
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD11	10	1.7	0.31	1.64
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD12	10	1.7	0.31	1.64
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD13	10	1.7	0.31	1.64
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD11	10	1.7	0.31	1.64
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD12	10	1.7	0.31	1.64
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD13	10	1.7	0.31	1.64
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD11	10	1.7	0.31	1.64
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD12	10	1.7	0.31	1.64
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD13	10	1.7	0.31	1.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	10	1.68	0.07	1.68
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	10	1.68	0.07	1.68
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	10	1.68	0.07	1.68
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	10	1.68	0.07	1.68
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	10	1.68	0.07	1.68
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	10	1.68	0.07	1.68
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	10	1.68	0.07	1.68
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	10	1.68	0.07	1.68
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	10	1.68	0.07	1.68
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD11	10	1.54	0.11	1.54
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD12	10	1.54	0.11	1.54
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD13	10	1.54	0.11	1.54
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	10	1.53	0.1	1.52
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	10	1.53	0.1	1.52
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	10	1.53	0.1	1.52
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	10	1.53	0.1	1.52
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	10	1.53	0.1	1.52
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	10	1.53	0.1	1.52
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD11	10	1.52	0.19	1.54
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD12	10	1.52	0.19	1.54
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD13	10	1.52	0.19	1.54
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD11	10	1.52	0.19	1.54
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD12	10	1.52	0.19	1.54
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD13	10	1.52	0.19	1.54
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	10	1.51	0.05	1.49
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	10	1.51	0.05	1.49
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	10	1.51	0.05	1.49
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	10	1.51	0.05	1.49
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	10	1.51	0.05	1.49
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	10	1.51	0.05	1.49
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	10	1.51	0.05	1.49
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	10	1.51	0.05	1.49
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	10	1.51	0.05	1.49
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD11	10	1.5	0.11	1.52
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD12	10	1.5	0.11	1.52
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD13	10	1.5	0.11	1.52
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD11	10	1.48	0.18	1.46
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD12	10	1.48	0.18	1.46
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD13	10	1.48	0.18	1.46
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD11	10	1.47	0.18	1.54
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD12	10	1.47	0.18	1.54
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD13	10	1.47	0.18	1.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD11	10	1.47	0.18	1.54
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD12	10	1.47	0.18	1.54
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD13	10	1.47	0.18	1.54
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD11	10	1.47	0.18	1.54
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD12	10	1.47	0.18	1.54
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD13	10	1.47	0.18	1.54
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD11	10	1.45	0.37	1.6
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD12	10	1.45	0.37	1.6
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD13	10	1.45	0.37	1.6
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD11	10	1.45	0.37	1.6
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD12	10	1.45	0.37	1.6
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD13	10	1.45	0.37	1.6
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD11	10	1.45	0.37	1.6
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD12	10	1.45	0.37	1.6
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD13	10	1.45	0.37	1.6
(1,104)	1:27:A:LEU:HD11	1:12:A:LEU:H	10	1.39	0.17	1.34
(1,104)	1:27:A:LEU:HD12	1:12:A:LEU:H	10	1.39	0.17	1.34
(1,104)	1:27:A:LEU:HD13	1:12:A:LEU:H	10	1.39	0.17	1.34
(1,1813)	1:26:A:ILE:HG13	2:14:C:GLY:HA3	10	1.36	0.11	1.34
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD11	10	1.3	0.06	1.3
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD12	10	1.3	0.06	1.3
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD13	10	1.3	0.06	1.3
(1,269)	1:27:A:LEU:HD11	1:13:A:ALA:HA	10	1.3	0.11	1.32
(1,269)	1:27:A:LEU:HD12	1:13:A:ALA:HA	10	1.3	0.11	1.32
(1,269)	1:27:A:LEU:HD13	1:13:A:ALA:HA	10	1.3	0.11	1.32
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD21	10	1.28	0.4	1.12
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD22	10	1.28	0.4	1.12
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD23	10	1.28	0.4	1.12
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD21	10	1.28	0.4	1.12
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD22	10	1.28	0.4	1.12
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD23	10	1.28	0.4	1.12
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD21	10	1.28	0.4	1.12
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD22	10	1.28	0.4	1.12
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD23	10	1.28	0.4	1.12
(1,1843)	2:19:B:LEU:HD21	2:22:B:LEU:HG	10	1.23	0.11	1.21
(1,1843)	2:19:B:LEU:HD22	2:22:B:LEU:HG	10	1.23	0.11	1.21
(1,1843)	2:19:B:LEU:HD23	2:22:B:LEU:HG	10	1.23	0.11	1.21
(1,1545)	1:27:A:LEU:HD21	2:15:C:GLU:HG2	10	1.23	0.25	1.27
(1,1545)	1:27:A:LEU:HD22	2:15:C:GLU:HG2	10	1.23	0.25	1.27
(1,1545)	1:27:A:LEU:HD23	2:15:C:GLU:HG2	10	1.23	0.25	1.27
(1,1405)	2:17:B:VAL:HG11	2:45:B:LEU:HG	10	1.19	0.2	1.23
(1,1405)	2:17:B:VAL:HG12	2:45:B:LEU:HG	10	1.19	0.2	1.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1405)	2:17:B:VAL:HG13	2:45:B:LEU:HG	10	1.19	0.2	1.23
(1,1844)	2:19:C:LEU:HD11	2:22:C:LEU:HG	10	1.19	0.25	1.25
(1,1844)	2:19:C:LEU:HD12	2:22:C:LEU:HG	10	1.19	0.25	1.25
(1,1844)	2:19:C:LEU:HD13	2:22:C:LEU:HG	10	1.19	0.25	1.25
(1,1862)	2:27:B:LEU:HD21	2:24:B:PRO:HA	10	1.18	0.22	1.23
(1,1862)	2:27:B:LEU:HD22	2:24:B:PRO:HA	10	1.18	0.22	1.23
(1,1862)	2:27:B:LEU:HD23	2:24:B:PRO:HA	10	1.18	0.22	1.23
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD11	10	1.16	0.21	1.16
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD12	10	1.16	0.21	1.16
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD13	10	1.16	0.21	1.16
(1,1873)	2:23:B:ASN:HD22	2:26:B:GLN:HG2	10	1.15	0.57	1.17
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB2	10	1.08	0.43	1.29
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB3	10	1.08	0.43	1.29
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	10	1.07	0.1	1.06
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	10	1.07	0.1	1.06
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	10	1.07	0.1	1.06
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	10	1.07	0.1	1.06
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	10	1.07	0.1	1.06
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	10	1.07	0.1	1.06
(1,813)	2:34:C:ILE:HG23	2:37:C:ASP:H	10	1.05	0.14	1.11
(1,813)	2:34:C:ILE:HG21	2:37:C:ASP:H	10	1.05	0.14	1.11
(1,813)	2:34:C:ILE:HG22	2:37:C:ASP:H	10	1.05	0.14	1.11
(1,1432)	1:24:A:GLY:HA3	2:19:C:LEU:HB2	10	1.05	0.38	1.15
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	10	1.03	0.07	1.04
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	10	1.03	0.07	1.04
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	10	1.03	0.07	1.04
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	10	1.03	0.07	1.04
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	10	1.03	0.07	1.04
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	10	1.03	0.07	1.04
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	10	1.03	0.07	1.04
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	10	1.03	0.07	1.04
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	10	1.03	0.07	1.04
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	10	1.01	0.38	1.12
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	10	1.01	0.38	1.12
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	10	1.01	0.38	1.12
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	10	1.01	0.38	1.12
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	10	1.01	0.38	1.12
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	10	1.01	0.38	1.12
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	10	1.01	0.38	1.12
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	10	1.01	0.38	1.12
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	10	1.01	0.38	1.12
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD11	10	0.97	0.19	1.05

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD12	10	0.97	0.19	1.05
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD13	10	0.97	0.19	1.05
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD21	10	0.93	0.15	0.95
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD22	10	0.93	0.15	0.95
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD23	10	0.93	0.15	0.95
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD11	10	0.92	0.02	0.92
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD12	10	0.92	0.02	0.92
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD13	10	0.92	0.02	0.92
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD21	10	0.92	0.18	0.94
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD22	10	0.92	0.18	0.94
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD23	10	0.92	0.18	0.94
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD21	10	0.92	0.18	0.94
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD22	10	0.92	0.18	0.94
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD23	10	0.92	0.18	0.94
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD21	10	0.92	0.18	0.94
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD22	10	0.92	0.18	0.94
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD23	10	0.92	0.18	0.94
(1,1931)	2:19:B:LEU:HD21	2:48:B:ALA:HA	10	0.91	0.18	0.93
(1,1931)	2:19:B:LEU:HD22	2:48:B:ALA:HA	10	0.91	0.18	0.93
(1,1931)	2:19:B:LEU:HD23	2:48:B:ALA:HA	10	0.91	0.18	0.93
(1,1605)	2:19:B:LEU:HD21	2:52:B:ASN:HB3	10	0.9	0.35	0.98
(1,1605)	2:19:B:LEU:HD22	2:52:B:ASN:HB3	10	0.9	0.35	0.98
(1,1605)	2:19:B:LEU:HD23	2:52:B:ASN:HB3	10	0.9	0.35	0.98
(1,953)	2:31:B:ILE:HG21	2:24:C:PRO:HB2	10	0.9	0.23	0.98
(1,953)	2:31:B:ILE:HG22	2:24:C:PRO:HB2	10	0.9	0.23	0.98
(1,953)	2:31:B:ILE:HG23	2:24:C:PRO:HB2	10	0.9	0.23	0.98
(1,372)	1:11:A:ARG:HG2	1:12:A:LEU:H	10	0.9	0.26	1.02
(1,1790)	2:56:C:ALA:HB3	2:53:C:ASP:HB2	10	0.88	0.18	0.92
(1,1790)	2:56:C:ALA:HB2	2:53:C:ASP:HB3	10	0.88	0.18	0.92
(1,1790)	2:56:C:ALA:HB1	2:53:C:ASP:HB2	10	0.88	0.18	0.92
(1,1790)	2:56:C:ALA:HB2	2:53:C:ASP:HB2	10	0.88	0.18	0.92
(1,1149)	2:35:B:HIS:HB3	2:34:B:ILE:HB	10	0.88	0.38	1.02
(1,810)	2:37:B:ASP:H	2:44:B:LEU:HD22	10	0.81	0.08	0.8
(1,810)	2:37:B:ASP:H	2:34:B:ILE:HG22	10	0.81	0.08	0.8
(1,810)	2:37:B:ASP:H	2:44:B:LEU:HD23	10	0.81	0.08	0.8
(1,810)	2:37:B:ASP:H	2:34:B:ILE:HG23	10	0.81	0.08	0.8
(1,810)	2:37:B:ASP:H	2:44:B:LEU:HD21	10	0.81	0.08	0.8
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD11	10	0.81	0.02	0.82
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD12	10	0.81	0.02	0.82
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD13	10	0.81	0.02	0.82
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD11	10	0.8	0.11	0.8
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD12	10	0.8	0.11	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD13	10	0.8	0.11	0.8
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	10	0.78	0.03	0.78
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	10	0.78	0.03	0.78
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	10	0.78	0.03	0.78
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	10	0.78	0.03	0.78
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	10	0.78	0.03	0.78
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	10	0.78	0.03	0.78
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	10	0.78	0.03	0.78
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	10	0.78	0.03	0.78
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	10	0.78	0.03	0.78
(1,1138)	2:24:B:PRO:HA	2:27:B:LEU:HB3	10	0.77	0.15	0.74
(1,1552)	2:17:B:VAL:HG21	2:15:B:GLU:HG2	10	0.76	0.23	0.78
(1,1552)	2:17:B:VAL:HG22	2:15:B:GLU:HG2	10	0.76	0.23	0.78
(1,1552)	2:17:B:VAL:HG23	2:15:B:GLU:HG2	10	0.76	0.23	0.78
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD11	10	0.74	0.06	0.77
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD12	10	0.74	0.06	0.77
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD13	10	0.74	0.06	0.77
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG21	10	0.72	0.03	0.74
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG22	10	0.72	0.03	0.74
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG23	10	0.72	0.03	0.74
(1,991)	2:16:C:ILE:HG22	1:26:A:ILE:HG13	10	0.7	0.13	0.7
(1,991)	2:16:C:ILE:HG23	1:26:A:ILE:HG13	10	0.7	0.13	0.7
(1,991)	2:16:C:ILE:HG21	1:26:A:ILE:HG13	10	0.7	0.13	0.7
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	10	0.65	0.57	0.45
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	10	0.65	0.57	0.45
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	10	0.65	0.57	0.45
(1,1836)	2:19:B:LEU:HD21	2:22:B:LEU:HA	10	0.64	0.16	0.6
(1,1836)	2:19:B:LEU:HD22	2:22:B:LEU:HA	10	0.64	0.16	0.6
(1,1836)	2:19:B:LEU:HD23	2:22:B:LEU:HA	10	0.64	0.16	0.6
(1,1604)	2:19:C:LEU:HD11	2:52:C:ASN:HB3	10	0.6	0.11	0.64
(1,1604)	2:19:C:LEU:HD12	2:52:C:ASN:HB3	10	0.6	0.11	0.64
(1,1604)	2:19:C:LEU:HD13	2:52:C:ASN:HB3	10	0.6	0.11	0.64
(1,1791)	2:54:B:ALA:HB2	2:53:B:ASP:HB3	10	0.6	0.07	0.58
(1,1791)	2:54:B:ALA:HB1	2:53:B:ASP:HB3	10	0.6	0.07	0.58
(1,1791)	2:54:B:ALA:HB3	2:53:B:ASP:HB3	10	0.6	0.07	0.58
(1,14)	1:17:A:VAL:H	1:16:A:LEU:HD21	10	0.59	0.02	0.6
(1,14)	1:17:A:VAL:H	1:16:A:LEU:HD22	10	0.59	0.02	0.6
(1,14)	1:17:A:VAL:H	1:16:A:LEU:HD23	10	0.59	0.02	0.6
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD11	10	0.58	0.46	0.4
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD12	10	0.58	0.46	0.4
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD13	10	0.58	0.46	0.4
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD11	10	0.57	0.36	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD12	10	0.57	0.36	0.42
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD13	10	0.57	0.36	0.42
(1,1204)	2:31:C:ILE:HD12	2:27:B:LEU:HG	10	0.56	0.03	0.56
(1,1204)	2:31:C:ILE:HD11	2:27:B:LEU:HG	10	0.56	0.03	0.56
(1,1204)	2:31:C:ILE:HD13	2:27:B:LEU:HG	10	0.56	0.03	0.56
(1,1713)	2:44:C:LEU:HD11	2:40:C:GLN:HG2	10	0.55	0.42	0.32
(1,1713)	2:44:C:LEU:HD12	2:40:C:GLN:HG2	10	0.55	0.42	0.32
(1,1713)	2:44:C:LEU:HD13	2:40:C:GLN:HG2	10	0.55	0.42	0.32
(1,962)	2:44:C:LEU:HD11	2:34:C:ILE:HB	10	0.53	0.22	0.61
(1,962)	2:44:C:LEU:HD12	2:34:C:ILE:HB	10	0.53	0.22	0.61
(1,962)	2:44:C:LEU:HD13	2:34:C:ILE:HB	10	0.53	0.22	0.61
(1,1829)	2:21:C:ASN:H	2:20:C:PRO:HG3	10	0.52	0.12	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD11	10	0.52	0.01	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD12	10	0.52	0.01	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD13	10	0.52	0.01	0.51
(1,1083)	2:34:C:ILE:HG21	2:34:C:ILE:HG12	10	0.5	0.0	0.5
(1,1083)	2:34:C:ILE:HG22	2:34:C:ILE:HG12	10	0.5	0.0	0.5
(1,1083)	2:34:C:ILE:HG23	2:34:C:ILE:HG12	10	0.5	0.0	0.5
(1,175)	1:27:A:LEU:HD11	1:27:A:LEU:HA	10	0.48	0.01	0.48
(1,175)	1:27:A:LEU:HD12	1:27:A:LEU:HA	10	0.48	0.01	0.48
(1,175)	1:27:A:LEU:HD13	1:27:A:LEU:HA	10	0.48	0.01	0.48
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD11	10	0.44	0.08	0.4
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD12	10	0.44	0.08	0.4
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD13	10	0.44	0.08	0.4
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	10	0.42	0.03	0.43
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	10	0.42	0.03	0.43
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	10	0.42	0.03	0.43
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	10	0.42	0.03	0.43
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	10	0.42	0.03	0.43
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	10	0.42	0.03	0.43
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	10	0.42	0.03	0.43
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	10	0.42	0.03	0.43
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	10	0.42	0.03	0.43
(1,1658)	2:35:B:HIS:HB2	2:36:B:ASP:H	10	0.41	0.13	0.46
(1,350)	1:10:A:GLN:HG2	1:10:A:GLN:HE22	10	0.4	0.04	0.4
(1,350)	1:10:A:GLN:HG3	1:10:A:GLN:HE22	10	0.4	0.04	0.4
(1,1777)	2:47:C:GLU:HG2	2:47:C:GLU:HB3	10	0.4	0.02	0.4
(1,1777)	2:47:B:GLU:HG3	2:47:B:GLU:HB2	10	0.4	0.02	0.4
(1,1393)	2:29:B:ALA:H	2:29:B:ALA:HB3	10	0.38	0.02	0.38
(1,1393)	2:29:B:ALA:H	2:29:B:ALA:HB1	10	0.38	0.02	0.38
(1,1393)	2:29:C:ALA:H	2:29:C:ALA:HB1	10	0.38	0.02	0.38
(1,1393)	2:29:C:ALA:H	2:29:C:ALA:HB3	10	0.38	0.02	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1196)	2:27:B:LEU:H	2:27:B:LEU:HB3	10	0.37	0.01	0.38
(1,1591)	2:39:B:SER:H	2:38:B:PRO:HG3	10	0.36	0.1	0.36
(1,46)	2:17:C:VAL:H	1:27:A:LEU:H	10	0.35	0.05	0.34
(1,46)	1:27:A:LEU:H	1:28:A:SER:H	10	0.35	0.05	0.34
(1,1534)	2:54:B:ALA:HA	2:54:B:ALA:HB3	10	0.34	0.02	0.34
(1,1534)	2:54:B:ALA:HA	2:54:B:ALA:HB2	10	0.34	0.02	0.34
(1,1534)	2:54:C:ALA:HA	2:54:C:ALA:HB2	10	0.34	0.02	0.34
(1,1534)	2:54:C:ALA:HA	2:54:C:ALA:HB1	10	0.34	0.02	0.34
(1,1534)	2:54:C:ALA:HA	2:54:C:ALA:HB3	10	0.34	0.02	0.34
(1,1595)	2:38:B:PRO:HB2	2:38:B:PRO:HD2	10	0.33	0.01	0.34
(1,1532)	2:54:B:ALA:HA	2:54:B:ALA:HB3	10	0.32	0.02	0.32
(1,1532)	2:54:B:ALA:HA	2:54:B:ALA:HB2	10	0.32	0.02	0.32
(1,1532)	2:54:C:ALA:HA	2:54:C:ALA:HB2	10	0.32	0.02	0.32
(1,1532)	2:54:C:ALA:HA	2:54:C:ALA:HB1	10	0.32	0.02	0.32
(1,1532)	2:54:C:ALA:HA	2:54:C:ALA:HB3	10	0.32	0.02	0.32
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD11	10	0.32	0.05	0.32
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD12	10	0.32	0.05	0.32
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD13	10	0.32	0.05	0.32
(1,1523)	2:46:B:ALA:HB2	2:46:B:ALA:HA	10	0.32	0.01	0.32
(1,1523)	2:46:B:ALA:HB1	2:46:B:ALA:HA	10	0.32	0.01	0.32
(1,1523)	2:46:B:ALA:HB3	2:46:B:ALA:HA	10	0.32	0.01	0.32
(1,1523)	2:46:C:ALA:HA	2:46:C:ALA:HB1	10	0.32	0.01	0.32
(1,1353)	2:22:B:LEU:HD22	2:22:B:LEU:HD12	10	0.31	0.03	0.31
(1,1353)	2:22:B:LEU:HD23	2:22:B:LEU:HD11	10	0.31	0.03	0.31
(1,1353)	2:22:B:LEU:HD23	2:22:B:LEU:HD13	10	0.31	0.03	0.31
(1,1353)	2:22:B:LEU:HD21	2:22:B:LEU:HD12	10	0.31	0.03	0.31
(1,1353)	2:22:B:LEU:HD22	2:22:B:LEU:HD13	10	0.31	0.03	0.31
(1,1613)	2:23:B:ASN:HB2	2:23:B:ASN:HD22	10	0.27	0.1	0.25
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG21	10	0.26	0.01	0.26
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG22	10	0.26	0.01	0.26
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG23	10	0.26	0.01	0.26
(1,1525)	2:55:B:GLN:H	2:54:B:ALA:HA	10	0.25	0.04	0.26
(1,1392)	2:29:C:ALA:HB3	2:29:C:ALA:HA	10	0.25	0.01	0.25
(1,1392)	2:29:B:ALA:HA	2:29:B:ALA:HB1	10	0.25	0.01	0.25
(1,1392)	2:29:C:ALA:HB2	2:29:C:ALA:HA	10	0.25	0.01	0.25
(1,1392)	2:29:C:ALA:HB1	2:29:C:ALA:HA	10	0.25	0.01	0.25
(1,1775)	2:47:B:GLU:HG2	2:47:B:GLU:HB2	10	0.24	0.02	0.23
(1,1775)	2:47:C:GLU:HG3	2:47:C:GLU:HB3	10	0.24	0.02	0.23
(1,1362)	2:51:B:LEU:H	2:51:B:LEU:HB3	10	0.23	0.01	0.24
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD11	10	0.23	0.02	0.23
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD12	10	0.23	0.02	0.23
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD13	10	0.23	0.02	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1524)	2:46:B:ALA:HB2	2:46:B:ALA:HA	10	0.23	0.01	0.23
(1,1524)	2:46:B:ALA:HB1	2:46:B:ALA:HA	10	0.23	0.01	0.23
(1,1524)	2:46:B:ALA:HB3	2:46:B:ALA:HA	10	0.23	0.01	0.23
(1,1524)	2:46:C:ALA:HA	2:46:C:ALA:HB1	10	0.23	0.01	0.23
(1,1211)	2:27:C:LEU:HD21	2:27:C:LEU:HG	10	0.23	0.01	0.22
(1,1211)	2:27:C:LEU:HD23	2:27:C:LEU:HG	10	0.23	0.01	0.22
(1,1211)	2:27:B:LEU:HD23	2:27:B:LEU:HG	10	0.23	0.01	0.22
(1,1211)	2:27:B:LEU:HD22	2:27:B:LEU:HG	10	0.23	0.01	0.22
(1,1211)	2:27:B:LEU:HD21	2:27:B:LEU:HG	10	0.23	0.01	0.22
(1,1776)	2:47:C:GLU:HG2	2:47:C:GLU:HB3	10	0.22	0.02	0.22
(1,1776)	2:47:B:GLU:HG3	2:47:B:GLU:HB2	10	0.22	0.02	0.22
(1,1206)	2:27:B:LEU:HB3	2:27:B:LEU:HG	10	0.22	0.0	0.22
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG21	10	0.21	0.02	0.21
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG22	10	0.21	0.02	0.21
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG23	10	0.21	0.02	0.21
(1,1216)	2:27:B:LEU:HD11	2:27:B:LEU:H	10	0.2	0.06	0.19
(1,1216)	2:27:B:LEU:HD12	2:27:B:LEU:H	10	0.2	0.06	0.19
(1,1216)	2:27:B:LEU:HD13	2:27:B:LEU:H	10	0.2	0.06	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG21	10	0.18	0.01	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG22	10	0.18	0.01	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG23	10	0.18	0.01	0.19
(1,1105)	2:31:C:ILE:HD11	2:31:C:ILE:HA	10	0.18	0.02	0.18
(1,1105)	2:31:C:ILE:HD12	2:31:C:ILE:HA	10	0.18	0.02	0.18
(1,1105)	2:31:C:ILE:HD13	2:31:C:ILE:HA	10	0.18	0.02	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG21	10	0.18	0.01	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG22	10	0.18	0.01	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG23	10	0.18	0.01	0.18
(1,1273)	2:27:C:LEU:H	2:27:C:LEU:HB2	10	0.16	0.02	0.16
(1,1391)	2:29:C:ALA:HB3	2:29:C:ALA:HA	10	0.15	0.01	0.15
(1,1391)	2:29:B:ALA:HA	2:29:B:ALA:HB1	10	0.15	0.01	0.15
(1,1391)	2:29:C:ALA:HB2	2:29:C:ALA:HA	10	0.15	0.01	0.15
(1,1391)	2:29:C:ALA:HB1	2:29:C:ALA:HA	10	0.15	0.01	0.15
(1,164)	2:17:C:VAL:H	1:25:A:ALA:HA	10	0.15	0.01	0.15
(1,1210)	2:27:B:LEU:HD21	2:27:B:LEU:HB3	10	0.14	0.03	0.14
(1,1210)	2:27:B:LEU:HD22	2:27:B:LEU:HB3	10	0.14	0.03	0.14
(1,1210)	2:27:B:LEU:HD23	2:27:B:LEU:HB3	10	0.14	0.03	0.14
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	9	1.23	0.13	1.27
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	9	1.23	0.13	1.27
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	9	1.23	0.13	1.27
(1,381)	1:27:A:LEU:HD11	1:11:A:ARG:HG2	9	1.09	0.46	1.29
(1,381)	1:27:A:LEU:HD12	1:11:A:ARG:HG2	9	1.09	0.46	1.29
(1,381)	1:27:A:LEU:HD13	1:11:A:ARG:HG2	9	1.09	0.46	1.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB1	9	1.03	0.15	1.09
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB2	9	1.03	0.15	1.09
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB3	9	1.03	0.15	1.09
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB1	9	1.03	0.15	1.09
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB2	9	1.03	0.15	1.09
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB3	9	1.03	0.15	1.09
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB1	9	1.03	0.15	1.09
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB2	9	1.03	0.15	1.09
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB3	9	1.03	0.15	1.09
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD11	9	0.91	0.11	0.91
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD12	9	0.91	0.11	0.91
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD13	9	0.91	0.11	0.91
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD11	9	0.91	0.11	0.91
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD12	9	0.91	0.11	0.91
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD13	9	0.91	0.11	0.91
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD11	9	0.91	0.11	0.91
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD12	9	0.91	0.11	0.91
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD13	9	0.91	0.11	0.91
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	9	0.89	0.13	0.94
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	9	0.89	0.13	0.94
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	9	0.89	0.13	0.94
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG21	9	0.83	0.32	0.67
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG22	9	0.83	0.32	0.67
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG23	9	0.83	0.32	0.67
(1,268)	1:27:A:LEU:HD21	2:45:C:LEU:HB3	9	0.68	0.45	0.32
(1,268)	1:27:A:LEU:HD22	2:45:C:LEU:HB3	9	0.68	0.45	0.32
(1,268)	1:27:A:LEU:HD23	2:45:C:LEU:HB3	9	0.68	0.45	0.32
(1,1895)	2:31:C:ILE:HG13	2:34:C:ILE:HD12	9	0.6	0.21	0.61
(1,1895)	2:31:C:ILE:HG13	2:34:C:ILE:HD11	9	0.6	0.21	0.61
(1,1895)	2:31:C:ILE:HG13	2:34:C:ILE:HD13	9	0.6	0.21	0.61
(1,1837)	2:19:C:LEU:HD11	2:22:C:LEU:HA	9	0.57	0.08	0.55
(1,1837)	2:19:C:LEU:HD12	2:22:C:LEU:HA	9	0.57	0.08	0.55
(1,1837)	2:19:C:LEU:HD13	2:22:C:LEU:HA	9	0.57	0.08	0.55
(1,307)	1:14:A:ASN:HB3	1:14:A:ASN:HD22	9	0.53	0.12	0.57
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD11	9	0.37	0.19	0.29
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD12	9	0.37	0.19	0.29
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD13	9	0.37	0.19	0.29
(1,1128)	2:31:C:ILE:HG21	2:27:B:LEU:HB3	9	0.28	0.07	0.28
(1,1128)	2:31:C:ILE:HG22	2:27:B:LEU:HB3	9	0.28	0.07	0.28
(1,1128)	2:31:C:ILE:HG23	2:27:B:LEU:HB3	9	0.28	0.07	0.28
(1,362)	1:11:A:ARG:HA	1:11:A:ARG:HG2	9	0.27	0.05	0.27
(1,253)	1:27:A:LEU:H	1:27:A:LEU:HD23	9	0.26	0.08	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,253)	1:27:A:LEU:H	1:27:A:LEU:HD21	9	0.26	0.08	0.23
(1,253)	1:27:A:LEU:H	1:27:A:LEU:HD22	9	0.26	0.08	0.23
(1,1615)	2:23:B:ASN:HB3	2:23:B:ASN:HD22	9	0.22	0.06	0.21
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD11	9	0.22	0.07	0.22
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD12	9	0.22	0.07	0.22
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD13	9	0.22	0.07	0.22
(1,1419)	2:25:C:ASP:H	2:24:C:PRO:HB3	9	0.16	0.02	0.16
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD11	9	0.15	0.02	0.15
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD12	9	0.15	0.02	0.15
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD13	9	0.15	0.02	0.15
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB2	9	0.15	0.02	0.15
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB3	9	0.15	0.02	0.15
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB2	9	0.15	0.02	0.15
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB3	9	0.15	0.02	0.15
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB2	9	0.15	0.02	0.15
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB3	9	0.15	0.02	0.15
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD11	9	0.14	0.02	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD12	9	0.14	0.02	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD13	9	0.14	0.02	0.13
(1,504)	2:51:B:LEU:H	2:51:B:LEU:HB3	9	0.12	0.01	0.12
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB1	9	0.11	0.01	0.11
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB2	9	0.11	0.01	0.11
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB3	9	0.11	0.01	0.11
(1,1230)	2:44:B:LEU:H	2:44:B:LEU:HB3	9	0.11	0.01	0.1
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD11	8	0.67	0.24	0.7
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD12	8	0.67	0.24	0.7
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD13	8	0.67	0.24	0.7
(1,407)	1:12:A:LEU:HD21	2:38:C:PRO:HB3	8	0.6	0.48	0.42
(1,407)	1:12:A:LEU:HD22	2:38:C:PRO:HB3	8	0.6	0.48	0.42
(1,407)	1:12:A:LEU:HD23	2:38:C:PRO:HB3	8	0.6	0.48	0.42
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD11	8	0.32	0.16	0.3
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD12	8	0.32	0.16	0.3
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD13	8	0.32	0.16	0.3
(1,1424)	2:48:B:ALA:HB1	2:19:B:LEU:HB2	8	0.21	0.04	0.22
(1,1424)	2:48:B:ALA:HB2	2:19:B:LEU:HB2	8	0.21	0.04	0.22
(1,1424)	2:48:B:ALA:HB3	2:19:B:LEU:HB2	8	0.21	0.04	0.22
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD21	8	0.13	0.01	0.13
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD22	8	0.13	0.01	0.13
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD23	8	0.13	0.01	0.13
(1,237)	1:26:A:ILE:HG13	1:26:A:ILE:HD11	8	0.13	0.01	0.13
(1,237)	1:26:A:ILE:HG13	1:26:A:ILE:HD12	8	0.13	0.01	0.13
(1,237)	1:26:A:ILE:HG23	1:26:A:ILE:HD13	8	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,237)	1:26:A:ILE:HG13	1:26:A:ILE:HD13	8	0.13	0.01	0.13
(1,237)	1:26:A:ILE:HG21	1:26:A:ILE:HD13	8	0.13	0.01	0.13
(1,274)	1:17:A:VAL:HB	2:17:B:VAL:HB	8	0.13	0.01	0.13
(1,1312)	2:49:B:LYS:HB2	2:49:B:LYS:HG2	8	0.13	0.0	0.13
(1,323)	1:23:A:PHE:H	1:23:A:PHE:HB2	8	0.12	0.01	0.12
(1,1710)	2:40:C:GLN:H	2:40:C:GLN:HG3	8	0.12	0.01	0.12
(1,1606)	2:19:B:LEU:HD21	2:52:B:ASN:HB2	7	0.89	0.34	0.85
(1,1606)	2:19:B:LEU:HD22	2:52:B:ASN:HB2	7	0.89	0.34	0.85
(1,1606)	2:19:B:LEU:HD23	2:52:B:ASN:HB2	7	0.89	0.34	0.85
(1,1809)	2:29:B:ALA:HB1	2:26:B:GLN:HG3	7	0.8	0.08	0.82
(1,1809)	2:29:B:ALA:HB2	2:26:B:GLN:HG3	7	0.8	0.08	0.82
(1,1809)	2:29:B:ALA:HB3	2:26:B:GLN:HG3	7	0.8	0.08	0.82
(1,63)	1:29:A:SER:H	1:29:A:SER:HB3	7	0.59	0.11	0.56
(1,1752)	2:44:C:LEU:HD21	2:43:C:ASN:HB2	7	0.56	0.14	0.61
(1,1752)	2:44:C:LEU:HD21	2:43:C:ASN:HB3	7	0.56	0.14	0.61
(1,1752)	2:44:C:LEU:HD22	2:43:C:ASN:HB2	7	0.56	0.14	0.61
(1,1752)	2:44:C:LEU:HD22	2:43:C:ASN:HB3	7	0.56	0.14	0.61
(1,1752)	2:44:C:LEU:HD23	2:43:C:ASN:HB2	7	0.56	0.14	0.61
(1,1752)	2:44:C:LEU:HD23	2:43:C:ASN:HB3	7	0.56	0.14	0.61
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	7	0.54	0.16	0.5
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	7	0.54	0.16	0.5
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	7	0.54	0.16	0.5
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	7	0.54	0.16	0.5
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	7	0.54	0.16	0.5
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	7	0.54	0.16	0.5
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	7	0.54	0.16	0.5
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	7	0.54	0.16	0.5
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	7	0.54	0.16	0.5
(1,1242)	2:44:B:LEU:HD22	2:44:B:LEU:HB3	7	0.54	0.05	0.56
(1,1242)	2:44:B:LEU:HD21	2:44:B:LEU:HB3	7	0.54	0.05	0.56
(1,1242)	2:44:C:LEU:HD12	2:44:C:LEU:HB3	7	0.54	0.05	0.56
(1,1242)	2:44:B:LEU:HD23	2:44:B:LEU:HB3	7	0.54	0.05	0.56
(1,1242)	2:44:C:LEU:HD13	2:44:C:LEU:HB3	7	0.54	0.05	0.56
(1,1427)	2:19:B:LEU:HD21	2:19:B:LEU:HB3	7	0.33	0.01	0.32
(1,1427)	2:19:B:LEU:HD22	2:19:B:LEU:HB3	7	0.33	0.01	0.32
(1,1427)	2:19:B:LEU:HD23	2:19:B:LEU:HB3	7	0.33	0.01	0.32
(1,1265)	2:31:B:ILE:HG21	2:24:C:PRO:HG2	7	0.18	0.02	0.19
(1,1265)	2:31:B:ILE:HG22	2:24:C:PRO:HG2	7	0.18	0.02	0.19
(1,1265)	2:31:B:ILE:HG23	2:24:C:PRO:HG2	7	0.18	0.02	0.19
(1,809)	2:37:C:ASP:H	2:38:C:PRO:HG2	7	0.15	0.03	0.17
(1,809)	2:37:C:ASP:H	2:38:C:PRO:HG3	7	0.15	0.03	0.17
(1,276)	1:27:A:LEU:HD11	2:45:C:LEU:HG	6	0.94	0.37	1.06

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,276)	1:27:A:LEU:HD12	2:45:C:LEU:HG	6	0.94	0.37	1.06
(1,276)	1:27:A:LEU:HD13	2:45:C:LEU:HG	6	0.94	0.37	1.06
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	6	0.73	0.53	0.58
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	6	0.73	0.53	0.58
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	6	0.73	0.53	0.58
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG21	6	0.7	0.11	0.72
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG22	6	0.7	0.11	0.72
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG23	6	0.7	0.11	0.72
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD11	6	0.6	0.03	0.57
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD12	6	0.6	0.03	0.57
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD13	6	0.6	0.03	0.57
(1,797)	2:37:B:ASP:H	2:38:B:PRO:HD2	6	0.24	0.05	0.22
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD11	6	0.21	0.07	0.24
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD12	6	0.21	0.07	0.24
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD13	6	0.21	0.07	0.24
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD21	6	0.19	0.07	0.18
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD22	6	0.19	0.07	0.18
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD23	6	0.19	0.07	0.18
(1,1798)	2:26:C:GLN:H	2:26:C:GLN:HG3	6	0.14	0.03	0.12
(1,1780)	2:51:B:LEU:HD11	2:47:B:GLU:HG2	6	0.13	0.01	0.14
(1,1780)	2:51:B:LEU:HD11	2:47:B:GLU:HG3	6	0.13	0.01	0.14
(1,1780)	2:51:B:LEU:HD12	2:47:B:GLU:HG2	6	0.13	0.01	0.14
(1,1780)	2:51:B:LEU:HD12	2:47:B:GLU:HG3	6	0.13	0.01	0.14
(1,1780)	2:51:B:LEU:HD13	2:47:B:GLU:HG2	6	0.13	0.01	0.14
(1,1780)	2:51:B:LEU:HD13	2:47:B:GLU:HG3	6	0.13	0.01	0.14
(1,1921)	2:37:B:ASP:HB3	2:40:B:GLN:HG2	5	1.25	0.25	1.24
(1,1778)	2:46:B:ALA:HB1	2:47:B:GLU:HG2	5	0.99	0.06	0.99
(1,1778)	2:46:B:ALA:HB2	2:47:B:GLU:HG2	5	0.99	0.06	0.99
(1,1778)	2:46:B:ALA:HB3	2:47:B:GLU:HG2	5	0.99	0.06	0.99
(1,1901)	2:37:B:ASP:HB3	2:44:B:LEU:HG	5	0.94	0.13	0.95
(1,1316)	2:17:B:VAL:HG21	2:49:B:LYS:HE2	5	0.74	0.24	0.73
(1,1316)	2:17:B:VAL:HG21	2:49:B:LYS:HE3	5	0.74	0.24	0.73
(1,1316)	2:17:B:VAL:HG22	2:49:B:LYS:HE2	5	0.74	0.24	0.73
(1,1316)	2:17:B:VAL:HG22	2:49:B:LYS:HE3	5	0.74	0.24	0.73
(1,1316)	2:17:B:VAL:HG23	2:49:B:LYS:HE2	5	0.74	0.24	0.73
(1,1316)	2:17:B:VAL:HG23	2:49:B:LYS:HE3	5	0.74	0.24	0.73
(1,1771)	2:47:B:GLU:H	2:47:B:GLU:HG2	5	0.65	0.04	0.65
(1,1902)	2:44:B:LEU:HD11	2:37:B:ASP:HB3	5	0.63	0.03	0.64
(1,1902)	2:44:B:LEU:HD12	2:37:B:ASP:HB3	5	0.63	0.03	0.64
(1,1902)	2:44:B:LEU:HD13	2:37:B:ASP:HB3	5	0.63	0.03	0.64
(1,1774)	2:47:B:GLU:HA	2:47:B:GLU:HG2	5	0.36	0.03	0.37
(1,1884)	2:51:C:LEU:HD21	2:26:C:GLN:HG2	5	0.3	0.01	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1884)	2:51:C:LEU:HD22	2:26:C:GLN:HG2	5	0.3	0.01	0.31
(1,1884)	2:51:C:LEU:HD23	2:26:C:GLN:HG2	5	0.3	0.01	0.31
(1,1618)	2:23:C:ASN:HB3	2:24:C:PRO:HD2	5	0.24	0.1	0.26
(1,1533)	2:51:C:LEU:HA	2:54:C:ALA:HB2	5	0.23	0.11	0.19
(1,1533)	2:51:C:LEU:HA	2:54:C:ALA:HB3	5	0.23	0.11	0.19
(1,1564)	2:19:C:LEU:HD21	2:49:C:LYS:HG2	5	0.17	0.06	0.17
(1,1564)	2:19:C:LEU:HD21	2:49:C:LYS:HG3	5	0.17	0.06	0.17
(1,1564)	2:19:C:LEU:HD22	2:49:C:LYS:HG2	5	0.17	0.06	0.17
(1,1564)	2:19:C:LEU:HD22	2:49:C:LYS:HG3	5	0.17	0.06	0.17
(1,1564)	2:19:C:LEU:HD23	2:49:C:LYS:HG2	5	0.17	0.06	0.17
(1,1564)	2:19:C:LEU:HD23	2:49:C:LYS:HG3	5	0.17	0.06	0.17
(1,1675)	2:37:B:ASP:H	2:37:B:ASP:HB3	5	0.16	0.03	0.16
(1,1179)	2:15:C:GLU:HB3	2:16:C:ILE:H	5	0.11	0.01	0.11
(1,1596)	2:38:C:PRO:HB2	2:38:C:PRO:HD3	5	0.11	0.01	0.11
(1,267)	1:27:A:LEU:HD11	2:45:C:LEU:HB3	4	0.66	0.02	0.66
(1,267)	1:27:A:LEU:HD12	2:45:C:LEU:HB3	4	0.66	0.02	0.66
(1,267)	1:27:A:LEU:HD13	2:45:C:LEU:HB3	4	0.66	0.02	0.66
(1,1619)	2:23:C:ASN:HB2	2:24:C:PRO:HD2	4	0.4	0.17	0.43
(1,1551)	2:17:B:VAL:HG21	2:15:B:GLU:HG3	4	0.29	0.08	0.31
(1,1551)	2:17:B:VAL:HG22	2:15:B:GLU:HG3	4	0.29	0.08	0.31
(1,1551)	2:17:B:VAL:HG23	2:15:B:GLU:HG3	4	0.29	0.08	0.31
(1,888)	2:21:C:ASN:H	2:20:C:PRO:HG3	4	0.2	0.09	0.18
(1,252)	1:27:A:LEU:HD21	2:42:C:ALA:H	4	0.19	0.09	0.16
(1,252)	1:27:A:LEU:HD22	2:42:C:ALA:H	4	0.19	0.09	0.16
(1,252)	1:27:A:LEU:HD23	2:42:C:ALA:H	4	0.19	0.09	0.16
(1,1439)	2:19:B:LEU:HD21	2:48:B:ALA:HB1	4	0.16	0.05	0.16
(1,1439)	2:19:B:LEU:HD21	2:48:B:ALA:HB2	4	0.16	0.05	0.16
(1,1439)	2:19:B:LEU:HD21	2:48:B:ALA:HB3	4	0.16	0.05	0.16
(1,1439)	2:19:B:LEU:HD22	2:48:B:ALA:HB1	4	0.16	0.05	0.16
(1,1439)	2:19:B:LEU:HD22	2:48:B:ALA:HB2	4	0.16	0.05	0.16
(1,1439)	2:19:B:LEU:HD22	2:48:B:ALA:HB3	4	0.16	0.05	0.16
(1,1439)	2:19:B:LEU:HD23	2:48:B:ALA:HB1	4	0.16	0.05	0.16
(1,1439)	2:19:B:LEU:HD23	2:48:B:ALA:HB2	4	0.16	0.05	0.16
(1,1439)	2:19:B:LEU:HD23	2:48:B:ALA:HB3	4	0.16	0.05	0.16
(1,1193)	2:31:C:ILE:HG21	2:27:B:LEU:HB3	4	0.16	0.03	0.16
(1,1193)	2:31:C:ILE:HG22	2:27:B:LEU:HB3	4	0.16	0.03	0.16
(1,1193)	2:31:C:ILE:HG23	2:27:B:LEU:HB3	4	0.16	0.03	0.16
(1,1517)	2:49:B:LYS:H	2:46:B:ALA:HA	4	0.15	0.06	0.12
(1,1517)	2:49:C:LYS:H	2:46:C:ALA:HA	4	0.15	0.06	0.12
(1,345)	1:10:A:GLN:HA	1:10:A:GLN:HG2	4	0.11	0.0	0.11
(1,345)	1:10:A:GLN:HA	1:10:A:GLN:HG3	4	0.11	0.0	0.11
(1,352)	1:10:A:GLN:HA	1:10:A:GLN:HG2	4	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,352)	1:10:A:GLN:HA	1:10:A:GLN:HG3	4	0.11	0.0	0.11
(1,1872)	2:23:B:ASN:HD22	2:26:B:GLN:HG3	3	1.27	0.04	1.26
(1,1849)	2:22:B:LEU:HD11	2:19:B:LEU:HG	3	1.1	0.09	1.07
(1,1559)	2:19:B:LEU:HD21	2:22:B:LEU:HD11	3	0.74	0.04	0.77
(1,1559)	2:19:B:LEU:HD21	2:22:B:LEU:HD12	3	0.74	0.04	0.77
(1,1559)	2:19:B:LEU:HD21	2:22:B:LEU:HD13	3	0.74	0.04	0.77
(1,1559)	2:19:B:LEU:HD22	2:22:B:LEU:HD11	3	0.74	0.04	0.77
(1,1559)	2:19:B:LEU:HD22	2:22:B:LEU:HD12	3	0.74	0.04	0.77
(1,1559)	2:19:B:LEU:HD22	2:22:B:LEU:HD13	3	0.74	0.04	0.77
(1,1559)	2:19:B:LEU:HD23	2:22:B:LEU:HD11	3	0.74	0.04	0.77
(1,1559)	2:19:B:LEU:HD23	2:22:B:LEU:HD12	3	0.74	0.04	0.77
(1,1559)	2:19:B:LEU:HD23	2:22:B:LEU:HD13	3	0.74	0.04	0.77
(1,1433)	2:19:B:LEU:HD21	2:19:B:LEU:HB2	3	0.61	0.02	0.61
(1,1433)	2:19:B:LEU:HD22	2:19:B:LEU:HB2	3	0.61	0.02	0.61
(1,1433)	2:19:B:LEU:HD23	2:19:B:LEU:HB2	3	0.61	0.02	0.61
(1,1714)	2:44:C:LEU:HD11	2:40:C:GLN:HG3	3	0.51	0.02	0.52
(1,1714)	2:44:C:LEU:HD12	2:40:C:GLN:HG3	3	0.51	0.02	0.52
(1,1714)	2:44:C:LEU:HD13	2:40:C:GLN:HG3	3	0.51	0.02	0.52
(1,1794)	2:23:C:ASN:HD22	2:26:C:GLN:HG2	3	0.47	0.09	0.54
(1,1213)	2:31:B:ILE:HD11	2:27:C:LEU:HD21	3	0.34	0.15	0.3
(1,1213)	2:31:B:ILE:HD13	2:27:C:LEU:HD22	3	0.34	0.15	0.3
(1,1628)	2:22:C:LEU:H	2:21:C:ASN:HB2	3	0.26	0.11	0.24
(1,1812)	2:51:C:LEU:HD11	2:26:C:GLN:HG2	3	0.24	0.09	0.26
(1,1812)	2:51:C:LEU:HD12	2:26:C:GLN:HG2	3	0.24	0.09	0.26
(1,1812)	2:51:C:LEU:HD13	2:26:C:GLN:HG2	3	0.24	0.09	0.26
(1,1612)	2:23:C:ASN:HB2	2:23:C:ASN:HD21	3	0.22	0.01	0.22
(1,501)	2:25:B:ASP:H	2:24:B:PRO:HD3	3	0.18	0.06	0.16
(1,1426)	2:19:B:LEU:HD21	2:19:B:LEU:HB2	3	0.17	0.02	0.17
(1,1426)	2:19:B:LEU:HD22	2:19:B:LEU:HB2	3	0.17	0.02	0.17
(1,1426)	2:19:B:LEU:HD23	2:19:B:LEU:HB2	3	0.17	0.02	0.17
(1,1795)	2:26:B:GLN:H	2:26:B:GLN:HG2	3	0.17	0.04	0.17
(1,1300)	2:39:B:SER:H	2:38:B:PRO:HB3	3	0.15	0.04	0.17
(1,1772)	2:48:B:ALA:H	2:47:B:GLU:HG2	3	0.13	0.01	0.12
(1,1772)	2:48:B:ALA:H	2:47:B:GLU:HG3	3	0.13	0.01	0.12
(1,94)	1:11:A:ARG:H	1:11:A:ARG:HB2	3	0.12	0.0	0.12
(1,94)	1:11:A:ARG:H	1:11:A:ARG:HB3	3	0.12	0.0	0.12
(1,964)	2:45:C:LEU:H	2:45:C:LEU:HB3	3	0.12	0.01	0.11
(1,100)	1:28:A:SER:HB2	1:12:A:LEU:H	2	0.64	0.2	0.64
(1,1643)	2:32:B:HIS:HA	2:24:C:PRO:HB2	2	0.61	0.27	0.61
(1,413)	1:11:A:ARG:HG2	1:12:A:LEU:HD11	2	0.44	0.23	0.44
(1,413)	1:11:A:ARG:HG2	1:12:A:LEU:HD12	2	0.44	0.23	0.44
(1,413)	1:11:A:ARG:HG2	1:12:A:LEU:HD13	2	0.44	0.23	0.44

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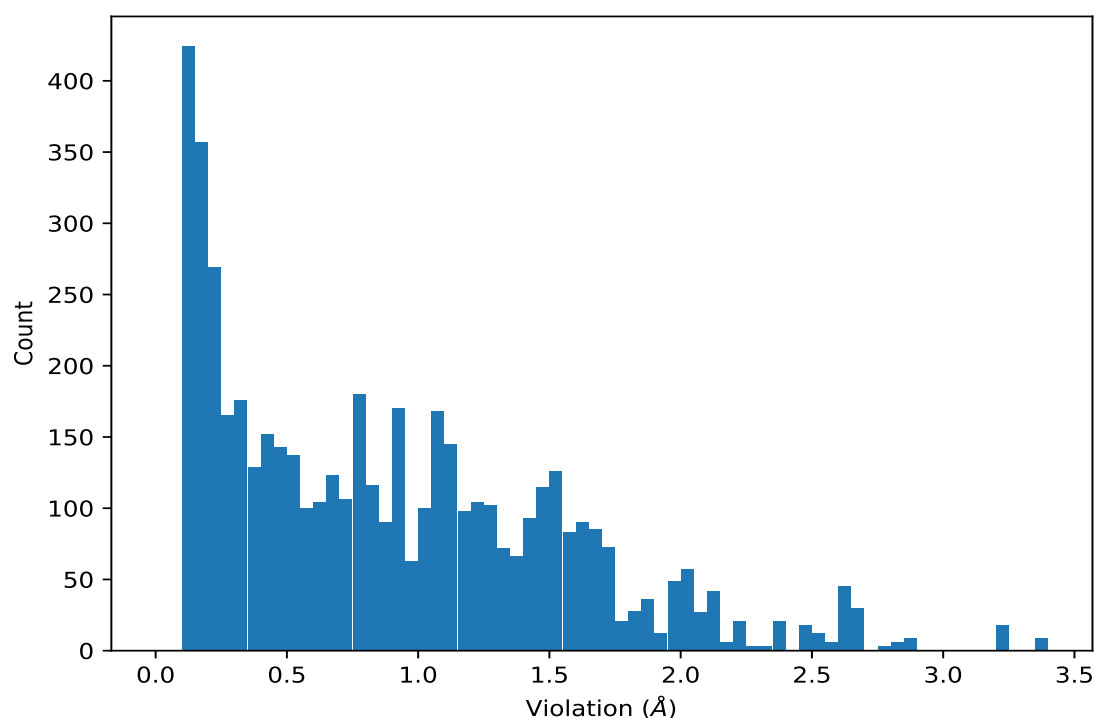
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,423)	1:28:A:SER:HB3	1:12:A:LEU:HB3	2	0.38	0.14	0.38
(1,423)	1:28:A:SER:HB2	1:12:A:LEU:HB2	2	0.38	0.14	0.38
(1,423)	1:28:A:SER:HB2	1:12:A:LEU:HB3	2	0.38	0.14	0.38
(1,1404)	2:17:C:VAL:HG11	2:45:C:LEU:HG	2	0.29	0.0	0.29
(1,1404)	2:17:C:VAL:HG12	2:45:C:LEU:HG	2	0.29	0.0	0.29
(1,1404)	2:17:C:VAL:HG13	2:45:C:LEU:HG	2	0.29	0.0	0.29
(1,1469)	2:45:C:LEU:HB2	2:45:C:LEU:HD21	2	0.26	0.01	0.26
(1,1469)	2:45:C:LEU:HB2	2:45:C:LEU:HD22	2	0.26	0.01	0.26
(1,1469)	2:45:C:LEU:HB2	2:45:C:LEU:HD23	2	0.26	0.01	0.26
(1,396)	1:12:A:LEU:HA	1:12:A:LEU:HD11	2	0.23	0.02	0.23
(1,396)	1:12:A:LEU:HA	1:12:A:LEU:HD12	2	0.23	0.02	0.23
(1,396)	1:12:A:LEU:HA	1:12:A:LEU:HD13	2	0.23	0.02	0.23
(1,66)	1:29:A:SER:HB2	1:30:A:THR:H	2	0.21	0.01	0.21
(1,1145)	2:17:B:VAL:HG21	2:15:B:GLU:HB2	2	0.2	0.04	0.2
(1,1145)	2:17:B:VAL:HG22	2:15:B:GLU:HB2	2	0.2	0.04	0.2
(1,1145)	2:17:B:VAL:HG23	2:15:B:GLU:HB2	2	0.2	0.04	0.2
(1,1470)	2:45:C:LEU:HA	2:45:C:LEU:HD21	2	0.2	0.01	0.2
(1,1470)	2:45:C:LEU:HA	2:45:C:LEU:HD22	2	0.2	0.01	0.2
(1,1470)	2:45:C:LEU:HA	2:45:C:LEU:HD23	2	0.2	0.01	0.2
(1,1537)	1:15:A:PHE:HD1	2:27:B:LEU:HD21	2	0.13	0.01	0.13
(1,1537)	1:15:A:PHE:HD1	2:27:B:LEU:HD22	2	0.13	0.01	0.13
(1,1537)	1:15:A:PHE:HD1	2:27:B:LEU:HD23	2	0.13	0.01	0.13
(1,1537)	1:15:A:PHE:HD2	2:27:B:LEU:HD21	2	0.13	0.01	0.13
(1,1537)	1:15:A:PHE:HD2	2:27:B:LEU:HD22	2	0.13	0.01	0.13
(1,1537)	1:15:A:PHE:HD2	2:27:B:LEU:HD23	2	0.13	0.01	0.13
(1,1388)	2:51:C:LEU:H	2:51:C:LEU:HD11	2	0.12	0.0	0.12
(1,1388)	2:51:C:LEU:H	2:51:C:LEU:HD12	2	0.12	0.0	0.12
(1,1388)	2:51:C:LEU:H	2:51:C:LEU:HD13	2	0.12	0.0	0.12
(1,83)	1:17:A:VAL:H	2:18:B:TYR:H	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)
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG11	8	3.36
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG12	8	3.36
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG13	8	3.36
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG11	8	3.36
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG12	8	3.36
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG13	8	3.36
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG11	8	3.36
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG12	8	3.36
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG13	8	3.36
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG11	10	3.24
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG12	10	3.24
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG13	10	3.24
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG11	10	3.24
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG12	10	3.24
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG13	10	3.24
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG11	10	3.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG12	10	3.24
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG13	10	3.24
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG11	1	3.22
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG12	1	3.22
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG13	1	3.22
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG11	1	3.22
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG12	1	3.22
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG13	1	3.22
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG11	1	3.22
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG12	1	3.22
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG13	1	3.22
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD11	1	2.88
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD12	1	2.88
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD13	1	2.88
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD11	5	2.87
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD12	5	2.87
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD13	5	2.87
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD11	7	2.87
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD12	7	2.87
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD13	7	2.87
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD11	4	2.84
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD12	4	2.84
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD13	4	2.84
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD11	8	2.83
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD12	8	2.83
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD13	8	2.83
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD11	6	2.75
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD12	6	2.75
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD13	6	2.75
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD21	7	2.68
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD22	7	2.68
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD23	7	2.68
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD21	7	2.68
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD22	7	2.68
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD23	7	2.68
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD21	7	2.68
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD22	7	2.68
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD23	7	2.68
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD21	3	2.67
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD22	3	2.67
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD23	3	2.67
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD21	3	2.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD22	3	2.67
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD23	3	2.67
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD21	3	2.67
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD22	3	2.67
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD23	3	2.67
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD21	8	2.67
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD22	8	2.67
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD23	8	2.67
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD21	8	2.67
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD22	8	2.67
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD23	8	2.67
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD21	8	2.67
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD22	8	2.67
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD23	8	2.67
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD11	9	2.65
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD12	9	2.65
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD13	9	2.65
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD21	2	2.64
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD22	2	2.64
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD23	2	2.64
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD21	2	2.64
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD22	2	2.64
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD23	2	2.64
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD21	2	2.64
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD22	2	2.64
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD23	2	2.64
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD21	4	2.64
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD22	4	2.64
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD23	4	2.64
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD21	4	2.64
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD22	4	2.64
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD23	4	2.64
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD21	4	2.64
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD22	4	2.64
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD23	4	2.64
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD21	1	2.63
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD22	1	2.63
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD23	1	2.63
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD21	1	2.63
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD22	1	2.63
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD23	1	2.63
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD21	1	2.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD22	1	2.63
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD23	1	2.63
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD21	6	2.62
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD22	6	2.62
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD23	6	2.62
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD21	6	2.62
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD22	6	2.62
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD23	6	2.62
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD21	6	2.62
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD22	6	2.62
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD23	6	2.62
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD21	9	2.62
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD22	9	2.62
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD23	9	2.62
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD21	9	2.62
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD22	9	2.62
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD23	9	2.62
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD21	9	2.62
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD22	9	2.62
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD23	9	2.62
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD11	2	2.58
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD12	2	2.58
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD13	2	2.58
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD11	2	2.55
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD12	2	2.55
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD13	2	2.55
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD21	5	2.54
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD22	5	2.54
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD23	5	2.54
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD21	5	2.54
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD22	5	2.54
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD23	5	2.54
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD21	5	2.54
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD22	5	2.54
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD23	5	2.54
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD11	3	2.51
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD12	3	2.51
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD13	3	2.51
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD11	4	2.49
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD12	4	2.49
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD13	4	2.49
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD11	10	2.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD12	10	2.49
(1,1080)	2:34:C:ILE:HG13	2:44:C:LEU:HD13	10	2.49
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD11	7	2.48
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD12	7	2.48
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD13	7	2.48
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD11	5	2.47
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD12	5	2.47
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD13	5	2.47
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD11	3	2.46
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD12	3	2.46
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD13	3	2.46
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD11	1	2.45
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD12	1	2.45
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD13	1	2.45
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD11	8	2.38
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD12	8	2.38
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD13	8	2.38
(1,1436)	2:19:B:LEU:HD21	2:52:B:ASN:H	3	2.38
(1,1436)	2:19:B:LEU:HD22	2:52:B:ASN:H	3	2.38
(1,1436)	2:19:B:LEU:HD23	2:52:B:ASN:H	3	2.38
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD11	10	2.37
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD12	10	2.37
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD13	10	2.37
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD11	6	2.36
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD12	6	2.36
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD13	6	2.36
(1,1436)	2:19:B:LEU:HD21	2:52:B:ASN:H	7	2.36
(1,1436)	2:19:B:LEU:HD22	2:52:B:ASN:H	7	2.36
(1,1436)	2:19:B:LEU:HD23	2:52:B:ASN:H	7	2.36
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG2	10	2.35
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG3	10	2.35
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG2	10	2.35
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG3	10	2.35
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG2	10	2.35
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG3	10	2.35
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD11	9	2.3
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD12	9	2.3
(1,1833)	2:22:C:LEU:HA	2:27:C:LEU:HD13	9	2.3
(1,1436)	2:19:B:LEU:HD21	2:52:B:ASN:H	6	2.29
(1,1436)	2:19:B:LEU:HD22	2:52:B:ASN:H	6	2.29
(1,1436)	2:19:B:LEU:HD23	2:52:B:ASN:H	6	2.29
(1,1436)	2:19:B:LEU:HD21	2:52:B:ASN:H	2	2.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1436)	2:19:B:LEU:HD22	2:52:B:ASN:H	2	2.21
(1,1436)	2:19:B:LEU:HD23	2:52:B:ASN:H	2	2.21
(1,399)	1:27:A:LEU:HD11	1:12:A:LEU:HA	7	2.21
(1,399)	1:27:A:LEU:HD12	1:12:A:LEU:HA	7	2.21
(1,399)	1:27:A:LEU:HD13	1:12:A:LEU:HA	7	2.21
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD21	10	2.21
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD22	10	2.21
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD23	10	2.21
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD21	10	2.21
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD22	10	2.21
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD23	10	2.21
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD21	10	2.21
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD22	10	2.21
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD23	10	2.21
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG2	5	2.2
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG3	5	2.2
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG2	5	2.2
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG3	5	2.2
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG2	5	2.2
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG3	5	2.2
(1,1436)	2:19:B:LEU:HD21	2:52:B:ASN:H	9	2.19
(1,1436)	2:19:B:LEU:HD22	2:52:B:ASN:H	9	2.19
(1,1436)	2:19:B:LEU:HD23	2:52:B:ASN:H	9	2.19
(1,399)	1:27:A:LEU:HD11	1:12:A:LEU:HA	2	2.15
(1,399)	1:27:A:LEU:HD12	1:12:A:LEU:HA	2	2.15
(1,399)	1:27:A:LEU:HD13	1:12:A:LEU:HA	2	2.15
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD11	7	2.13
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD12	7	2.13
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD13	7	2.13
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD11	7	2.13
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD12	7	2.13
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD13	7	2.13
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD11	7	2.13
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD12	7	2.13
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD13	7	2.13
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD11	9	2.12
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD12	9	2.12
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD13	9	2.12
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD11	9	2.12
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD12	9	2.12
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD13	9	2.12
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD11	9	2.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD12	9	2.12
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD13	9	2.12
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	1	2.12
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	1	2.12
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	1	2.12
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	1	2.12
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	1	2.12
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	1	2.12
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	1	2.12
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	1	2.12
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	1	2.12
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG2	2	2.11
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG3	2	2.11
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG2	2	2.11
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG3	2	2.11
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG2	2	2.11
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG3	2	2.11
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	9	2.1
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	9	2.1
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	9	2.1
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	9	2.1
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	9	2.1
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	9	2.1
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	9	2.1
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	9	2.1
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	9	2.1
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG2	6	2.08
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG3	6	2.08
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG2	6	2.08
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG3	6	2.08
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG2	6	2.08
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG3	6	2.08
(1,1436)	2:19:B:LEU:HD21	2:52:B:ASN:H	4	2.07
(1,1436)	2:19:B:LEU:HD22	2:52:B:ASN:H	4	2.07
(1,1436)	2:19:B:LEU:HD23	2:52:B:ASN:H	4	2.07
(1,1436)	2:19:B:LEU:HD21	2:52:B:ASN:H	5	2.07
(1,1436)	2:19:B:LEU:HD22	2:52:B:ASN:H	5	2.07
(1,1436)	2:19:B:LEU:HD23	2:52:B:ASN:H	5	2.07
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG2	3	2.06
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG3	3	2.06
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG2	3	2.06
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG3	3	2.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG2	3	2.06
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG3	3	2.06
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	4	2.06
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	4	2.06
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	4	2.06
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	4	2.06
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	4	2.06
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	4	2.06
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	4	2.06
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	4	2.06
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	4	2.06
(1,399)	1:27:A:LEU:HD11	1:12:A:LEU:HA	4	2.04
(1,399)	1:27:A:LEU:HD12	1:12:A:LEU:HA	4	2.04
(1,399)	1:27:A:LEU:HD13	1:12:A:LEU:HA	4	2.04
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG2	4	2.03
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG3	4	2.03
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG2	4	2.03
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG3	4	2.03
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG2	4	2.03
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG3	4	2.03
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	5	2.03
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	5	2.03
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	5	2.03
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	5	2.03
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	5	2.03
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	5	2.03
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	5	2.03
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	5	2.03
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	5	2.03
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD11	2	2.02
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD12	2	2.02
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD13	2	2.02
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD11	2	2.02
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD12	2	2.02
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD13	2	2.02
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD11	2	2.02
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD12	2	2.02
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD13	2	2.02
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	6	2.01
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	6	2.01
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	6	2.01
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	6	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	6	2.01
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	6	2.01
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	6	2.01
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	6	2.01
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	6	2.01
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	8	2.01
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	8	2.01
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	8	2.01
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	8	2.01
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	8	2.01
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	8	2.01
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	8	2.01
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	8	2.01
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	8	2.01
(1,399)	1:27:A:LEU:HD11	1:12:A:LEU:HA	6	2.01
(1,399)	1:27:A:LEU:HD12	1:12:A:LEU:HA	6	2.01
(1,399)	1:27:A:LEU:HD13	1:12:A:LEU:HA	6	2.01
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	3	2.0
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	3	2.0
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	3	2.0
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	3	2.0
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	3	2.0
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	3	2.0
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	3	2.0
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	3	2.0
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	3	2.0
(1,1930)	2:19:C:LEU:HD11	2:48:C:ALA:HA	5	1.99
(1,1930)	2:19:C:LEU:HD12	2:48:C:ALA:HA	5	1.99
(1,1930)	2:19:C:LEU:HD13	2:48:C:ALA:HA	5	1.99
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	2	1.98
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	2	1.98
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	2	1.98
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	2	1.98
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	2	1.98
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	2	1.98
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	2	1.98
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	2	1.98
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	2	1.98
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	10	1.98
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	10	1.98
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	10	1.98
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	10	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	10	1.98
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	10	1.98
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	10	1.98
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	10	1.98
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	10	1.98
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD11	5	1.97
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD12	5	1.97
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD13	5	1.97
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD11	5	1.97
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD12	5	1.97
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD13	5	1.97
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD11	5	1.97
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD12	5	1.97
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD13	5	1.97
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	7	1.97
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	7	1.97
(1,1212)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	7	1.97
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	7	1.97
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	7	1.97
(1,1212)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	7	1.97
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	7	1.97
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	7	1.97
(1,1212)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	7	1.97
(1,399)	1:27:A:LEU:HD11	1:12:A:LEU:HA	3	1.97
(1,399)	1:27:A:LEU:HD12	1:12:A:LEU:HA	3	1.97
(1,399)	1:27:A:LEU:HD13	1:12:A:LEU:HA	3	1.97
(1,1930)	2:19:C:LEU:HD11	2:48:C:ALA:HA	9	1.96
(1,1930)	2:19:C:LEU:HD12	2:48:C:ALA:HA	9	1.96
(1,1930)	2:19:C:LEU:HD13	2:48:C:ALA:HA	9	1.96
(1,1930)	2:19:C:LEU:HD11	2:48:C:ALA:HA	3	1.95
(1,1930)	2:19:C:LEU:HD12	2:48:C:ALA:HA	3	1.95
(1,1930)	2:19:C:LEU:HD13	2:48:C:ALA:HA	3	1.95
(1,1873)	2:23:B:ASN:HD22	2:26:B:GLN:HG2	9	1.95
(1,399)	1:27:A:LEU:HD11	1:12:A:LEU:HA	1	1.92
(1,399)	1:27:A:LEU:HD12	1:12:A:LEU:HA	1	1.92
(1,399)	1:27:A:LEU:HD13	1:12:A:LEU:HA	1	1.92
(1,1930)	2:19:C:LEU:HD11	2:48:C:ALA:HA	6	1.91
(1,1930)	2:19:C:LEU:HD12	2:48:C:ALA:HA	6	1.91
(1,1930)	2:19:C:LEU:HD13	2:48:C:ALA:HA	6	1.91
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG2	8	1.9
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG3	8	1.9
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG2	8	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG3	8	1.9
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG2	8	1.9
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG3	8	1.9
(1,1930)	2:19:C:LEU:HD11	2:48:C:ALA:HA	2	1.89
(1,1930)	2:19:C:LEU:HD12	2:48:C:ALA:HA	2	1.89
(1,1930)	2:19:C:LEU:HD13	2:48:C:ALA:HA	2	1.89
(1,1930)	2:19:C:LEU:HD11	2:48:C:ALA:HA	8	1.88
(1,1930)	2:19:C:LEU:HD12	2:48:C:ALA:HA	8	1.88
(1,1930)	2:19:C:LEU:HD13	2:48:C:ALA:HA	8	1.88
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD11	4	1.88
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD12	4	1.88
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD13	4	1.88
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD11	4	1.88
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD12	4	1.88
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD13	4	1.88
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD11	4	1.88
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD12	4	1.88
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD13	4	1.88
(1,399)	1:27:A:LEU:HD11	1:12:A:LEU:HA	5	1.88
(1,399)	1:27:A:LEU:HD12	1:12:A:LEU:HA	5	1.88
(1,399)	1:27:A:LEU:HD13	1:12:A:LEU:HA	5	1.88
(1,399)	1:27:A:LEU:HD11	1:12:A:LEU:HA	8	1.87
(1,399)	1:27:A:LEU:HD12	1:12:A:LEU:HA	8	1.87
(1,399)	1:27:A:LEU:HD13	1:12:A:LEU:HA	8	1.87
(1,399)	1:27:A:LEU:HD11	1:12:A:LEU:HA	9	1.87
(1,399)	1:27:A:LEU:HD12	1:12:A:LEU:HA	9	1.87
(1,399)	1:27:A:LEU:HD13	1:12:A:LEU:HA	9	1.87
(1,407)	1:12:A:LEU:HD21	2:38:C:PRO:HB3	3	1.86
(1,407)	1:12:A:LEU:HD22	2:38:C:PRO:HB3	3	1.86
(1,407)	1:12:A:LEU:HD23	2:38:C:PRO:HB3	3	1.86
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG2	7	1.85
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG3	7	1.85
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG2	7	1.85
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG3	7	1.85
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG2	7	1.85
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG3	7	1.85
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD11	7	1.85
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD12	7	1.85
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD13	7	1.85
(1,399)	1:27:A:LEU:HD11	1:12:A:LEU:HA	10	1.83
(1,399)	1:27:A:LEU:HD12	1:12:A:LEU:HA	10	1.83
(1,399)	1:27:A:LEU:HD13	1:12:A:LEU:HA	10	1.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1930)	2:19:C:LEU:HD11	2:48:C:ALA:HA	7	1.81
(1,1930)	2:19:C:LEU:HD12	2:48:C:ALA:HA	7	1.81
(1,1930)	2:19:C:LEU:HD13	2:48:C:ALA:HA	7	1.81
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD11	3	1.81
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD12	3	1.81
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD13	3	1.81
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD11	3	1.81
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD12	3	1.81
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD13	3	1.81
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD11	3	1.81
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD12	3	1.81
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD13	3	1.81
(1,1873)	2:23:B:ASN:HD22	2:26:B:GLN:HG2	8	1.81
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG2	1	1.81
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG3	1	1.81
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG2	1	1.81
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG3	1	1.81
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG2	1	1.81
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG3	1	1.81
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD11	9	1.81
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD12	9	1.81
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD13	9	1.81
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD11	9	1.81
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD12	9	1.81
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD13	9	1.81
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	10	1.79
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	10	1.79
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	10	1.79
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	2	1.79
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	2	1.79
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	2	1.79
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	2	1.79
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	2	1.79
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	2	1.79
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	2	1.79
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	2	1.79
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	2	1.79
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG2	9	1.77
(1,1779)	2:44:C:LEU:HD21	2:47:C:GLU:HG3	9	1.77
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG2	9	1.77
(1,1779)	2:44:C:LEU:HD22	2:47:C:GLU:HG3	9	1.77
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG2	9	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1779)	2:44:C:LEU:HD23	2:47:C:GLU:HG3	9	1.77
(1,1930)	2:19:C:LEU:HD11	2:48:C:ALA:HA	1	1.76
(1,1930)	2:19:C:LEU:HD12	2:48:C:ALA:HA	1	1.76
(1,1930)	2:19:C:LEU:HD13	2:48:C:ALA:HA	1	1.76
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	3	1.74
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	3	1.74
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	3	1.74
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	3	1.74
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	3	1.74
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	3	1.74
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	3	1.74
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	3	1.74
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	3	1.74
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	6	1.73
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	6	1.73
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	6	1.73
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	6	1.73
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	6	1.73
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	6	1.73
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	6	1.73
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	6	1.73
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	6	1.73
(1,1873)	2:23:B:ASN:HD22	2:26:B:GLN:HG2	1	1.72
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD11	3	1.72
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD12	3	1.72
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD13	3	1.72
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD11	4	1.72
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD12	4	1.72
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD13	4	1.72
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD11	4	1.72
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD12	4	1.72
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD13	4	1.72
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD11	4	1.72
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD12	4	1.72
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD13	4	1.72
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD11	8	1.71
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD12	8	1.71
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD13	8	1.71
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	7	1.71
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	7	1.71
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	7	1.71
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	7	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	7	1.71
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	7	1.71
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	7	1.71
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	7	1.71
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	7	1.71
(1,1930)	2:19:C:LEU:HD11	2:48:C:ALA:HA	4	1.7
(1,1930)	2:19:C:LEU:HD12	2:48:C:ALA:HA	4	1.7
(1,1930)	2:19:C:LEU:HD13	2:48:C:ALA:HA	4	1.7
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG11	3	1.7
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG12	3	1.7
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG13	3	1.7
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG11	3	1.7
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG12	3	1.7
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG13	3	1.7
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG11	3	1.7
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG12	3	1.7
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG13	3	1.7
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD21	4	1.7
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD22	4	1.7
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD23	4	1.7
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD21	4	1.7
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD22	4	1.7
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD23	4	1.7
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD21	4	1.7
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD22	4	1.7
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD23	4	1.7
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	4	1.7
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	4	1.7
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	4	1.7
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	4	1.7
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	4	1.7
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	4	1.7
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	4	1.7
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	4	1.7
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	4	1.7
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG11	7	1.69
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG12	7	1.69
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG13	7	1.69
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG11	7	1.69
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG12	7	1.69
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG13	7	1.69
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG11	7	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG12	7	1.69
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG13	7	1.69
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	10	1.68
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	10	1.68
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	10	1.68
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	10	1.68
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	10	1.68
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	10	1.68
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD11	9	1.68
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD12	9	1.68
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD13	9	1.68
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD11	9	1.68
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD12	9	1.68
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD13	9	1.68
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD11	9	1.68
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD12	9	1.68
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD13	9	1.68
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	5	1.67
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	5	1.67
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	5	1.67
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	5	1.67
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	5	1.67
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	5	1.67
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD11	9	1.67
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD12	9	1.67
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD13	9	1.67
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	10	1.67
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	10	1.67
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	10	1.67
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	10	1.67
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	10	1.67
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	10	1.67
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	10	1.67
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	10	1.67
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	10	1.67
(1,104)	1:27:A:LEU:HD11	1:12:A:LEU:H	9	1.67
(1,104)	1:27:A:LEU:HD12	1:12:A:LEU:H	9	1.67
(1,104)	1:27:A:LEU:HD13	1:12:A:LEU:H	9	1.67
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	6	1.66
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	6	1.66
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	6	1.66
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	6	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	6	1.66
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	6	1.66
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD11	9	1.66
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD12	9	1.66
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD13	9	1.66
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	1	1.66
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	1	1.66
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	1	1.66
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	1	1.66
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	1	1.66
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	1	1.66
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	1	1.66
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	1	1.66
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	1	1.66
(1,1813)	1:26:A:ILE:HG13	2:14:C:GLY:HA3	6	1.65
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD11	5	1.65
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD12	5	1.65
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD13	5	1.65
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD11	5	1.65
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD12	5	1.65
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD13	5	1.65
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD11	8	1.65
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD12	8	1.65
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD13	8	1.65
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD11	8	1.65
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD12	8	1.65
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD13	8	1.65
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	5	1.65
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	5	1.65
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	5	1.65
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	5	1.65
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	5	1.65
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	5	1.65
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	5	1.65
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	5	1.65
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	5	1.65
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD11	6	1.64
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD12	6	1.64
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD13	6	1.64
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD11	6	1.64
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD12	6	1.64
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD13	6	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD11	6	1.64
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD12	6	1.64
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD13	6	1.64
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD11	8	1.64
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD12	8	1.64
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD13	8	1.64
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD11	8	1.64
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD12	8	1.64
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD13	8	1.64
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD11	8	1.64
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD12	8	1.64
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD13	8	1.64
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD11	7	1.64
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD12	7	1.64
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD13	7	1.64
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD11	7	1.64
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD12	7	1.64
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD13	7	1.64
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD11	7	1.64
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD12	7	1.64
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD13	7	1.64
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD11	7	1.63
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD12	7	1.63
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD13	7	1.63
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD11	7	1.63
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD12	7	1.63
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD13	7	1.63
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD11	7	1.63
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD12	7	1.63
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD13	7	1.63
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD11	2	1.63
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD12	2	1.63
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD13	2	1.63
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD11	2	1.63
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD12	2	1.63
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD13	2	1.63
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD11	2	1.63
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD12	2	1.63
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD13	2	1.63
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD11	2	1.63
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD12	2	1.63
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD13	2	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	8	1.63
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	8	1.63
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	8	1.63
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	8	1.63
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	8	1.63
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	8	1.63
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	8	1.63
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	8	1.63
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	8	1.63
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD11	1	1.62
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD12	1	1.62
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD13	1	1.62
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD21	1	1.62
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD22	1	1.62
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD23	1	1.62
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD21	1	1.62
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD22	1	1.62
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD23	1	1.62
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD21	1	1.62
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD22	1	1.62
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD23	1	1.62
(1,1545)	1:27:A:LEU:HD21	2:15:C:GLU:HG2	3	1.6
(1,1545)	1:27:A:LEU:HD22	2:15:C:GLU:HG2	3	1.6
(1,1545)	1:27:A:LEU:HD23	2:15:C:GLU:HG2	3	1.6
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD11	6	1.6
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD12	6	1.6
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD13	6	1.6
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD11	6	1.6
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD12	6	1.6
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD13	6	1.6
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD11	10	1.6
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD12	10	1.6
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD13	10	1.6
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	1	1.6
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	1	1.6
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	1	1.6
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	1	1.6
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	1	1.6
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	1	1.6
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	1	1.6
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	1	1.6
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	1	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD11	9	1.59
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD12	9	1.59
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD13	9	1.59
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	9	1.59
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	9	1.59
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	9	1.59
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	9	1.59
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	9	1.59
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	9	1.59
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	9	1.59
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	9	1.59
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	9	1.59
(1,104)	1:27:A:LEU:HD11	1:12:A:LEU:H	2	1.59
(1,104)	1:27:A:LEU:HD12	1:12:A:LEU:H	2	1.59
(1,104)	1:27:A:LEU:HD13	1:12:A:LEU:H	2	1.59
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD11	9	1.58
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD12	9	1.58
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD13	9	1.58
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD11	9	1.58
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD12	9	1.58
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD13	9	1.58
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD11	9	1.58
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD12	9	1.58
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD13	9	1.58
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD11	8	1.58
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD12	8	1.58
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD13	8	1.58
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD11	10	1.58
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD12	10	1.58
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD13	10	1.58
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD11	10	1.58
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD12	10	1.58
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD13	10	1.58
(1,1873)	2:23:B:ASN:HD22	2:26:B:GLN:HG2	10	1.57
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD11	4	1.57
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD12	4	1.57
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD13	4	1.57
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD11	10	1.57
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD12	10	1.57
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD13	10	1.57
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD11	3	1.57
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD12	3	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD13	3	1.57
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD11	3	1.57
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD12	3	1.57
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD13	3	1.57
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD11	3	1.57
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD12	3	1.57
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD13	3	1.57
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD11	6	1.57
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD12	6	1.57
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD13	6	1.57
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD11	6	1.57
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD12	6	1.57
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD13	6	1.57
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD11	6	1.57
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD12	6	1.57
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD13	6	1.57
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG21	7	1.57
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG22	7	1.57
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG23	7	1.57
(1,1921)	2:37:B:ASP:HB3	2:40:B:GLN:HG2	2	1.56
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	4	1.56
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	4	1.56
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	4	1.56
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	4	1.56
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	4	1.56
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	4	1.56
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD11	6	1.56
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD12	6	1.56
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD13	6	1.56
(1,381)	1:27:A:LEU:HD11	1:11:A:ARG:HG2	3	1.56
(1,381)	1:27:A:LEU:HD12	1:11:A:ARG:HG2	3	1.56
(1,381)	1:27:A:LEU:HD13	1:11:A:ARG:HG2	3	1.56
(1,381)	1:27:A:LEU:HD11	1:11:A:ARG:HG2	9	1.56
(1,381)	1:27:A:LEU:HD12	1:11:A:ARG:HG2	9	1.56
(1,381)	1:27:A:LEU:HD13	1:11:A:ARG:HG2	9	1.56
(1,104)	1:27:A:LEU:HD11	1:12:A:LEU:H	4	1.56
(1,104)	1:27:A:LEU:HD12	1:12:A:LEU:H	4	1.56
(1,104)	1:27:A:LEU:HD13	1:12:A:LEU:H	4	1.56
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	10	1.55
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	10	1.55
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	10	1.55
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD11	2	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD12	2	1.54
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD13	2	1.54
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD11	2	1.54
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD12	2	1.54
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD13	2	1.54
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD11	2	1.54
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD12	2	1.54
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD13	2	1.54
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	4	1.54
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	4	1.54
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	4	1.54
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	4	1.54
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	4	1.54
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	4	1.54
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	4	1.54
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	4	1.54
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	4	1.54
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG11	6	1.54
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG12	6	1.54
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG13	6	1.54
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG11	6	1.54
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG12	6	1.54
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG13	6	1.54
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG11	6	1.54
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG12	6	1.54
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG13	6	1.54
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD11	5	1.53
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD12	5	1.53
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD13	5	1.53
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD11	5	1.53
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD12	5	1.53
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD13	5	1.53
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD11	5	1.53
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD12	5	1.53
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD13	5	1.53
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	7	1.53
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	7	1.53
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	7	1.53
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	7	1.53
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	7	1.53
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	7	1.53
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD11	6	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD12	6	1.53
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD13	6	1.53
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD11	3	1.53
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD12	3	1.53
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD13	3	1.53
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD21	10	1.52
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD22	10	1.52
(1,1566)	2:19:C:LEU:HD11	2:22:C:LEU:HD23	10	1.52
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD21	10	1.52
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD22	10	1.52
(1,1566)	2:19:C:LEU:HD12	2:22:C:LEU:HD23	10	1.52
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD21	10	1.52
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD22	10	1.52
(1,1566)	2:19:C:LEU:HD13	2:22:C:LEU:HD23	10	1.52
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	2	1.52
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	2	1.52
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	2	1.52
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	2	1.52
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	2	1.52
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	2	1.52
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	2	1.52
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	2	1.52
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	2	1.52
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	9	1.52
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	9	1.52
(1,147)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	9	1.52
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	9	1.52
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	9	1.52
(1,147)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	9	1.52
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	9	1.52
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	9	1.52
(1,147)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	9	1.52
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD11	10	1.51
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD12	10	1.51
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD13	10	1.51
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD11	10	1.51
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD12	10	1.51
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD13	10	1.51
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD11	10	1.51
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD12	10	1.51
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD13	10	1.51
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	8	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	8	1.51
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	8	1.51
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	8	1.51
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	8	1.51
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	8	1.51
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD11	2	1.51
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD12	2	1.51
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD13	2	1.51
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD11	1	1.51
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD12	1	1.51
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD13	1	1.51
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD11	1	1.51
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD12	1	1.51
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD13	1	1.51
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD11	5	1.51
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD12	5	1.51
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD13	5	1.51
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	5	1.51
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	5	1.51
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	5	1.51
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	5	1.51
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	5	1.51
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	5	1.51
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	5	1.51
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	5	1.51
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	5	1.51
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG11	2	1.51
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG12	2	1.51
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG13	2	1.51
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG11	2	1.51
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG12	2	1.51
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG13	2	1.51
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG11	2	1.51
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG12	2	1.51
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG13	2	1.51
(1,104)	1:27:A:LEU:HD11	1:12:A:LEU:H	6	1.51
(1,104)	1:27:A:LEU:HD12	1:12:A:LEU:H	6	1.51
(1,104)	1:27:A:LEU:HD13	1:12:A:LEU:H	6	1.51
(1,1606)	2:19:B:LEU:HD21	2:52:B:ASN:HB2	7	1.5
(1,1606)	2:19:B:LEU:HD22	2:52:B:ASN:HB2	7	1.5
(1,1606)	2:19:B:LEU:HD23	2:52:B:ASN:HB2	7	1.5
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD11	4	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD12	4	1.49
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD13	4	1.49
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD11	4	1.49
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD12	4	1.49
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD13	4	1.49
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	6	1.49
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	6	1.49
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	6	1.49
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	6	1.49
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	6	1.49
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	6	1.49
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	6	1.49
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	6	1.49
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	6	1.49
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	8	1.49
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	8	1.49
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	8	1.49
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	8	1.49
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	8	1.49
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	8	1.49
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	8	1.49
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	8	1.49
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	8	1.49
(1,1862)	2:27:B:LEU:HD21	2:24:B:PRO:HA	8	1.48
(1,1862)	2:27:B:LEU:HD22	2:24:B:PRO:HA	8	1.48
(1,1862)	2:27:B:LEU:HD23	2:24:B:PRO:HA	8	1.48
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	5	1.48
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	5	1.48
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	5	1.48
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	9	1.48
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	9	1.48
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	9	1.48
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	9	1.48
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	9	1.48
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	9	1.48
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD11	1	1.48
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD12	1	1.48
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD13	1	1.48
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD11	7	1.48
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD12	7	1.48
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD13	7	1.48
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD11	7	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD12	7	1.48
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD13	7	1.48
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	3	1.48
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	3	1.48
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	3	1.48
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	3	1.48
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	3	1.48
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	3	1.48
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	3	1.48
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	3	1.48
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	3	1.48
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD11	1	1.47
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD12	1	1.47
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD13	1	1.47
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD11	1	1.47
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD12	1	1.47
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD13	1	1.47
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD11	1	1.47
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD12	1	1.47
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD13	1	1.47
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD11	3	1.47
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD12	3	1.47
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD13	3	1.47
(1,1432)	1:24:A:GLY:HA3	2:19:C:LEU:HB2	8	1.47
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD11	1	1.47
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD12	1	1.47
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD13	1	1.47
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD11	8	1.46
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD12	8	1.46
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD13	8	1.46
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD11	8	1.46
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD12	8	1.46
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD13	8	1.46
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD11	8	1.46
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD12	8	1.46
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD13	8	1.46
(1,1545)	1:27:A:LEU:HD21	2:15:C:GLU:HG2	5	1.46
(1,1545)	1:27:A:LEU:HD22	2:15:C:GLU:HG2	5	1.46
(1,1545)	1:27:A:LEU:HD23	2:15:C:GLU:HG2	5	1.46
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	2	1.46
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	2	1.46
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	2	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	2	1.46
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	2	1.46
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	2	1.46
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	2	1.46
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	2	1.46
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	2	1.46
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	10	1.46
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	10	1.46
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	10	1.46
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	10	1.46
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	10	1.46
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	10	1.46
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	10	1.46
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	10	1.46
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	10	1.46
(1,1843)	2:19:B:LEU:HD21	2:22:B:LEU:HG	8	1.45
(1,1843)	2:19:B:LEU:HD22	2:22:B:LEU:HG	8	1.45
(1,1843)	2:19:B:LEU:HD23	2:22:B:LEU:HG	8	1.45
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD11	9	1.45
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD12	9	1.45
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD13	9	1.45
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG21	7	1.45
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG22	7	1.45
(1,1126)	2:27:B:LEU:HD21	2:31:C:ILE:HG23	7	1.45
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG21	7	1.45
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG22	7	1.45
(1,1126)	2:27:B:LEU:HD22	2:31:C:ILE:HG23	7	1.45
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG21	7	1.45
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG22	7	1.45
(1,1126)	2:27:B:LEU:HD23	2:31:C:ILE:HG23	7	1.45
(1,1605)	2:19:B:LEU:HD21	2:52:B:ASN:HB3	7	1.44
(1,1605)	2:19:B:LEU:HD22	2:52:B:ASN:HB3	7	1.44
(1,1605)	2:19:B:LEU:HD23	2:52:B:ASN:HB3	7	1.44
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD11	2	1.44
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD12	2	1.44
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD13	2	1.44
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD11	6	1.44
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD12	6	1.44
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD13	6	1.44
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD11	6	1.43
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD12	6	1.43
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD13	6	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD11	6	1.43
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD12	6	1.43
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD13	6	1.43
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD11	6	1.43
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD12	6	1.43
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD13	6	1.43
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	6	1.43
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	6	1.43
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	6	1.43
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	1	1.43
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	1	1.43
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	1	1.43
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	1	1.43
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	1	1.43
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	1	1.43
(1,1405)	2:17:B:VAL:HG11	2:45:B:LEU:HG	2	1.43
(1,1405)	2:17:B:VAL:HG12	2:45:B:LEU:HG	2	1.43
(1,1405)	2:17:B:VAL:HG13	2:45:B:LEU:HG	2	1.43
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	5	1.43
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	5	1.43
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	5	1.43
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	5	1.43
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	5	1.43
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	5	1.43
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	5	1.43
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	5	1.43
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	5	1.43
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD11	3	1.43
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD12	3	1.43
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD13	3	1.43
(1,269)	1:27:A:LEU:HD11	1:13:A:ALA:HA	6	1.43
(1,269)	1:27:A:LEU:HD12	1:13:A:ALA:HA	6	1.43
(1,269)	1:27:A:LEU:HD13	1:13:A:ALA:HA	6	1.43
(1,1921)	2:37:B:ASP:HB3	2:40:B:GLN:HG2	7	1.42
(1,1844)	2:19:C:LEU:HD11	2:22:C:LEU:HG	7	1.42
(1,1844)	2:19:C:LEU:HD12	2:22:C:LEU:HG	7	1.42
(1,1844)	2:19:C:LEU:HD13	2:22:C:LEU:HG	7	1.42
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD11	5	1.41
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD12	5	1.41
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD13	5	1.41
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD11	5	1.41
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD12	5	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD13	5	1.41
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD11	5	1.41
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD12	5	1.41
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD13	5	1.41
(1,1813)	1:26:A:ILE:HG13	2:14:C:GLY:HA3	5	1.41
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	2	1.41
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	2	1.41
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	2	1.41
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	2	1.41
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	2	1.41
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	2	1.41
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD11	5	1.41
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD12	5	1.41
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD13	5	1.41
(1,1545)	1:27:A:LEU:HD21	2:15:C:GLU:HG2	8	1.41
(1,1545)	1:27:A:LEU:HD22	2:15:C:GLU:HG2	8	1.41
(1,1545)	1:27:A:LEU:HD23	2:15:C:GLU:HG2	8	1.41
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD11	1	1.41
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD12	1	1.41
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD13	1	1.41
(1,269)	1:27:A:LEU:HD11	1:13:A:ALA:HA	3	1.41
(1,269)	1:27:A:LEU:HD12	1:13:A:ALA:HA	3	1.41
(1,269)	1:27:A:LEU:HD13	1:13:A:ALA:HA	3	1.41
(1,1432)	1:24:A:GLY:HA3	2:19:C:LEU:HB2	2	1.4
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD11	4	1.4
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD12	4	1.4
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD13	4	1.4
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD11	7	1.4
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD12	7	1.4
(1,1345)	2:23:C:ASN:H	2:22:C:LEU:HD13	7	1.4
(1,381)	1:27:A:LEU:HD11	1:11:A:ARG:HG2	1	1.4
(1,381)	1:27:A:LEU:HD12	1:11:A:ARG:HG2	1	1.4
(1,381)	1:27:A:LEU:HD13	1:11:A:ARG:HG2	1	1.4
(1,269)	1:27:A:LEU:HD11	1:13:A:ALA:HA	7	1.4
(1,269)	1:27:A:LEU:HD12	1:13:A:ALA:HA	7	1.4
(1,269)	1:27:A:LEU:HD13	1:13:A:ALA:HA	7	1.4
(1,104)	1:27:A:LEU:HD11	1:12:A:LEU:H	8	1.4
(1,104)	1:27:A:LEU:HD12	1:12:A:LEU:H	8	1.4
(1,104)	1:27:A:LEU:HD13	1:12:A:LEU:H	8	1.4
(1,1862)	2:27:B:LEU:HD21	2:24:B:PRO:HA	9	1.39
(1,1862)	2:27:B:LEU:HD22	2:24:B:PRO:HA	9	1.39
(1,1862)	2:27:B:LEU:HD23	2:24:B:PRO:HA	9	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1843)	2:19:B:LEU:HD21	2:22:B:LEU:HG	1	1.39
(1,1843)	2:19:B:LEU:HD22	2:22:B:LEU:HG	1	1.39
(1,1843)	2:19:B:LEU:HD23	2:22:B:LEU:HG	1	1.39
(1,1813)	1:26:A:ILE:HG13	2:14:C:GLY:HA3	3	1.39
(1,1813)	1:26:A:ILE:HG13	2:14:C:GLY:HA3	7	1.39
(1,1436)	2:19:B:LEU:HD21	2:52:B:ASN:H	1	1.39
(1,1436)	2:19:B:LEU:HD22	2:52:B:ASN:H	1	1.39
(1,1436)	2:19:B:LEU:HD23	2:52:B:ASN:H	1	1.39
(1,1432)	1:24:A:GLY:HA3	2:19:C:LEU:HB2	1	1.39
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG11	5	1.39
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG12	5	1.39
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG13	5	1.39
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG11	5	1.39
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG12	5	1.39
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG13	5	1.39
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG11	5	1.39
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG12	5	1.39
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG13	5	1.39
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	3	1.38
(1,1766)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	3	1.38
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	3	1.38
(1,1766)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	3	1.38
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	3	1.38
(1,1766)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	3	1.38
(1,269)	1:27:A:LEU:HD11	1:13:A:ALA:HA	2	1.38
(1,269)	1:27:A:LEU:HD12	1:13:A:ALA:HA	2	1.38
(1,269)	1:27:A:LEU:HD13	1:13:A:ALA:HA	2	1.38
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	3	1.37
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	3	1.37
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	3	1.37
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD11	7	1.37
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD12	7	1.37
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD13	7	1.37
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD11	3	1.37
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD12	3	1.37
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD13	3	1.37
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD11	3	1.37
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD12	3	1.37
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD13	3	1.37
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD11	9	1.37
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD12	9	1.37
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD13	9	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,381)	1:27:A:LEU:HD11	1:11:A:ARG:HG2	6	1.37
(1,381)	1:27:A:LEU:HD12	1:11:A:ARG:HG2	6	1.37
(1,381)	1:27:A:LEU:HD13	1:11:A:ARG:HG2	6	1.37
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD11	8	1.36
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD12	8	1.36
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD13	8	1.36
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD11	2	1.36
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD12	2	1.36
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD13	2	1.36
(1,1813)	1:26:A:ILE:HG13	2:14:C:GLY:HA3	4	1.35
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB2	8	1.35
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB3	8	1.35
(1,1545)	1:27:A:LEU:HD21	2:15:C:GLU:HG2	6	1.35
(1,1545)	1:27:A:LEU:HD22	2:15:C:GLU:HG2	6	1.35
(1,1545)	1:27:A:LEU:HD23	2:15:C:GLU:HG2	6	1.35
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD11	3	1.35
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD12	3	1.35
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD13	3	1.35
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD11	8	1.35
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD12	8	1.35
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD13	8	1.35
(1,1862)	2:27:B:LEU:HD21	2:24:B:PRO:HA	1	1.34
(1,1862)	2:27:B:LEU:HD22	2:24:B:PRO:HA	1	1.34
(1,1862)	2:27:B:LEU:HD23	2:24:B:PRO:HA	1	1.34
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB2	3	1.34
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB3	3	1.34
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD11	6	1.34
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD12	6	1.34
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD13	6	1.34
(1,276)	1:27:A:LEU:HD11	2:45:C:LEU:HG	1	1.34
(1,276)	1:27:A:LEU:HD12	2:45:C:LEU:HG	1	1.34
(1,276)	1:27:A:LEU:HD13	2:45:C:LEU:HG	1	1.34
(1,1872)	2:23:B:ASN:HD22	2:26:B:GLN:HG3	3	1.33
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD11	3	1.33
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD12	3	1.33
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD13	3	1.33
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD11	3	1.33
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD12	3	1.33
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD13	3	1.33
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD11	3	1.33
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD12	3	1.33
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD13	3	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG11	4	1.33
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG12	4	1.33
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG13	4	1.33
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG11	4	1.33
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG12	4	1.33
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG13	4	1.33
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG11	4	1.33
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG12	4	1.33
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG13	4	1.33
(1,1844)	2:19:C:LEU:HD11	2:22:C:LEU:HG	3	1.32
(1,1844)	2:19:C:LEU:HD12	2:22:C:LEU:HG	3	1.32
(1,1844)	2:19:C:LEU:HD13	2:22:C:LEU:HG	3	1.32
(1,1813)	1:26:A:ILE:HG13	2:14:C:GLY:HA3	2	1.32
(1,269)	1:27:A:LEU:HD11	1:13:A:ALA:HA	10	1.32
(1,269)	1:27:A:LEU:HD12	1:13:A:ALA:HA	10	1.32
(1,269)	1:27:A:LEU:HD13	1:13:A:ALA:HA	10	1.32
(1,1843)	2:19:B:LEU:HD21	2:22:B:LEU:HG	10	1.31
(1,1843)	2:19:B:LEU:HD22	2:22:B:LEU:HG	10	1.31
(1,1843)	2:19:B:LEU:HD23	2:22:B:LEU:HG	10	1.31
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD11	5	1.31
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD12	5	1.31
(1,1597)	2:52:C:ASN:HA	2:22:C:LEU:HD13	5	1.31
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD11	5	1.31
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD12	5	1.31
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD13	5	1.31
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG11	9	1.31
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG12	9	1.31
(1,1037)	2:19:B:LEU:HD11	2:17:B:VAL:HG13	9	1.31
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG11	9	1.31
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG12	9	1.31
(1,1037)	2:19:B:LEU:HD12	2:17:B:VAL:HG13	9	1.31
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG11	9	1.31
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG12	9	1.31
(1,1037)	2:19:B:LEU:HD13	2:17:B:VAL:HG13	9	1.31
(1,276)	1:27:A:LEU:HD11	2:45:C:LEU:HG	5	1.31
(1,276)	1:27:A:LEU:HD12	2:45:C:LEU:HG	5	1.31
(1,276)	1:27:A:LEU:HD13	2:45:C:LEU:HG	5	1.31
(1,269)	1:27:A:LEU:HD11	1:13:A:ALA:HA	4	1.31
(1,269)	1:27:A:LEU:HD12	1:13:A:ALA:HA	4	1.31
(1,269)	1:27:A:LEU:HD13	1:13:A:ALA:HA	4	1.31
(1,1813)	1:26:A:ILE:HG13	2:14:C:GLY:HA3	10	1.3
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB2	1	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB3	1	1.3
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB2	7	1.3
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB3	7	1.3
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD11	4	1.3
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD12	4	1.3
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD13	4	1.3
(1,1405)	2:17:B:VAL:HG11	2:45:B:LEU:HG	10	1.3
(1,1405)	2:17:B:VAL:HG12	2:45:B:LEU:HG	10	1.3
(1,1405)	2:17:B:VAL:HG13	2:45:B:LEU:HG	10	1.3
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD11	10	1.29
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD12	10	1.29
(1,1888)	2:51:C:LEU:HD21	2:22:C:LEU:HD13	10	1.29
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD11	10	1.29
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD12	10	1.29
(1,1888)	2:51:C:LEU:HD22	2:22:C:LEU:HD13	10	1.29
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD11	10	1.29
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD12	10	1.29
(1,1888)	2:51:C:LEU:HD23	2:22:C:LEU:HD13	10	1.29
(1,1844)	2:19:C:LEU:HD11	2:22:C:LEU:HG	4	1.29
(1,1844)	2:19:C:LEU:HD12	2:22:C:LEU:HG	4	1.29
(1,1844)	2:19:C:LEU:HD13	2:22:C:LEU:HG	4	1.29
(1,1813)	1:26:A:ILE:HG13	2:14:C:GLY:HA3	8	1.29
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB2	9	1.29
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB3	9	1.29
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB2	10	1.29
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB3	10	1.29
(1,1405)	2:17:B:VAL:HG11	2:45:B:LEU:HG	4	1.29
(1,1405)	2:17:B:VAL:HG12	2:45:B:LEU:HG	4	1.29
(1,1405)	2:17:B:VAL:HG13	2:45:B:LEU:HG	4	1.29
(1,381)	1:27:A:LEU:HD11	1:11:A:ARG:HG2	4	1.29
(1,381)	1:27:A:LEU:HD12	1:11:A:ARG:HG2	4	1.29
(1,381)	1:27:A:LEU:HD13	1:11:A:ARG:HG2	4	1.29
(1,104)	1:27:A:LEU:HD11	1:12:A:LEU:H	5	1.29
(1,104)	1:27:A:LEU:HD12	1:12:A:LEU:H	5	1.29
(1,104)	1:27:A:LEU:HD13	1:12:A:LEU:H	5	1.29
(1,104)	1:27:A:LEU:HD11	1:12:A:LEU:H	7	1.29
(1,104)	1:27:A:LEU:HD12	1:12:A:LEU:H	7	1.29
(1,104)	1:27:A:LEU:HD13	1:12:A:LEU:H	7	1.29
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	4	1.28
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	4	1.28
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	4	1.28
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	9	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	9	1.28
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	9	1.28
(1,1813)	1:26:A:ILE:HG13	2:14:C:GLY:HA3	9	1.28
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB2	6	1.28
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB3	6	1.28
(1,1545)	1:27:A:LEU:HD21	2:15:C:GLU:HG2	2	1.28
(1,1545)	1:27:A:LEU:HD22	2:15:C:GLU:HG2	2	1.28
(1,1545)	1:27:A:LEU:HD23	2:15:C:GLU:HG2	2	1.28
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD11	1	1.28
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD12	1	1.28
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD13	1	1.28
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD11	10	1.28
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD12	10	1.28
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD13	10	1.28
(1,1862)	2:27:B:LEU:HD21	2:24:B:PRO:HA	7	1.27
(1,1862)	2:27:B:LEU:HD22	2:24:B:PRO:HA	7	1.27
(1,1862)	2:27:B:LEU:HD23	2:24:B:PRO:HA	7	1.27
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	2	1.27
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	2	1.27
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	2	1.27
(1,1436)	2:19:B:LEU:HD21	2:52:B:ASN:H	8	1.27
(1,1436)	2:19:B:LEU:HD22	2:52:B:ASN:H	8	1.27
(1,1436)	2:19:B:LEU:HD23	2:52:B:ASN:H	8	1.27
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD11	4	1.27
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD12	4	1.27
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD13	4	1.27
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD11	6	1.27
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD12	6	1.27
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD13	6	1.27
(1,1872)	2:23:B:ASN:HD22	2:26:B:GLN:HG3	6	1.26
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	8	1.26
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	8	1.26
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	8	1.26
(1,1844)	2:19:C:LEU:HD11	2:22:C:LEU:HG	5	1.26
(1,1844)	2:19:C:LEU:HD12	2:22:C:LEU:HG	5	1.26
(1,1844)	2:19:C:LEU:HD13	2:22:C:LEU:HG	5	1.26
(1,1843)	2:19:B:LEU:HD21	2:22:B:LEU:HG	7	1.26
(1,1843)	2:19:B:LEU:HD22	2:22:B:LEU:HG	7	1.26
(1,1843)	2:19:B:LEU:HD23	2:22:B:LEU:HG	7	1.26
(1,1605)	2:19:B:LEU:HD21	2:52:B:ASN:HB3	5	1.26
(1,1605)	2:19:B:LEU:HD22	2:52:B:ASN:HB3	5	1.26
(1,1605)	2:19:B:LEU:HD23	2:52:B:ASN:HB3	5	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1545)	1:27:A:LEU:HD21	2:15:C:GLU:HG2	7	1.26
(1,1545)	1:27:A:LEU:HD22	2:15:C:GLU:HG2	7	1.26
(1,1545)	1:27:A:LEU:HD23	2:15:C:GLU:HG2	7	1.26
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB1	5	1.26
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB2	5	1.26
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB3	5	1.26
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB1	5	1.26
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB2	5	1.26
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB3	5	1.26
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB1	5	1.26
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB2	5	1.26
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB3	5	1.26
(1,1405)	2:17:B:VAL:HG11	2:45:B:LEU:HG	1	1.26
(1,1405)	2:17:B:VAL:HG12	2:45:B:LEU:HG	1	1.26
(1,1405)	2:17:B:VAL:HG13	2:45:B:LEU:HG	1	1.26
(1,269)	1:27:A:LEU:HD11	1:13:A:ALA:HA	5	1.26
(1,269)	1:27:A:LEU:HD12	1:13:A:ALA:HA	5	1.26
(1,269)	1:27:A:LEU:HD13	1:13:A:ALA:HA	5	1.26
(1,1844)	2:19:C:LEU:HD11	2:22:C:LEU:HG	6	1.25
(1,1844)	2:19:C:LEU:HD12	2:22:C:LEU:HG	6	1.25
(1,1844)	2:19:C:LEU:HD13	2:22:C:LEU:HG	6	1.25
(1,1844)	2:19:C:LEU:HD11	2:22:C:LEU:HG	9	1.25
(1,1844)	2:19:C:LEU:HD12	2:22:C:LEU:HG	9	1.25
(1,1844)	2:19:C:LEU:HD13	2:22:C:LEU:HG	9	1.25
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD11	4	1.25
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD12	4	1.25
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD13	4	1.25
(1,1921)	2:37:B:ASP:HB3	2:40:B:GLN:HG2	9	1.24
(1,1862)	2:27:B:LEU:HD21	2:24:B:PRO:HA	5	1.24
(1,1862)	2:27:B:LEU:HD22	2:24:B:PRO:HA	5	1.24
(1,1862)	2:27:B:LEU:HD23	2:24:B:PRO:HA	5	1.24
(1,1813)	1:26:A:ILE:HG13	2:14:C:GLY:HA3	1	1.24
(1,1713)	2:44:C:LEU:HD11	2:40:C:GLN:HG2	10	1.24
(1,1713)	2:44:C:LEU:HD12	2:40:C:GLN:HG2	10	1.24
(1,1713)	2:44:C:LEU:HD13	2:40:C:GLN:HG2	10	1.24
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB2	4	1.24
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB3	4	1.24
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	5	1.24
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	5	1.24
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	5	1.24
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	9	1.24
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	9	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	9	1.24
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	9	1.24
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	9	1.24
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	9	1.24
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	9	1.24
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	9	1.24
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	9	1.24
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD11	2	1.24
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD12	2	1.24
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD13	2	1.24
(1,268)	1:27:A:LEU:HD21	2:45:C:LEU:HB3	2	1.24
(1,268)	1:27:A:LEU:HD22	2:45:C:LEU:HB3	2	1.24
(1,268)	1:27:A:LEU:HD23	2:45:C:LEU:HB3	2	1.24
(1,104)	1:27:A:LEU:HD11	1:12:A:LEU:H	10	1.24
(1,104)	1:27:A:LEU:HD12	1:12:A:LEU:H	10	1.24
(1,104)	1:27:A:LEU:HD13	1:12:A:LEU:H	10	1.24
(1,1873)	2:23:B:ASN:HD22	2:26:B:GLN:HG2	7	1.23
(1,1872)	2:23:B:ASN:HD22	2:26:B:GLN:HG3	4	1.23
(1,1862)	2:27:B:LEU:HD21	2:24:B:PRO:HA	3	1.23
(1,1862)	2:27:B:LEU:HD22	2:24:B:PRO:HA	3	1.23
(1,1862)	2:27:B:LEU:HD23	2:24:B:PRO:HA	3	1.23
(1,1843)	2:19:B:LEU:HD21	2:22:B:LEU:HG	4	1.23
(1,1843)	2:19:B:LEU:HD22	2:22:B:LEU:HG	4	1.23
(1,1843)	2:19:B:LEU:HD23	2:22:B:LEU:HG	4	1.23
(1,1405)	2:17:B:VAL:HG11	2:45:B:LEU:HG	9	1.23
(1,1405)	2:17:B:VAL:HG12	2:45:B:LEU:HG	9	1.23
(1,1405)	2:17:B:VAL:HG13	2:45:B:LEU:HG	9	1.23
(1,813)	2:34:C:ILE:HG21	2:37:C:ASP:H	7	1.23
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	10	1.22
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	10	1.22
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	10	1.22
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	10	1.22
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	10	1.22
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	10	1.22
(1,1921)	2:37:B:ASP:HB3	2:40:B:GLN:HG2	3	1.22
(1,1849)	2:22:B:LEU:HD11	2:19:B:LEU:HG	10	1.22
(1,1844)	2:19:C:LEU:HD11	2:22:C:LEU:HG	2	1.22
(1,1844)	2:19:C:LEU:HD12	2:22:C:LEU:HG	2	1.22
(1,1844)	2:19:C:LEU:HD13	2:22:C:LEU:HG	2	1.22
(1,1405)	2:17:B:VAL:HG11	2:45:B:LEU:HG	8	1.22
(1,1405)	2:17:B:VAL:HG12	2:45:B:LEU:HG	8	1.22
(1,1405)	2:17:B:VAL:HG13	2:45:B:LEU:HG	8	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,269)	1:27:A:LEU:HD11	1:13:A:ALA:HA	8	1.22
(1,269)	1:27:A:LEU:HD12	1:13:A:ALA:HA	8	1.22
(1,269)	1:27:A:LEU:HD13	1:13:A:ALA:HA	8	1.22
(1,1862)	2:27:B:LEU:HD21	2:24:B:PRO:HA	10	1.21
(1,1862)	2:27:B:LEU:HD22	2:24:B:PRO:HA	10	1.21
(1,1862)	2:27:B:LEU:HD23	2:24:B:PRO:HA	10	1.21
(1,1405)	2:17:B:VAL:HG11	2:45:B:LEU:HG	3	1.21
(1,1405)	2:17:B:VAL:HG12	2:45:B:LEU:HG	3	1.21
(1,1405)	2:17:B:VAL:HG13	2:45:B:LEU:HG	3	1.21
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD11	7	1.21
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD12	7	1.21
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD13	7	1.21
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	5	1.2
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	5	1.2
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	5	1.2
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	5	1.2
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	5	1.2
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	5	1.2
(1,1844)	2:19:C:LEU:HD11	2:22:C:LEU:HG	1	1.2
(1,1844)	2:19:C:LEU:HD12	2:22:C:LEU:HG	1	1.2
(1,1844)	2:19:C:LEU:HD13	2:22:C:LEU:HG	1	1.2
(1,1844)	2:19:C:LEU:HD11	2:22:C:LEU:HG	8	1.2
(1,1844)	2:19:C:LEU:HD12	2:22:C:LEU:HG	8	1.2
(1,1844)	2:19:C:LEU:HD13	2:22:C:LEU:HG	8	1.2
(1,1843)	2:19:B:LEU:HD21	2:22:B:LEU:HG	3	1.2
(1,1843)	2:19:B:LEU:HD22	2:22:B:LEU:HG	3	1.2
(1,1843)	2:19:B:LEU:HD23	2:22:B:LEU:HG	3	1.2
(1,1713)	2:44:C:LEU:HD11	2:40:C:GLN:HG2	2	1.2
(1,1713)	2:44:C:LEU:HD12	2:40:C:GLN:HG2	2	1.2
(1,1713)	2:44:C:LEU:HD13	2:40:C:GLN:HG2	2	1.2
(1,1605)	2:19:B:LEU:HD21	2:52:B:ASN:HB3	3	1.2
(1,1605)	2:19:B:LEU:HD22	2:52:B:ASN:HB3	3	1.2
(1,1605)	2:19:B:LEU:HD23	2:52:B:ASN:HB3	3	1.2
(1,1432)	1:24:A:GLY:HA3	2:19:C:LEU:HB2	3	1.2
(1,1432)	1:24:A:GLY:HA3	2:19:C:LEU:HB2	7	1.2
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	3	1.2
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	3	1.2
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	3	1.2
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	3	1.2
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	3	1.2
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	3	1.2
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	3	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	3	1.2
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	3	1.2
(1,269)	1:27:A:LEU:HD11	1:13:A:ALA:HA	9	1.2
(1,269)	1:27:A:LEU:HD12	1:13:A:ALA:HA	9	1.2
(1,269)	1:27:A:LEU:HD13	1:13:A:ALA:HA	9	1.2
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	6	1.19
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	6	1.19
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	6	1.19
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	6	1.19
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	6	1.19
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	6	1.19
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD11	1	1.19
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD12	1	1.19
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD13	1	1.19
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD11	1	1.19
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD12	1	1.19
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD13	1	1.19
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD11	1	1.19
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD12	1	1.19
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD13	1	1.19
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD11	10	1.19
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD12	10	1.19
(1,1598)	2:52:B:ASN:HA	2:22:B:LEU:HD13	10	1.19
(1,1545)	1:27:A:LEU:HD21	2:15:C:GLU:HG2	9	1.19
(1,1545)	1:27:A:LEU:HD22	2:15:C:GLU:HG2	9	1.19
(1,1545)	1:27:A:LEU:HD23	2:15:C:GLU:HG2	9	1.19
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB1	9	1.19
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB2	9	1.19
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB3	9	1.19
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB1	9	1.19
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB2	9	1.19
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB3	9	1.19
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB1	9	1.19
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB2	9	1.19
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB3	9	1.19
(1,1405)	2:17:B:VAL:HG11	2:45:B:LEU:HG	6	1.19
(1,1405)	2:17:B:VAL:HG12	2:45:B:LEU:HG	6	1.19
(1,1405)	2:17:B:VAL:HG13	2:45:B:LEU:HG	6	1.19
(1,1149)	2:35:B:HIS:HB3	2:34:B:ILE:HB	7	1.19
(1,813)	2:34:C:ILE:HG23	2:37:C:ASP:H	10	1.19
(1,104)	1:27:A:LEU:HD11	1:12:A:LEU:H	1	1.19
(1,104)	1:27:A:LEU:HD12	1:12:A:LEU:H	1	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:27:A:LEU:HD13	1:12:A:LEU:H	1	1.19
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD11	2	1.18
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD12	2	1.18
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD13	2	1.18
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD11	7	1.18
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD12	7	1.18
(1,1346)	2:52:C:ASN:H	2:22:C:LEU:HD13	7	1.18
(1,1931)	2:19:B:LEU:HD21	2:48:B:ALA:HA	3	1.17
(1,1931)	2:19:B:LEU:HD22	2:48:B:ALA:HA	3	1.17
(1,1931)	2:19:B:LEU:HD23	2:48:B:ALA:HA	3	1.17
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG21	5	1.17
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG22	5	1.17
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG23	5	1.17
(1,953)	2:31:B:ILE:HG21	2:24:C:PRO:HB2	9	1.17
(1,953)	2:31:B:ILE:HG22	2:24:C:PRO:HB2	9	1.17
(1,953)	2:31:B:ILE:HG23	2:24:C:PRO:HB2	9	1.17
(1,268)	1:27:A:LEU:HD21	2:45:C:LEU:HB3	3	1.17
(1,268)	1:27:A:LEU:HD22	2:45:C:LEU:HB3	3	1.17
(1,268)	1:27:A:LEU:HD23	2:45:C:LEU:HB3	3	1.17
(1,268)	1:27:A:LEU:HD21	2:45:C:LEU:HB3	4	1.17
(1,268)	1:27:A:LEU:HD22	2:45:C:LEU:HB3	4	1.17
(1,268)	1:27:A:LEU:HD23	2:45:C:LEU:HB3	4	1.17
(1,104)	1:27:A:LEU:HD11	1:12:A:LEU:H	3	1.17
(1,104)	1:27:A:LEU:HD12	1:12:A:LEU:H	3	1.17
(1,104)	1:27:A:LEU:HD13	1:12:A:LEU:H	3	1.17
(1,1606)	2:19:B:LEU:HD21	2:52:B:ASN:HB2	3	1.16
(1,1606)	2:19:B:LEU:HD22	2:52:B:ASN:HB2	3	1.16
(1,1606)	2:19:B:LEU:HD23	2:52:B:ASN:HB2	3	1.16
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD21	7	1.16
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD22	7	1.16
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD23	7	1.16
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD21	7	1.16
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD22	7	1.16
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD23	7	1.16
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD21	7	1.16
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD22	7	1.16
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD23	7	1.16
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD11	7	1.16
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD12	7	1.16
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD13	7	1.16
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD21	7	1.16
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD22	7	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD23	7	1.16
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD21	7	1.16
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD22	7	1.16
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD23	7	1.16
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD21	7	1.16
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD22	7	1.16
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD23	7	1.16
(1,1843)	2:19:B:LEU:HD21	2:22:B:LEU:HG	6	1.15
(1,1843)	2:19:B:LEU:HD22	2:22:B:LEU:HG	6	1.15
(1,1843)	2:19:B:LEU:HD23	2:22:B:LEU:HG	6	1.15
(1,1405)	2:17:B:VAL:HG11	2:45:B:LEU:HG	7	1.15
(1,1405)	2:17:B:VAL:HG12	2:45:B:LEU:HG	7	1.15
(1,1405)	2:17:B:VAL:HG13	2:45:B:LEU:HG	7	1.15
(1,1149)	2:35:B:HIS:HB3	2:34:B:ILE:HB	9	1.15
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD21	2	1.15
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD22	2	1.15
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD23	2	1.15
(1,813)	2:34:C:ILE:HG21	2:37:C:ASP:H	3	1.15
(1,813)	2:34:C:ILE:HG23	2:37:C:ASP:H	5	1.15
(1,1843)	2:19:B:LEU:HD21	2:22:B:LEU:HG	9	1.14
(1,1843)	2:19:B:LEU:HD22	2:22:B:LEU:HG	9	1.14
(1,1843)	2:19:B:LEU:HD23	2:22:B:LEU:HG	9	1.14
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD11	5	1.14
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD12	5	1.14
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD13	5	1.14
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD11	5	1.14
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD12	5	1.14
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD13	5	1.14
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD11	5	1.14
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD12	5	1.14
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD13	5	1.14
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD21	4	1.14
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD22	4	1.14
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD23	4	1.14
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD21	4	1.14
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD22	4	1.14
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD23	4	1.14
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD21	4	1.14
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD22	4	1.14
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD23	4	1.14
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	2	1.14
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	2	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	2	1.14
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	2	1.14
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	2	1.14
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	2	1.14
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	2	1.14
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	2	1.14
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	2	1.14
(1,1436)	2:19:B:LEU:HD21	2:52:B:ASN:H	10	1.13
(1,1436)	2:19:B:LEU:HD22	2:52:B:ASN:H	10	1.13
(1,1436)	2:19:B:LEU:HD23	2:52:B:ASN:H	10	1.13
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	7	1.13
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	7	1.13
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	7	1.13
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	7	1.13
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	7	1.13
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	7	1.13
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	7	1.13
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	7	1.13
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	7	1.13
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD11	10	1.13
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD12	10	1.13
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD13	10	1.13
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD11	4	1.12
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD12	4	1.12
(1,1851)	2:51:C:LEU:HD11	2:22:C:LEU:HD13	4	1.12
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD11	4	1.12
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD12	4	1.12
(1,1851)	2:51:C:LEU:HD12	2:22:C:LEU:HD13	4	1.12
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD11	4	1.12
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD12	4	1.12
(1,1851)	2:51:C:LEU:HD13	2:22:C:LEU:HD13	4	1.12
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	7	1.12
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	7	1.12
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	7	1.12
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	4	1.12
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	4	1.12
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	4	1.12
(1,1843)	2:19:B:LEU:HD21	2:22:B:LEU:HG	2	1.12
(1,1843)	2:19:B:LEU:HD22	2:22:B:LEU:HG	2	1.12
(1,1843)	2:19:B:LEU:HD23	2:22:B:LEU:HG	2	1.12
(1,1790)	2:56:C:ALA:HB3	2:53:C:ASP:HB2	1	1.12
(1,1713)	2:44:C:LEU:HD11	2:40:C:GLN:HG2	3	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1713)	2:44:C:LEU:HD12	2:40:C:GLN:HG2	3	1.12
(1,1713)	2:44:C:LEU:HD13	2:40:C:GLN:HG2	3	1.12
(1,1552)	2:17:B:VAL:HG21	2:15:B:GLU:HG2	3	1.12
(1,1552)	2:17:B:VAL:HG22	2:15:B:GLU:HG2	3	1.12
(1,1552)	2:17:B:VAL:HG23	2:15:B:GLU:HG2	3	1.12
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD11	3	1.12
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD12	3	1.12
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD13	3	1.12
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD11	3	1.12
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD12	3	1.12
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD13	3	1.12
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD11	2	1.12
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD12	2	1.12
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD13	2	1.12
(1,268)	1:27:A:LEU:HD21	2:45:C:LEU:HB3	10	1.12
(1,268)	1:27:A:LEU:HD22	2:45:C:LEU:HB3	10	1.12
(1,268)	1:27:A:LEU:HD23	2:45:C:LEU:HB3	10	1.12
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD21	2	1.12
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD22	2	1.12
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD23	2	1.12
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD21	2	1.12
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD22	2	1.12
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD23	2	1.12
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD21	2	1.12
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD22	2	1.12
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD23	2	1.12
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD21	6	1.12
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD22	6	1.12
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD23	6	1.12
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD21	6	1.12
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD22	6	1.12
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD23	6	1.12
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD21	6	1.12
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD22	6	1.12
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD23	6	1.12
(1,1873)	2:23:B:ASN:HD22	2:26:B:GLN:HG2	5	1.11
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	6	1.11
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	6	1.11
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	6	1.11
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	6	1.11
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	6	1.11
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	6	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	6	1.11
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	6	1.11
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	6	1.11
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD11	6	1.11
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD12	6	1.11
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD13	6	1.11
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD11	9	1.11
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD12	9	1.11
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD13	9	1.11
(1,953)	2:31:B:ILE:HG21	2:24:C:PRO:HB2	5	1.11
(1,953)	2:31:B:ILE:HG22	2:24:C:PRO:HB2	5	1.11
(1,953)	2:31:B:ILE:HG23	2:24:C:PRO:HB2	5	1.11
(1,953)	2:31:B:ILE:HG21	2:24:C:PRO:HB2	6	1.11
(1,953)	2:31:B:ILE:HG22	2:24:C:PRO:HB2	6	1.11
(1,953)	2:31:B:ILE:HG23	2:24:C:PRO:HB2	6	1.11
(1,813)	2:34:C:ILE:HG23	2:37:C:ASP:H	1	1.11
(1,813)	2:34:C:ILE:HG23	2:37:C:ASP:H	2	1.11
(1,372)	1:11:A:ARG:HG2	1:12:A:LEU:H	3	1.11
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD21	3	1.11
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD22	3	1.11
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD23	3	1.11
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD21	3	1.11
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD22	3	1.11
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD23	3	1.11
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD21	3	1.11
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD22	3	1.11
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD23	3	1.11
(1,1931)	2:19:B:LEU:HD21	2:48:B:ALA:HA	6	1.1
(1,1931)	2:19:B:LEU:HD22	2:48:B:ALA:HA	6	1.1
(1,1931)	2:19:B:LEU:HD23	2:48:B:ALA:HA	6	1.1
(1,1778)	2:46:B:ALA:HB1	2:47:B:GLU:HG2	4	1.1
(1,1778)	2:46:B:ALA:HB2	2:47:B:GLU:HG2	4	1.1
(1,1778)	2:46:B:ALA:HB3	2:47:B:GLU:HG2	4	1.1
(1,1432)	1:24:A:GLY:HA3	2:19:C:LEU:HB2	5	1.1
(1,1149)	2:35:B:HIS:HB3	2:34:B:ILE:HB	3	1.1
(1,953)	2:31:B:ILE:HG21	2:24:C:PRO:HB2	10	1.1
(1,953)	2:31:B:ILE:HG22	2:24:C:PRO:HB2	10	1.1
(1,953)	2:31:B:ILE:HG23	2:24:C:PRO:HB2	10	1.1
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	4	1.09
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	4	1.09
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	4	1.09
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	4	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	4	1.09
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	4	1.09
(1,1901)	2:37:B:ASP:HB3	2:44:B:LEU:HG	4	1.09
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	6	1.09
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	6	1.09
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	6	1.09
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	5	1.09
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	5	1.09
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	5	1.09
(1,1843)	2:19:B:LEU:HD21	2:22:B:LEU:HG	5	1.09
(1,1843)	2:19:B:LEU:HD22	2:22:B:LEU:HG	5	1.09
(1,1843)	2:19:B:LEU:HD23	2:22:B:LEU:HG	5	1.09
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD21	1	1.09
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD22	1	1.09
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD23	1	1.09
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD21	1	1.09
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD22	1	1.09
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD23	1	1.09
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD21	1	1.09
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD22	1	1.09
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD23	1	1.09
(1,1552)	2:17:B:VAL:HG21	2:15:B:GLU:HG2	8	1.09
(1,1552)	2:17:B:VAL:HG22	2:15:B:GLU:HG2	8	1.09
(1,1552)	2:17:B:VAL:HG23	2:15:B:GLU:HG2	8	1.09
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB1	3	1.09
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB2	3	1.09
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB3	3	1.09
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB1	3	1.09
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB2	3	1.09
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB3	3	1.09
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB1	3	1.09
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB2	3	1.09
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB3	3	1.09
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB1	6	1.09
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB2	6	1.09
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB3	6	1.09
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB1	6	1.09
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB2	6	1.09
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB3	6	1.09
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB1	6	1.09
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB2	6	1.09
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB3	6	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB1	8	1.09
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB2	8	1.09
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB3	8	1.09
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB1	8	1.09
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB2	8	1.09
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB3	8	1.09
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB1	8	1.09
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB2	8	1.09
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB3	8	1.09
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD11	5	1.09
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD12	5	1.09
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD13	5	1.09
(1,1149)	2:35:B:HIS:HB3	2:34:B:ILE:HB	6	1.09
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	3	1.09
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	3	1.09
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	3	1.09
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	3	1.09
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	3	1.09
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	3	1.09
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	3	1.09
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	3	1.09
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	3	1.09
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD11	2	1.08
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD12	2	1.08
(1,1541)	1:23:A:PHE:HD1	2:27:C:LEU:HD13	2	1.08
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD11	2	1.08
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD12	2	1.08
(1,1541)	1:23:A:PHE:HD2	2:27:C:LEU:HD13	2	1.08
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	4	1.08
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	4	1.08
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	4	1.08
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	4	1.08
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	4	1.08
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	4	1.08
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	4	1.08
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	4	1.08
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	4	1.08
(1,276)	1:27:A:LEU:HD11	2:45:C:LEU:HG	10	1.08
(1,276)	1:27:A:LEU:HD12	2:45:C:LEU:HG	10	1.08
(1,276)	1:27:A:LEU:HD13	2:45:C:LEU:HG	10	1.08
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	6	1.08
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	6	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	6	1.08
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	6	1.08
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	6	1.08
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	6	1.08
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	6	1.08
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	6	1.08
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	6	1.08
(1,1901)	2:37:B:ASP:HB3	2:44:B:LEU:HG	1	1.07
(1,1849)	2:22:B:LEU:HD11	2:19:B:LEU:HG	8	1.07
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD21	7	1.07
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD22	7	1.07
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD23	7	1.07
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	7	1.06
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	7	1.06
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	7	1.06
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	7	1.06
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	7	1.06
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	7	1.06
(1,1605)	2:19:B:LEU:HD21	2:52:B:ASN:HB3	6	1.06
(1,1605)	2:19:B:LEU:HD22	2:52:B:ASN:HB3	6	1.06
(1,1605)	2:19:B:LEU:HD23	2:52:B:ASN:HB3	6	1.06
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD21	8	1.06
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD22	8	1.06
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD23	8	1.06
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD21	8	1.06
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD22	8	1.06
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD23	8	1.06
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD21	8	1.06
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD22	8	1.06
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD23	8	1.06
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB1	2	1.06
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB2	2	1.06
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB3	2	1.06
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB1	2	1.06
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB2	2	1.06
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB3	2	1.06
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB1	2	1.06
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB2	2	1.06
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB3	2	1.06
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD11	10	1.06
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD12	10	1.06
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD13	10	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD21	3	1.06
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD22	3	1.06
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD23	3	1.06
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD11	3	1.06
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD12	3	1.06
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD13	3	1.06
(1,372)	1:11:A:ARG:HG2	1:12:A:LEU:H	2	1.06
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	7	1.06
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	7	1.06
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	7	1.06
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	7	1.06
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	7	1.06
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	7	1.06
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	7	1.06
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	7	1.06
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	7	1.06
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	8	1.05
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	8	1.05
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	8	1.05
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	8	1.05
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	8	1.05
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	8	1.05
(1,1862)	2:27:B:LEU:HD21	2:24:B:PRO:HA	2	1.05
(1,1862)	2:27:B:LEU:HD22	2:24:B:PRO:HA	2	1.05
(1,1862)	2:27:B:LEU:HD23	2:24:B:PRO:HA	2	1.05
(1,1790)	2:56:C:ALA:HB2	2:53:C:ASP:HB2	8	1.05
(1,276)	1:27:A:LEU:HD11	2:45:C:LEU:HG	4	1.05
(1,276)	1:27:A:LEU:HD12	2:45:C:LEU:HG	4	1.05
(1,276)	1:27:A:LEU:HD13	2:45:C:LEU:HG	4	1.05
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	4	1.05
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	4	1.05
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	4	1.05
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	4	1.05
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	4	1.05
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	4	1.05
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	4	1.05
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	4	1.05
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	4	1.05
(1,1931)	2:19:B:LEU:HD21	2:48:B:ALA:HA	7	1.04
(1,1931)	2:19:B:LEU:HD22	2:48:B:ALA:HA	7	1.04
(1,1931)	2:19:B:LEU:HD23	2:48:B:ALA:HA	7	1.04
(1,813)	2:34:C:ILE:HG23	2:37:C:ASP:H	6	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,372)	1:11:A:ARG:HG2	1:12:A:LEU:H	1	1.04
(1,269)	1:27:A:LEU:HD11	1:13:A:ALA:HA	1	1.04
(1,269)	1:27:A:LEU:HD12	1:13:A:ALA:HA	1	1.04
(1,269)	1:27:A:LEU:HD13	1:13:A:ALA:HA	1	1.04
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	3	1.03
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	3	1.03
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	3	1.03
(1,1606)	2:19:B:LEU:HD21	2:52:B:ASN:HB2	6	1.03
(1,1606)	2:19:B:LEU:HD22	2:52:B:ASN:HB2	6	1.03
(1,1606)	2:19:B:LEU:HD23	2:52:B:ASN:HB2	6	1.03
(1,1605)	2:19:B:LEU:HD21	2:52:B:ASN:HB3	4	1.03
(1,1605)	2:19:B:LEU:HD22	2:52:B:ASN:HB3	4	1.03
(1,1605)	2:19:B:LEU:HD23	2:52:B:ASN:HB3	4	1.03
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD21	5	1.03
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD22	5	1.03
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD23	5	1.03
(1,372)	1:11:A:ARG:HG2	1:12:A:LEU:H	5	1.03
(1,372)	1:11:A:ARG:HG2	1:12:A:LEU:H	8	1.03
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	9	1.02
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	9	1.02
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	9	1.02
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	9	1.02
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	9	1.02
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	9	1.02
(1,1790)	2:56:C:ALA:HB1	2:53:C:ASP:HB2	10	1.02
(1,1316)	2:17:B:VAL:HG21	2:49:B:LYS:HE2	5	1.02
(1,1316)	2:17:B:VAL:HG21	2:49:B:LYS:HE3	5	1.02
(1,1316)	2:17:B:VAL:HG22	2:49:B:LYS:HE2	5	1.02
(1,1316)	2:17:B:VAL:HG22	2:49:B:LYS:HE3	5	1.02
(1,1316)	2:17:B:VAL:HG23	2:49:B:LYS:HE2	5	1.02
(1,1316)	2:17:B:VAL:HG23	2:49:B:LYS:HE3	5	1.02
(1,1149)	2:35:B:HIS:HB3	2:34:B:ILE:HB	10	1.02
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	10	1.02
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	10	1.02
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	10	1.02
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	10	1.02
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	10	1.02
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	10	1.02
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	10	1.02
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	10	1.02
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	10	1.02
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD21	8	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD22	8	1.02
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD23	8	1.02
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD21	8	1.02
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD22	8	1.02
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD23	8	1.02
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD21	8	1.02
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD22	8	1.02
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD23	8	1.02
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD11	8	1.01
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD12	8	1.01
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD13	8	1.01
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD11	8	1.01
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD12	8	1.01
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD13	8	1.01
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD11	8	1.01
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD12	8	1.01
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD13	8	1.01
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD11	9	1.01
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD12	9	1.01
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD13	9	1.01
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD11	9	1.01
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD12	9	1.01
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD13	9	1.01
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD11	9	1.01
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD12	9	1.01
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD13	9	1.01
(1,1149)	2:35:B:HIS:HB3	2:34:B:ILE:HB	4	1.01
(1,1138)	2:24:B:PRO:HA	2:27:B:LEU:HB3	7	1.01
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	1	1.01
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	1	1.01
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	1	1.01
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	1	1.01
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	1	1.01
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	1	1.01
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	1	1.01
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	1	1.01
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	1	1.01
(1,1849)	2:22:B:LEU:HD11	2:19:B:LEU:HG	1	1.0
(1,1778)	2:46:B:ALA:HB1	2:47:B:GLU:HG2	10	1.0
(1,1778)	2:46:B:ALA:HB2	2:47:B:GLU:HG2	10	1.0
(1,1778)	2:46:B:ALA:HB3	2:47:B:GLU:HG2	10	1.0
(1,1545)	1:27:A:LEU:HD21	2:15:C:GLU:HG2	4	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1545)	1:27:A:LEU:HD22	2:15:C:GLU:HG2	4	1.0
(1,1545)	1:27:A:LEU:HD23	2:15:C:GLU:HG2	4	1.0
(1,372)	1:11:A:ARG:HG2	1:12:A:LEU:H	10	1.0
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	5	1.0
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	5	1.0
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	5	1.0
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	5	1.0
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	5	1.0
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	5	1.0
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	5	1.0
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	5	1.0
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	5	1.0
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	1	0.99
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	1	0.99
(1,1846)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	1	0.99
(1,1778)	2:46:B:ALA:HB1	2:47:B:GLU:HG2	3	0.99
(1,1778)	2:46:B:ALA:HB2	2:47:B:GLU:HG2	3	0.99
(1,1778)	2:46:B:ALA:HB3	2:47:B:GLU:HG2	3	0.99
(1,1545)	1:27:A:LEU:HD21	2:15:C:GLU:HG2	1	0.99
(1,1545)	1:27:A:LEU:HD22	2:15:C:GLU:HG2	1	0.99
(1,1545)	1:27:A:LEU:HD23	2:15:C:GLU:HG2	1	0.99
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD11	2	0.99
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD12	2	0.99
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD13	2	0.99
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD11	5	0.99
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD12	5	0.99
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD13	5	0.99
(1,1149)	2:35:B:HIS:HB3	2:34:B:ILE:HB	1	0.99
(1,1138)	2:24:B:PRO:HA	2:27:B:LEU:HB3	2	0.99
(1,1931)	2:19:B:LEU:HD21	2:48:B:ALA:HA	4	0.98
(1,1931)	2:19:B:LEU:HD22	2:48:B:ALA:HA	4	0.98
(1,1931)	2:19:B:LEU:HD23	2:48:B:ALA:HA	4	0.98
(1,953)	2:31:B:ILE:HG21	2:24:C:PRO:HB2	8	0.98
(1,953)	2:31:B:ILE:HG22	2:24:C:PRO:HB2	8	0.98
(1,953)	2:31:B:ILE:HG23	2:24:C:PRO:HB2	8	0.98
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD11	8	0.98
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD12	8	0.98
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD13	8	0.98
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	8	0.98
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	8	0.98
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	8	0.98
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	8	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	8	0.98
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	8	0.98
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	8	0.98
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	8	0.98
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	8	0.98
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	1	0.97
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	1	0.97
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	1	0.97
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	1	0.97
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	1	0.97
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	1	0.97
(1,1149)	2:35:B:HIS:HB3	2:34:B:ILE:HB	8	0.97
(1,953)	2:31:B:ILE:HG21	2:24:C:PRO:HB2	1	0.97
(1,953)	2:31:B:ILE:HG22	2:24:C:PRO:HB2	1	0.97
(1,953)	2:31:B:ILE:HG23	2:24:C:PRO:HB2	1	0.97
(1,810)	2:37:B:ASP:H	2:34:B:ILE:HG23	5	0.97
(1,1895)	2:31:C:ILE:HG13	2:34:C:ILE:HD11	2	0.96
(1,1432)	1:24:A:GLY:HA3	2:19:C:LEU:HB2	6	0.96
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD21	1	0.96
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD22	1	0.96
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD23	1	0.96
(1,381)	1:27:A:LEU:HD11	1:11:A:ARG:HG2	5	0.96
(1,381)	1:27:A:LEU:HD12	1:11:A:ARG:HG2	5	0.96
(1,381)	1:27:A:LEU:HD13	1:11:A:ARG:HG2	5	0.96
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD11	1	0.96
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD12	1	0.96
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD13	1	0.96
(1,1901)	2:37:B:ASP:HB3	2:44:B:LEU:HG	10	0.95
(1,1790)	2:56:C:ALA:HB2	2:53:C:ASP:HB2	7	0.95
(1,1552)	2:17:B:VAL:HG21	2:15:B:GLU:HG2	7	0.95
(1,1552)	2:17:B:VAL:HG22	2:15:B:GLU:HG2	7	0.95
(1,1552)	2:17:B:VAL:HG23	2:15:B:GLU:HG2	7	0.95
(1,1432)	1:24:A:GLY:HA3	2:19:C:LEU:HB2	4	0.95
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	2	0.94
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	2	0.94
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	2	0.94
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	2	0.94
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	2	0.94
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	2	0.94
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	2	0.94
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	2	0.94
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	2	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	4	0.94
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	4	0.94
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	4	0.94
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	9	0.94
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	9	0.94
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	9	0.94
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD21	9	0.94
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD22	9	0.94
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD23	9	0.94
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD21	9	0.94
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD22	9	0.94
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD23	9	0.94
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD21	9	0.94
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD22	9	0.94
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD23	9	0.94
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB1	7	0.94
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB2	7	0.94
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB3	7	0.94
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB1	7	0.94
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB2	7	0.94
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB3	7	0.94
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB1	7	0.94
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB2	7	0.94
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB3	7	0.94
(1,1316)	2:17:B:VAL:HG21	2:49:B:LYS:HE2	3	0.94
(1,1316)	2:17:B:VAL:HG21	2:49:B:LYS:HE3	3	0.94
(1,1316)	2:17:B:VAL:HG22	2:49:B:LYS:HE2	3	0.94
(1,1316)	2:17:B:VAL:HG22	2:49:B:LYS:HE3	3	0.94
(1,1316)	2:17:B:VAL:HG23	2:49:B:LYS:HE2	3	0.94
(1,1316)	2:17:B:VAL:HG23	2:49:B:LYS:HE3	3	0.94
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD21	8	0.94
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD22	8	0.94
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD23	8	0.94
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD11	10	0.94
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD12	10	0.94
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD13	10	0.94
(1,1931)	2:19:B:LEU:HD21	2:48:B:ALA:HA	2	0.93
(1,1931)	2:19:B:LEU:HD22	2:48:B:ALA:HA	2	0.93
(1,1931)	2:19:B:LEU:HD23	2:48:B:ALA:HA	2	0.93
(1,1931)	2:19:B:LEU:HD21	2:48:B:ALA:HA	9	0.93
(1,1931)	2:19:B:LEU:HD22	2:48:B:ALA:HA	9	0.93
(1,1931)	2:19:B:LEU:HD23	2:48:B:ALA:HA	9	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1790)	2:56:C:ALA:HB2	2:53:C:ASP:HB2	5	0.93
(1,1778)	2:46:B:ALA:HB1	2:47:B:GLU:HG2	5	0.93
(1,1778)	2:46:B:ALA:HB2	2:47:B:GLU:HG2	5	0.93
(1,1778)	2:46:B:ALA:HB3	2:47:B:GLU:HG2	5	0.93
(1,1778)	2:46:B:ALA:HB1	2:47:B:GLU:HG2	6	0.93
(1,1778)	2:46:B:ALA:HB2	2:47:B:GLU:HG2	6	0.93
(1,1778)	2:46:B:ALA:HB3	2:47:B:GLU:HG2	6	0.93
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD11	2	0.93
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD12	2	0.93
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD13	2	0.93
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD11	2	0.93
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD12	2	0.93
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD13	2	0.93
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD11	2	0.93
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD12	2	0.93
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD13	2	0.93
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD11	8	0.93
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD12	8	0.93
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD13	8	0.93
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD11	8	0.93
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD12	8	0.93
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD13	8	0.93
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD11	8	0.93
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD12	8	0.93
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD13	8	0.93
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD21	6	0.93
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD22	6	0.93
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD23	6	0.93
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD21	6	0.93
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD22	6	0.93
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD23	6	0.93
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD21	6	0.93
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD22	6	0.93
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD23	6	0.93
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD11	9	0.93
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD12	9	0.93
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD13	9	0.93
(1,810)	2:37:B:ASP:H	2:34:B:ILE:HG22	2	0.93
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD11	7	0.93
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD12	7	0.93
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD13	7	0.93
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB2	3	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1929)	2:44:C:LEU:HD21	2:47:C:GLU:HB3	3	0.92
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB2	3	0.92
(1,1929)	2:44:C:LEU:HD22	2:47:C:GLU:HB3	3	0.92
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB2	3	0.92
(1,1929)	2:44:C:LEU:HD23	2:47:C:GLU:HB3	3	0.92
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	8	0.92
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	8	0.92
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	8	0.92
(1,1605)	2:19:B:LEU:HD21	2:52:B:ASN:HB3	9	0.92
(1,1605)	2:19:B:LEU:HD22	2:52:B:ASN:HB3	9	0.92
(1,1605)	2:19:B:LEU:HD23	2:52:B:ASN:HB3	9	0.92
(1,813)	2:34:C:ILE:HG23	2:37:C:ASP:H	4	0.92
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD11	4	0.92
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD12	4	0.92
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD13	4	0.92
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD11	5	0.92
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD12	5	0.92
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD13	5	0.92
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD11	6	0.92
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD12	6	0.92
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD13	6	0.92
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD11	9	0.92
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD12	9	0.92
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD13	9	0.92
(1,1790)	2:56:C:ALA:HB2	2:53:C:ASP:HB2	9	0.91
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD11	10	0.91
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD12	10	0.91
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD13	10	0.91
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD11	10	0.91
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD12	10	0.91
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD13	10	0.91
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD11	10	0.91
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD12	10	0.91
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD13	10	0.91
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD11	3	0.91
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD12	3	0.91
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD13	3	0.91
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD11	3	0.91
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD12	3	0.91
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD13	3	0.91
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD11	3	0.91
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD12	3	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD13	3	0.91
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD11	6	0.91
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD12	6	0.91
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD13	6	0.91
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD11	6	0.91
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD12	6	0.91
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD13	6	0.91
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD11	6	0.91
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD12	6	0.91
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD13	6	0.91
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD11	2	0.91
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD12	2	0.91
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD13	2	0.91
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD11	8	0.91
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD12	8	0.91
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD13	8	0.91
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD21	5	0.91
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD22	5	0.91
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD23	5	0.91
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD21	5	0.91
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD22	5	0.91
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD23	5	0.91
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD21	5	0.91
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD22	5	0.91
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD23	5	0.91
(1,1836)	2:19:B:LEU:HD21	2:22:B:LEU:HA	8	0.9
(1,1836)	2:19:B:LEU:HD22	2:22:B:LEU:HA	8	0.9
(1,1836)	2:19:B:LEU:HD23	2:22:B:LEU:HA	8	0.9
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD11	1	0.9
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD12	1	0.9
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD13	1	0.9
(1,1138)	2:24:B:PRO:HA	2:27:B:LEU:HB3	1	0.9
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD11	3	0.9
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD12	3	0.9
(1,249)	1:28:A:SER:H	1:27:A:LEU:HD13	3	0.9
(1,1809)	2:29:B:ALA:HB1	2:26:B:GLN:HG3	5	0.89
(1,1809)	2:29:B:ALA:HB2	2:26:B:GLN:HG3	5	0.89
(1,1809)	2:29:B:ALA:HB3	2:26:B:GLN:HG3	5	0.89
(1,953)	2:31:B:ILE:HG21	2:24:C:PRO:HB2	7	0.89
(1,953)	2:31:B:ILE:HG22	2:24:C:PRO:HB2	7	0.89
(1,953)	2:31:B:ILE:HG23	2:24:C:PRO:HB2	7	0.89
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD11	2	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD12	2	0.89
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD13	2	0.89
(1,381)	1:27:A:LEU:HD11	1:11:A:ARG:HG2	8	0.89
(1,381)	1:27:A:LEU:HD12	1:11:A:ARG:HG2	8	0.89
(1,381)	1:27:A:LEU:HD13	1:11:A:ARG:HG2	8	0.89
(1,1931)	2:19:B:LEU:HD21	2:48:B:ALA:HA	1	0.88
(1,1931)	2:19:B:LEU:HD22	2:48:B:ALA:HA	1	0.88
(1,1931)	2:19:B:LEU:HD23	2:48:B:ALA:HA	1	0.88
(1,1643)	2:32:B:HIS:HA	2:24:C:PRO:HB2	5	0.88
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	4	0.88
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	4	0.88
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	4	0.88
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG21	6	0.88
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG22	6	0.88
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG23	6	0.88
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD21	10	0.88
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD22	10	0.88
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD23	10	0.88
(1,372)	1:11:A:ARG:HG2	1:12:A:LEU:H	4	0.88
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD21	9	0.88
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD22	9	0.88
(1,171)	1:25:A:ALA:HB1	2:19:C:LEU:HD23	9	0.88
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD21	9	0.88
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD22	9	0.88
(1,171)	1:25:A:ALA:HB2	2:19:C:LEU:HD23	9	0.88
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD21	9	0.88
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD22	9	0.88
(1,171)	1:25:A:ALA:HB3	2:19:C:LEU:HD23	9	0.88
(1,1931)	2:19:B:LEU:HD21	2:48:B:ALA:HA	5	0.87
(1,1931)	2:19:B:LEU:HD22	2:48:B:ALA:HA	5	0.87
(1,1931)	2:19:B:LEU:HD23	2:48:B:ALA:HA	5	0.87
(1,1836)	2:19:B:LEU:HD21	2:22:B:LEU:HA	1	0.87
(1,1836)	2:19:B:LEU:HD22	2:22:B:LEU:HA	1	0.87
(1,1836)	2:19:B:LEU:HD23	2:22:B:LEU:HA	1	0.87
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD11	7	0.87
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD12	7	0.87
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD13	7	0.87
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD11	7	0.87
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD12	7	0.87
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD13	7	0.87
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD11	7	0.87
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD12	7	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD13	7	0.87
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD11	10	0.87
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD12	10	0.87
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD13	10	0.87
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB1	9	0.87
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB2	9	0.87
(1,248)	1:27:A:LEU:HD11	1:13:A:ALA:HB3	9	0.87
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB1	9	0.87
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB2	9	0.87
(1,248)	1:27:A:LEU:HD12	1:13:A:ALA:HB3	9	0.87
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB1	9	0.87
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB2	9	0.87
(1,248)	1:27:A:LEU:HD13	1:13:A:ALA:HB3	9	0.87
(1,1809)	2:29:B:ALA:HB1	2:26:B:GLN:HG3	7	0.86
(1,1809)	2:29:B:ALA:HB2	2:26:B:GLN:HG3	7	0.86
(1,1809)	2:29:B:ALA:HB3	2:26:B:GLN:HG3	7	0.86
(1,1790)	2:56:C:ALA:HB3	2:53:C:ASP:HB2	3	0.86
(1,1862)	2:27:B:LEU:HD21	2:24:B:PRO:HA	6	0.85
(1,1862)	2:27:B:LEU:HD22	2:24:B:PRO:HA	6	0.85
(1,1862)	2:27:B:LEU:HD23	2:24:B:PRO:HA	6	0.85
(1,1606)	2:19:B:LEU:HD21	2:52:B:ASN:HB2	9	0.85
(1,1606)	2:19:B:LEU:HD22	2:52:B:ASN:HB2	9	0.85
(1,1606)	2:19:B:LEU:HD23	2:52:B:ASN:HB2	9	0.85
(1,1605)	2:19:B:LEU:HD21	2:52:B:ASN:HB3	2	0.85
(1,1605)	2:19:B:LEU:HD22	2:52:B:ASN:HB3	2	0.85
(1,1605)	2:19:B:LEU:HD23	2:52:B:ASN:HB3	2	0.85
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD11	1	0.85
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD12	1	0.85
(1,1565)	1:17:A:VAL:HG11	2:19:B:LEU:HD13	1	0.85
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD11	1	0.85
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD12	1	0.85
(1,1565)	1:17:A:VAL:HG12	2:19:B:LEU:HD13	1	0.85
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD11	1	0.85
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD12	1	0.85
(1,1565)	1:17:A:VAL:HG13	2:19:B:LEU:HD13	1	0.85
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD11	7	0.85
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD12	7	0.85
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD13	7	0.85
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD11	8	0.85
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD12	8	0.85
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD13	8	0.85
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD11	4	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD12	4	0.84
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD13	4	0.84
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD11	4	0.84
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD12	4	0.84
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD13	4	0.84
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD11	4	0.84
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD12	4	0.84
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD13	4	0.84
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD11	1	0.84
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD12	1	0.84
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD13	1	0.84
(1,813)	2:34:C:ILE:HG22	2:37:C:ASP:H	8	0.84
(1,372)	1:11:A:ARG:HG2	1:12:A:LEU:H	6	0.84
(1,372)	1:11:A:ARG:HG2	1:12:A:LEU:H	9	0.84
(1,100)	1:28:A:SER:HB2	1:12:A:LEU:H	9	0.84
(1,1790)	2:56:C:ALA:HB1	2:53:C:ASP:HB2	4	0.83
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD11	5	0.83
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD12	5	0.83
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD13	5	0.83
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD11	3	0.83
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD12	3	0.83
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD13	3	0.83
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD11	4	0.83
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD12	4	0.83
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD13	4	0.83
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG21	8	0.83
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG22	8	0.83
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG23	8	0.83
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD21	6	0.83
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD22	6	0.83
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD23	6	0.83
(1,991)	2:16:C:ILE:HG22	1:26:A:ILE:HG13	3	0.83
(1,1809)	2:29:B:ALA:HB1	2:26:B:GLN:HG3	8	0.82
(1,1809)	2:29:B:ALA:HB2	2:26:B:GLN:HG3	8	0.82
(1,1809)	2:29:B:ALA:HB3	2:26:B:GLN:HG3	8	0.82
(1,1809)	2:29:B:ALA:HB1	2:26:B:GLN:HG3	10	0.82
(1,1809)	2:29:B:ALA:HB2	2:26:B:GLN:HG3	10	0.82
(1,1809)	2:29:B:ALA:HB3	2:26:B:GLN:HG3	10	0.82
(1,1552)	2:17:B:VAL:HG21	2:15:B:GLU:HG2	4	0.82
(1,1552)	2:17:B:VAL:HG22	2:15:B:GLU:HG2	4	0.82
(1,1552)	2:17:B:VAL:HG23	2:15:B:GLU:HG2	4	0.82
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	2	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	2	0.82
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	2	0.82
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	2	0.82
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	2	0.82
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	2	0.82
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	2	0.82
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	2	0.82
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	2	0.82
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD11	6	0.82
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD12	6	0.82
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD13	6	0.82
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD11	10	0.82
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD12	10	0.82
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD13	10	0.82
(1,991)	2:16:C:ILE:HG22	1:26:A:ILE:HG13	8	0.82
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD11	6	0.82
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD12	6	0.82
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD13	6	0.82
(1,810)	2:37:B:ASP:H	2:44:B:LEU:HD22	1	0.82
(1,810)	2:37:B:ASP:H	2:44:B:LEU:HD23	3	0.82
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	1	0.82
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	1	0.82
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	1	0.82
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	1	0.82
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	1	0.82
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	1	0.82
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	1	0.82
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	1	0.82
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	1	0.82
(1,1921)	2:37:B:ASP:HB3	2:40:B:GLN:HG2	5	0.81
(1,1901)	2:37:B:ASP:HB3	2:44:B:LEU:HG	8	0.81
(1,1809)	2:29:B:ALA:HB1	2:26:B:GLN:HG3	1	0.81
(1,1809)	2:29:B:ALA:HB2	2:26:B:GLN:HG3	1	0.81
(1,1809)	2:29:B:ALA:HB3	2:26:B:GLN:HG3	1	0.81
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD11	5	0.81
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD12	5	0.81
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD13	5	0.81
(1,1138)	2:24:B:PRO:HA	2:27:B:LEU:HB3	9	0.81
(1,991)	2:16:C:ILE:HG22	1:26:A:ILE:HG13	7	0.81
(1,962)	2:44:C:LEU:HD11	2:34:C:ILE:HB	1	0.81
(1,962)	2:44:C:LEU:HD12	2:34:C:ILE:HB	1	0.81
(1,962)	2:44:C:LEU:HD13	2:34:C:ILE:HB	1	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,810)	2:37:B:ASP:H	2:44:B:LEU:HD21	9	0.81
(1,447)	1:19:A:SER:HB2	2:45:B:LEU:HD22	4	0.81
(1,63)	1:29:A:SER:H	1:29:A:SER:HB3	10	0.81
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD11	1	0.8
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD12	1	0.8
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD13	1	0.8
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD11	2	0.8
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD12	2	0.8
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD13	2	0.8
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD11	9	0.8
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD12	9	0.8
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD13	9	0.8
(1,810)	2:37:B:ASP:H	2:44:B:LEU:HD23	6	0.8
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	5	0.8
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	5	0.8
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	5	0.8
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	5	0.8
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	5	0.8
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	5	0.8
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	5	0.8
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	5	0.8
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	5	0.8
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	8	0.8
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	8	0.8
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	8	0.8
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	8	0.8
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	8	0.8
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	8	0.8
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	8	0.8
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	8	0.8
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	8	0.8
(1,1901)	2:37:B:ASP:HB3	2:44:B:LEU:HG	6	0.79
(1,1836)	2:19:B:LEU:HD21	2:22:B:LEU:HA	10	0.79
(1,1836)	2:19:B:LEU:HD22	2:22:B:LEU:HA	10	0.79
(1,1836)	2:19:B:LEU:HD23	2:22:B:LEU:HA	10	0.79
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD11	2	0.79
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD12	2	0.79
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD13	2	0.79
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD11	5	0.79
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD12	5	0.79
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD13	5	0.79
(1,1809)	2:29:B:ALA:HB1	2:26:B:GLN:HG3	9	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1809)	2:29:B:ALA:HB2	2:26:B:GLN:HG3	9	0.79
(1,1809)	2:29:B:ALA:HB3	2:26:B:GLN:HG3	9	0.79
(1,1552)	2:17:B:VAL:HG21	2:15:B:GLU:HG2	6	0.79
(1,1552)	2:17:B:VAL:HG22	2:15:B:GLU:HG2	6	0.79
(1,1552)	2:17:B:VAL:HG23	2:15:B:GLU:HG2	6	0.79
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB1	1	0.79
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB2	1	0.79
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB3	1	0.79
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB1	1	0.79
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB2	1	0.79
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB3	1	0.79
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB1	1	0.79
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB2	1	0.79
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB3	1	0.79
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB1	4	0.79
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB2	4	0.79
(1,1438)	2:19:C:LEU:HD11	2:48:C:ALA:HB3	4	0.79
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB1	4	0.79
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB2	4	0.79
(1,1438)	2:19:C:LEU:HD12	2:48:C:ALA:HB3	4	0.79
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB1	4	0.79
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB2	4	0.79
(1,1438)	2:19:C:LEU:HD13	2:48:C:ALA:HB3	4	0.79
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD11	8	0.79
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD12	8	0.79
(1,1344)	2:23:B:ASN:H	2:22:B:LEU:HD13	8	0.79
(1,1138)	2:24:B:PRO:HA	2:27:B:LEU:HB3	5	0.79
(1,962)	2:44:C:LEU:HD11	2:34:C:ILE:HB	5	0.79
(1,962)	2:44:C:LEU:HD12	2:34:C:ILE:HB	5	0.79
(1,962)	2:44:C:LEU:HD13	2:34:C:ILE:HB	5	0.79
(1,813)	2:34:C:ILE:HG21	2:37:C:ASP:H	9	0.79
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	6	0.79
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	6	0.79
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	6	0.79
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	6	0.79
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	6	0.79
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	6	0.79
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	6	0.79
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	6	0.79
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	6	0.79
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	7	0.78
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	7	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	7	0.78
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD11	9	0.78
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD12	9	0.78
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD13	9	0.78
(1,1829)	2:21:C:ASN:H	2:20:C:PRO:HG3	7	0.78
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD11	8	0.78
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD12	8	0.78
(1,1357)	2:22:C:LEU:HA	2:22:C:LEU:HD13	8	0.78
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	2	0.78
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	2	0.78
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	2	0.78
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	2	0.78
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	2	0.78
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	2	0.78
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	2	0.78
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	2	0.78
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	2	0.78
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	7	0.78
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	7	0.78
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	7	0.78
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	7	0.78
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	7	0.78
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	7	0.78
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	7	0.78
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	7	0.78
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	7	0.78
(1,1873)	2:23:B:ASN:HD22	2:26:B:GLN:HG2	2	0.77
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD11	4	0.77
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD12	4	0.77
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD13	4	0.77
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD11	6	0.77
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD12	6	0.77
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD13	6	0.77
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD11	7	0.77
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD12	7	0.77
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD13	7	0.77
(1,1559)	2:19:B:LEU:HD21	2:22:B:LEU:HD11	1	0.77
(1,1559)	2:19:B:LEU:HD21	2:22:B:LEU:HD12	1	0.77
(1,1559)	2:19:B:LEU:HD21	2:22:B:LEU:HD13	1	0.77
(1,1559)	2:19:B:LEU:HD22	2:22:B:LEU:HD11	1	0.77
(1,1559)	2:19:B:LEU:HD22	2:22:B:LEU:HD12	1	0.77
(1,1559)	2:19:B:LEU:HD22	2:22:B:LEU:HD13	1	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1559)	2:19:B:LEU:HD23	2:22:B:LEU:HD11	1	0.77
(1,1559)	2:19:B:LEU:HD23	2:22:B:LEU:HD12	1	0.77
(1,1559)	2:19:B:LEU:HD23	2:22:B:LEU:HD13	1	0.77
(1,1559)	2:19:B:LEU:HD21	2:22:B:LEU:HD11	8	0.77
(1,1559)	2:19:B:LEU:HD21	2:22:B:LEU:HD12	8	0.77
(1,1559)	2:19:B:LEU:HD21	2:22:B:LEU:HD13	8	0.77
(1,1559)	2:19:B:LEU:HD22	2:22:B:LEU:HD11	8	0.77
(1,1559)	2:19:B:LEU:HD22	2:22:B:LEU:HD12	8	0.77
(1,1559)	2:19:B:LEU:HD22	2:22:B:LEU:HD13	8	0.77
(1,1559)	2:19:B:LEU:HD23	2:22:B:LEU:HD11	8	0.77
(1,1559)	2:19:B:LEU:HD23	2:22:B:LEU:HD12	8	0.77
(1,1559)	2:19:B:LEU:HD23	2:22:B:LEU:HD13	8	0.77
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD21	2	0.77
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD22	2	0.77
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD23	2	0.77
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD21	2	0.77
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD22	2	0.77
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD23	2	0.77
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD21	2	0.77
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD22	2	0.77
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD23	2	0.77
(1,1552)	2:17:B:VAL:HG21	2:15:B:GLU:HG2	5	0.77
(1,1552)	2:17:B:VAL:HG22	2:15:B:GLU:HG2	5	0.77
(1,1552)	2:17:B:VAL:HG23	2:15:B:GLU:HG2	5	0.77
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD11	7	0.77
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD12	7	0.77
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD13	7	0.77
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD11	4	0.77
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD12	4	0.77
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD13	4	0.77
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG21	1	0.77
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG22	1	0.77
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG23	1	0.77
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG21	10	0.77
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG22	10	0.77
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG23	10	0.77
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD11	5	0.77
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD12	5	0.77
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD13	5	0.77
(1,810)	2:37:B:ASP:H	2:44:B:LEU:HD23	7	0.77
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	9	0.77
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	9	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	9	0.77
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	9	0.77
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	9	0.77
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	9	0.77
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	9	0.77
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	9	0.77
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	9	0.77
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	5	0.76
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	5	0.76
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	5	0.76
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD11	3	0.76
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD12	3	0.76
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD13	3	0.76
(1,1752)	2:44:C:LEU:HD21	2:43:C:ASN:HB2	1	0.76
(1,1752)	2:44:C:LEU:HD21	2:43:C:ASN:HB3	1	0.76
(1,1752)	2:44:C:LEU:HD22	2:43:C:ASN:HB2	1	0.76
(1,1752)	2:44:C:LEU:HD22	2:43:C:ASN:HB3	1	0.76
(1,1752)	2:44:C:LEU:HD23	2:43:C:ASN:HB2	1	0.76
(1,1752)	2:44:C:LEU:HD23	2:43:C:ASN:HB3	1	0.76
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG21	9	0.76
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG22	9	0.76
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG23	9	0.76
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD21	3	0.75
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD22	3	0.75
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD23	3	0.75
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD21	3	0.75
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD22	3	0.75
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD23	3	0.75
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD21	3	0.75
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD22	3	0.75
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD23	3	0.75
(1,991)	2:16:C:ILE:HG22	1:26:A:ILE:HG13	1	0.75
(1,810)	2:37:B:ASP:H	2:44:B:LEU:HD23	8	0.75
(1,810)	2:37:B:ASP:H	2:44:B:LEU:HD22	10	0.75
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	4	0.75
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	4	0.75
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	4	0.75
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	4	0.75
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	4	0.75
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	4	0.75
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	4	0.75
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	4	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	4	0.75
(1,1895)	2:31:C:ILE:HG13	2:34:C:ILE:HD13	4	0.74
(1,1791)	2:54:B:ALA:HB1	2:53:B:ASP:HB3	9	0.74
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG21	2	0.74
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG22	2	0.74
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG23	2	0.74
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG21	1	0.74
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG22	1	0.74
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG23	1	0.74
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG21	5	0.74
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG22	5	0.74
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG23	5	0.74
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG21	8	0.74
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG22	8	0.74
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG23	8	0.74
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG21	9	0.74
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG22	9	0.74
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG23	9	0.74
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	3	0.74
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	3	0.74
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	3	0.74
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	3	0.74
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	3	0.74
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	3	0.74
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	3	0.74
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	3	0.74
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	3	0.74
(1,1862)	2:27:B:LEU:HD21	2:24:B:PRO:HA	4	0.73
(1,1862)	2:27:B:LEU:HD22	2:24:B:PRO:HA	4	0.73
(1,1862)	2:27:B:LEU:HD23	2:24:B:PRO:HA	4	0.73
(1,1545)	1:27:A:LEU:HD21	2:15:C:GLU:HG2	10	0.73
(1,1545)	1:27:A:LEU:HD22	2:15:C:GLU:HG2	10	0.73
(1,1545)	1:27:A:LEU:HD23	2:15:C:GLU:HG2	10	0.73
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	5	0.73
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	5	0.73
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	5	0.73
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	5	0.73
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	5	0.73
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	5	0.73
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	5	0.73
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	5	0.73
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	5	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD11	3	0.73
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD12	3	0.73
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD13	3	0.73
(1,1316)	2:17:B:VAL:HG21	2:49:B:LYS:HE2	6	0.73
(1,1316)	2:17:B:VAL:HG21	2:49:B:LYS:HE3	6	0.73
(1,1316)	2:17:B:VAL:HG22	2:49:B:LYS:HE2	6	0.73
(1,1316)	2:17:B:VAL:HG22	2:49:B:LYS:HE3	6	0.73
(1,1316)	2:17:B:VAL:HG23	2:49:B:LYS:HE2	6	0.73
(1,1316)	2:17:B:VAL:HG23	2:49:B:LYS:HE3	6	0.73
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD21	9	0.73
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD22	9	0.73
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD23	9	0.73
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG21	2	0.73
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG22	2	0.73
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG23	2	0.73
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD11	1	0.73
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD12	1	0.73
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD13	1	0.73
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	10	0.73
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	10	0.73
(1,256)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	10	0.73
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	10	0.73
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	10	0.73
(1,256)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	10	0.73
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	10	0.73
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	10	0.73
(1,256)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	10	0.73
(1,1895)	2:31:C:ILE:HG13	2:34:C:ILE:HD11	10	0.72
(1,1790)	2:56:C:ALA:HB1	2:53:C:ASP:HB2	6	0.72
(1,1606)	2:19:B:LEU:HD21	2:52:B:ASN:HB2	2	0.72
(1,1606)	2:19:B:LEU:HD22	2:52:B:ASN:HB2	2	0.72
(1,1606)	2:19:B:LEU:HD23	2:52:B:ASN:HB2	2	0.72
(1,991)	2:16:C:ILE:HG21	1:26:A:ILE:HG13	10	0.72
(1,810)	2:37:B:ASP:H	2:44:B:LEU:HD23	4	0.72
(1,1837)	2:19:C:LEU:HD11	2:22:C:LEU:HA	7	0.71
(1,1837)	2:19:C:LEU:HD12	2:22:C:LEU:HA	7	0.71
(1,1837)	2:19:C:LEU:HD13	2:22:C:LEU:HA	7	0.71
(1,1771)	2:47:B:GLU:H	2:47:B:GLU:HG2	4	0.71
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD21	10	0.71
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD22	10	0.71
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD23	10	0.71
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD21	10	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD22	10	0.71
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD23	10	0.71
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD21	10	0.71
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD22	10	0.71
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD23	10	0.71
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG21	4	0.71
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG22	4	0.71
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG23	4	0.71
(1,1895)	2:31:C:ILE:HG13	2:34:C:ILE:HD12	6	0.7
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD11	2	0.7
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD12	2	0.7
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD13	2	0.7
(1,1604)	2:19:C:LEU:HD11	2:52:C:ASN:HB3	1	0.7
(1,1604)	2:19:C:LEU:HD12	2:52:C:ASN:HB3	1	0.7
(1,1604)	2:19:C:LEU:HD13	2:52:C:ASN:HB3	1	0.7
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG21	10	0.7
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG22	10	0.7
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG23	10	0.7
(1,1138)	2:24:B:PRO:HA	2:27:B:LEU:HB3	6	0.7
(1,962)	2:44:C:LEU:HD11	2:34:C:ILE:HB	7	0.7
(1,962)	2:44:C:LEU:HD12	2:34:C:ILE:HB	7	0.7
(1,962)	2:44:C:LEU:HD13	2:34:C:ILE:HB	7	0.7
(1,63)	1:29:A:SER:H	1:29:A:SER:HB3	7	0.7
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD11	8	0.69
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD12	8	0.69
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD13	8	0.69
(1,1604)	2:19:C:LEU:HD11	2:52:C:ASN:HB3	4	0.69
(1,1604)	2:19:C:LEU:HD12	2:52:C:ASN:HB3	4	0.69
(1,1604)	2:19:C:LEU:HD13	2:52:C:ASN:HB3	4	0.69
(1,1604)	2:19:C:LEU:HD11	2:52:C:ASN:HB3	10	0.69
(1,1604)	2:19:C:LEU:HD12	2:52:C:ASN:HB3	10	0.69
(1,1604)	2:19:C:LEU:HD13	2:52:C:ASN:HB3	10	0.69
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD11	1	0.69
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD12	1	0.69
(1,1558)	2:19:C:LEU:HD11	2:22:C:LEU:HD13	1	0.69
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD11	1	0.69
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD12	1	0.69
(1,1558)	2:19:C:LEU:HD12	2:22:C:LEU:HD13	1	0.69
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD11	1	0.69
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD12	1	0.69
(1,1558)	2:19:C:LEU:HD13	2:22:C:LEU:HD13	1	0.69
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG21	4	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG22	4	0.69
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG23	4	0.69
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG21	3	0.69
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG22	3	0.69
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG23	3	0.69
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG21	6	0.69
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG22	6	0.69
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG23	6	0.69
(1,991)	2:16:C:ILE:HG22	1:26:A:ILE:HG13	2	0.69
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD11	3	0.69
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD12	3	0.69
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD13	3	0.69
(1,1604)	2:19:C:LEU:HD11	2:52:C:ASN:HB3	7	0.68
(1,1604)	2:19:C:LEU:HD12	2:52:C:ASN:HB3	7	0.68
(1,1604)	2:19:C:LEU:HD13	2:52:C:ASN:HB3	7	0.68
(1,1559)	2:19:B:LEU:HD21	2:22:B:LEU:HD11	10	0.68
(1,1559)	2:19:B:LEU:HD21	2:22:B:LEU:HD12	10	0.68
(1,1559)	2:19:B:LEU:HD21	2:22:B:LEU:HD13	10	0.68
(1,1559)	2:19:B:LEU:HD22	2:22:B:LEU:HD11	10	0.68
(1,1559)	2:19:B:LEU:HD22	2:22:B:LEU:HD12	10	0.68
(1,1559)	2:19:B:LEU:HD22	2:22:B:LEU:HD13	10	0.68
(1,1559)	2:19:B:LEU:HD23	2:22:B:LEU:HD11	10	0.68
(1,1559)	2:19:B:LEU:HD23	2:22:B:LEU:HD12	10	0.68
(1,1559)	2:19:B:LEU:HD23	2:22:B:LEU:HD13	10	0.68
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG21	7	0.68
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG22	7	0.68
(1,1023)	2:18:B:TYR:H	2:17:B:VAL:HG23	7	0.68
(1,991)	2:16:C:ILE:HG23	1:26:A:ILE:HG13	9	0.68
(1,1902)	2:44:B:LEU:HD11	2:37:B:ASP:HB3	10	0.67
(1,1902)	2:44:B:LEU:HD12	2:37:B:ASP:HB3	10	0.67
(1,1902)	2:44:B:LEU:HD13	2:37:B:ASP:HB3	10	0.67
(1,1771)	2:47:B:GLU:H	2:47:B:GLU:HG2	10	0.67
(1,1432)	1:24:A:GLY:HA3	2:19:C:LEU:HB2	9	0.67
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD11	9	0.67
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD12	9	0.67
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD13	9	0.67
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG21	8	0.67
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG22	8	0.67
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG23	8	0.67
(1,1316)	2:17:B:VAL:HG21	2:49:B:LYS:HE2	7	0.67
(1,1316)	2:17:B:VAL:HG21	2:49:B:LYS:HE3	7	0.67
(1,1316)	2:17:B:VAL:HG22	2:49:B:LYS:HE2	7	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1316)	2:17:B:VAL:HG22	2:49:B:LYS:HE3	7	0.67
(1,1316)	2:17:B:VAL:HG23	2:49:B:LYS:HE2	7	0.67
(1,1316)	2:17:B:VAL:HG23	2:49:B:LYS:HE3	7	0.67
(1,1138)	2:24:B:PRO:HA	2:27:B:LEU:HB3	8	0.67
(1,991)	2:16:C:ILE:HG23	1:26:A:ILE:HG13	5	0.67
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD11	9	0.67
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD12	9	0.67
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD13	9	0.67
(1,267)	1:27:A:LEU:HD11	2:45:C:LEU:HB3	10	0.67
(1,267)	1:27:A:LEU:HD12	2:45:C:LEU:HB3	10	0.67
(1,267)	1:27:A:LEU:HD13	2:45:C:LEU:HB3	10	0.67
(1,1791)	2:54:B:ALA:HB1	2:53:B:ASP:HB3	6	0.66
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD21	5	0.66
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD22	5	0.66
(1,1556)	2:17:C:VAL:HG11	2:19:C:LEU:HD23	5	0.66
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD21	5	0.66
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD22	5	0.66
(1,1556)	2:17:C:VAL:HG12	2:19:C:LEU:HD23	5	0.66
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD21	5	0.66
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD22	5	0.66
(1,1556)	2:17:C:VAL:HG13	2:19:C:LEU:HD23	5	0.66
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD11	4	0.66
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD12	4	0.66
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD13	4	0.66
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD11	7	0.66
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD12	7	0.66
(1,912)	2:23:C:ASN:H	2:22:C:LEU:HD13	7	0.66
(1,413)	1:11:A:ARG:HG2	1:12:A:LEU:HD11	10	0.66
(1,413)	1:11:A:ARG:HG2	1:12:A:LEU:HD12	10	0.66
(1,413)	1:11:A:ARG:HG2	1:12:A:LEU:HD13	10	0.66
(1,267)	1:27:A:LEU:HD11	2:45:C:LEU:HB3	2	0.66
(1,267)	1:27:A:LEU:HD12	2:45:C:LEU:HB3	2	0.66
(1,267)	1:27:A:LEU:HD13	2:45:C:LEU:HB3	2	0.66
(1,267)	1:27:A:LEU:HD11	2:45:C:LEU:HB3	4	0.66
(1,267)	1:27:A:LEU:HD12	2:45:C:LEU:HB3	4	0.66
(1,267)	1:27:A:LEU:HD13	2:45:C:LEU:HB3	4	0.66
(1,1931)	2:19:B:LEU:HD21	2:48:B:ALA:HA	8	0.65
(1,1931)	2:19:B:LEU:HD22	2:48:B:ALA:HA	8	0.65
(1,1931)	2:19:B:LEU:HD23	2:48:B:ALA:HA	8	0.65
(1,1902)	2:44:B:LEU:HD11	2:37:B:ASP:HB3	1	0.65
(1,1902)	2:44:B:LEU:HD12	2:37:B:ASP:HB3	1	0.65
(1,1902)	2:44:B:LEU:HD13	2:37:B:ASP:HB3	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD11	1	0.65
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD12	1	0.65
(1,1879)	2:52:C:ASN:HB3	2:22:C:LEU:HD13	1	0.65
(1,1837)	2:19:C:LEU:HD11	2:22:C:LEU:HA	3	0.65
(1,1837)	2:19:C:LEU:HD12	2:22:C:LEU:HA	3	0.65
(1,1837)	2:19:C:LEU:HD13	2:22:C:LEU:HA	3	0.65
(1,1836)	2:19:B:LEU:HD21	2:22:B:LEU:HA	7	0.65
(1,1836)	2:19:B:LEU:HD22	2:22:B:LEU:HA	7	0.65
(1,1836)	2:19:B:LEU:HD23	2:22:B:LEU:HA	7	0.65
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD11	1	0.65
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD12	1	0.65
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD13	1	0.65
(1,1791)	2:54:B:ALA:HB1	2:53:B:ASP:HB3	3	0.65
(1,1771)	2:47:B:GLU:H	2:47:B:GLU:HG2	5	0.65
(1,1604)	2:19:C:LEU:HD11	2:52:C:ASN:HB3	2	0.65
(1,1604)	2:19:C:LEU:HD12	2:52:C:ASN:HB3	2	0.65
(1,1604)	2:19:C:LEU:HD13	2:52:C:ASN:HB3	2	0.65
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD11	6	0.65
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD12	6	0.65
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD13	6	0.65
(1,1902)	2:44:B:LEU:HD11	2:37:B:ASP:HB3	4	0.64
(1,1902)	2:44:B:LEU:HD12	2:37:B:ASP:HB3	4	0.64
(1,1902)	2:44:B:LEU:HD13	2:37:B:ASP:HB3	4	0.64
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD11	2	0.64
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD12	2	0.64
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD13	2	0.64
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD11	3	0.64
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD12	3	0.64
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD13	3	0.64
(1,1433)	2:19:B:LEU:HD21	2:19:B:LEU:HB2	1	0.64
(1,1433)	2:19:B:LEU:HD22	2:19:B:LEU:HB2	1	0.64
(1,1433)	2:19:B:LEU:HD23	2:19:B:LEU:HB2	1	0.64
(1,1405)	2:17:B:VAL:HG11	2:45:B:LEU:HG	5	0.64
(1,1405)	2:17:B:VAL:HG12	2:45:B:LEU:HG	5	0.64
(1,1405)	2:17:B:VAL:HG13	2:45:B:LEU:HG	5	0.64
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG21	4	0.64
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG22	4	0.64
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG23	4	0.64
(1,991)	2:16:C:ILE:HG23	1:26:A:ILE:HG13	4	0.64
(1,962)	2:44:C:LEU:HD11	2:34:C:ILE:HB	4	0.64
(1,962)	2:44:C:LEU:HD12	2:34:C:ILE:HB	4	0.64
(1,962)	2:44:C:LEU:HD13	2:34:C:ILE:HB	4	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,953)	2:31:B:ILE:HG21	2:24:C:PRO:HB2	4	0.64
(1,953)	2:31:B:ILE:HG22	2:24:C:PRO:HB2	4	0.64
(1,953)	2:31:B:ILE:HG23	2:24:C:PRO:HB2	4	0.64
(1,1837)	2:19:C:LEU:HD11	2:22:C:LEU:HA	4	0.63
(1,1837)	2:19:C:LEU:HD12	2:22:C:LEU:HA	4	0.63
(1,1837)	2:19:C:LEU:HD13	2:22:C:LEU:HA	4	0.63
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD11	10	0.63
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD12	10	0.63
(1,1835)	2:22:B:LEU:HA	2:22:B:LEU:HD13	10	0.63
(1,1752)	2:44:C:LEU:HD21	2:43:C:ASN:HB2	7	0.63
(1,1752)	2:44:C:LEU:HD21	2:43:C:ASN:HB3	7	0.63
(1,1752)	2:44:C:LEU:HD22	2:43:C:ASN:HB2	7	0.63
(1,1752)	2:44:C:LEU:HD22	2:43:C:ASN:HB3	7	0.63
(1,1752)	2:44:C:LEU:HD23	2:43:C:ASN:HB2	7	0.63
(1,1752)	2:44:C:LEU:HD23	2:43:C:ASN:HB3	7	0.63
(1,1752)	2:44:C:LEU:HD21	2:43:C:ASN:HB2	9	0.63
(1,1752)	2:44:C:LEU:HD21	2:43:C:ASN:HB3	9	0.63
(1,1752)	2:44:C:LEU:HD22	2:43:C:ASN:HB2	9	0.63
(1,1752)	2:44:C:LEU:HD22	2:43:C:ASN:HB3	9	0.63
(1,1752)	2:44:C:LEU:HD23	2:43:C:ASN:HB2	9	0.63
(1,1752)	2:44:C:LEU:HD23	2:43:C:ASN:HB3	9	0.63
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD11	10	0.63
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD12	10	0.63
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD13	10	0.63
(1,1604)	2:19:C:LEU:HD11	2:52:C:ASN:HB3	3	0.63
(1,1604)	2:19:C:LEU:HD12	2:52:C:ASN:HB3	3	0.63
(1,1604)	2:19:C:LEU:HD13	2:52:C:ASN:HB3	3	0.63
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG21	9	0.63
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG22	9	0.63
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG23	9	0.63
(1,1138)	2:24:B:PRO:HA	2:27:B:LEU:HB3	4	0.63
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD21	4	0.63
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD22	4	0.63
(1,1107)	2:31:C:ILE:HA	2:27:C:LEU:HD23	4	0.63
(1,962)	2:44:C:LEU:HD11	2:34:C:ILE:HB	8	0.63
(1,962)	2:44:C:LEU:HD12	2:34:C:ILE:HB	8	0.63
(1,962)	2:44:C:LEU:HD13	2:34:C:ILE:HB	8	0.63
(1,408)	1:12:A:LEU:HD21	2:38:C:PRO:HB2	3	0.63
(1,408)	1:12:A:LEU:HD22	2:38:C:PRO:HB2	3	0.63
(1,408)	1:12:A:LEU:HD23	2:38:C:PRO:HB2	3	0.63
(1,381)	1:27:A:LEU:HD11	1:11:A:ARG:HG2	2	0.63
(1,381)	1:27:A:LEU:HD12	1:11:A:ARG:HG2	2	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,381)	1:27:A:LEU:HD13	1:11:A:ARG:HG2	2	0.63
(1,267)	1:27:A:LEU:HD11	2:45:C:LEU:HB3	3	0.63
(1,267)	1:27:A:LEU:HD12	2:45:C:LEU:HB3	3	0.63
(1,267)	1:27:A:LEU:HD13	2:45:C:LEU:HB3	3	0.63
(1,1902)	2:44:B:LEU:HD11	2:37:B:ASP:HB3	8	0.62
(1,1902)	2:44:B:LEU:HD12	2:37:B:ASP:HB3	8	0.62
(1,1902)	2:44:B:LEU:HD13	2:37:B:ASP:HB3	8	0.62
(1,1836)	2:19:B:LEU:HD21	2:22:B:LEU:HA	4	0.62
(1,1836)	2:19:B:LEU:HD22	2:22:B:LEU:HA	4	0.62
(1,1836)	2:19:B:LEU:HD23	2:22:B:LEU:HA	4	0.62
(1,1829)	2:21:C:ASN:H	2:20:C:PRO:HG3	4	0.62
(1,14)	1:17:A:VAL:H	1:16:A:LEU:HD21	1	0.62
(1,14)	1:17:A:VAL:H	1:16:A:LEU:HD22	4	0.62
(1,14)	1:17:A:VAL:H	1:16:A:LEU:HD21	5	0.62
(1,1895)	2:31:C:ILE:HG13	2:34:C:ILE:HD12	5	0.61
(1,1809)	2:29:B:ALA:HB1	2:26:B:GLN:HG3	2	0.61
(1,1809)	2:29:B:ALA:HB2	2:26:B:GLN:HG3	2	0.61
(1,1809)	2:29:B:ALA:HB3	2:26:B:GLN:HG3	2	0.61
(1,1771)	2:47:B:GLU:H	2:47:B:GLU:HG2	3	0.61
(1,1752)	2:44:C:LEU:HD21	2:43:C:ASN:HB2	6	0.61
(1,1752)	2:44:C:LEU:HD21	2:43:C:ASN:HB3	6	0.61
(1,1752)	2:44:C:LEU:HD22	2:43:C:ASN:HB2	6	0.61
(1,1752)	2:44:C:LEU:HD22	2:43:C:ASN:HB3	6	0.61
(1,1752)	2:44:C:LEU:HD23	2:43:C:ASN:HB2	6	0.61
(1,1752)	2:44:C:LEU:HD23	2:43:C:ASN:HB3	6	0.61
(1,1552)	2:17:B:VAL:HG21	2:15:B:GLU:HG2	1	0.61
(1,1552)	2:17:B:VAL:HG22	2:15:B:GLU:HG2	1	0.61
(1,1552)	2:17:B:VAL:HG23	2:15:B:GLU:HG2	1	0.61
(1,1433)	2:19:B:LEU:HD21	2:19:B:LEU:HB2	8	0.61
(1,1433)	2:19:B:LEU:HD22	2:19:B:LEU:HB2	8	0.61
(1,1433)	2:19:B:LEU:HD23	2:19:B:LEU:HB2	8	0.61
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD11	10	0.61
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD12	10	0.61
(1,1347)	2:52:B:ASN:H	2:22:B:LEU:HD13	10	0.61
(1,1829)	2:21:C:ASN:H	2:20:C:PRO:HG3	5	0.6
(1,1791)	2:54:B:ALA:HB2	2:53:B:ASP:HB3	4	0.6
(1,1204)	2:31:C:ILE:HD13	2:27:B:LEU:HG	10	0.6
(1,1138)	2:24:B:PRO:HA	2:27:B:LEU:HB3	10	0.6
(1,14)	1:17:A:VAL:H	1:16:A:LEU:HD23	7	0.6
(1,14)	1:17:A:VAL:H	1:16:A:LEU:HD22	8	0.6
(1,1791)	2:54:B:ALA:HB2	2:53:B:ASP:HB3	1	0.59
(1,1771)	2:47:B:GLU:H	2:47:B:GLU:HG2	6	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1619)	2:23:C:ASN:HB2	2:24:C:PRO:HD2	10	0.59
(1,1433)	2:19:B:LEU:HD21	2:19:B:LEU:HB2	10	0.59
(1,1433)	2:19:B:LEU:HD22	2:19:B:LEU:HB2	10	0.59
(1,1433)	2:19:B:LEU:HD23	2:19:B:LEU:HB2	10	0.59
(1,1204)	2:31:C:ILE:HD12	2:27:B:LEU:HG	4	0.59
(1,962)	2:44:C:LEU:HD11	2:34:C:ILE:HB	6	0.59
(1,962)	2:44:C:LEU:HD12	2:34:C:ILE:HB	6	0.59
(1,962)	2:44:C:LEU:HD13	2:34:C:ILE:HB	6	0.59
(1,14)	1:17:A:VAL:H	1:16:A:LEU:HD22	2	0.59
(1,14)	1:17:A:VAL:H	1:16:A:LEU:HD22	3	0.59
(1,1836)	2:19:B:LEU:HD21	2:22:B:LEU:HA	3	0.58
(1,1836)	2:19:B:LEU:HD22	2:22:B:LEU:HA	3	0.58
(1,1836)	2:19:B:LEU:HD23	2:22:B:LEU:HA	3	0.58
(1,1791)	2:54:B:ALA:HB1	2:53:B:ASP:HB3	8	0.58
(1,1604)	2:19:C:LEU:HD11	2:52:C:ASN:HB3	6	0.58
(1,1604)	2:19:C:LEU:HD12	2:52:C:ASN:HB3	6	0.58
(1,1604)	2:19:C:LEU:HD13	2:52:C:ASN:HB3	6	0.58
(1,1604)	2:19:C:LEU:HD11	2:52:C:ASN:HB3	8	0.58
(1,1604)	2:19:C:LEU:HD12	2:52:C:ASN:HB3	8	0.58
(1,1604)	2:19:C:LEU:HD13	2:52:C:ASN:HB3	8	0.58
(1,1552)	2:17:B:VAL:HG21	2:15:B:GLU:HG2	2	0.58
(1,1552)	2:17:B:VAL:HG22	2:15:B:GLU:HG2	2	0.58
(1,1552)	2:17:B:VAL:HG23	2:15:B:GLU:HG2	2	0.58
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD11	7	0.58
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD12	7	0.58
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD13	7	0.58
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD11	4	0.58
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD12	4	0.58
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD13	4	0.58
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD11	1	0.58
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD12	1	0.58
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD13	1	0.58
(1,307)	1:14:A:ASN:HB3	1:14:A:ASN:HD22	8	0.58
(1,63)	1:29:A:SER:H	1:29:A:SER:HB3	9	0.58
(1,1902)	2:44:B:LEU:HD11	2:37:B:ASP:HB3	6	0.57
(1,1902)	2:44:B:LEU:HD12	2:37:B:ASP:HB3	6	0.57
(1,1902)	2:44:B:LEU:HD13	2:37:B:ASP:HB3	6	0.57
(1,1837)	2:19:C:LEU:HD11	2:22:C:LEU:HA	1	0.57
(1,1837)	2:19:C:LEU:HD12	2:22:C:LEU:HA	1	0.57
(1,1837)	2:19:C:LEU:HD13	2:22:C:LEU:HA	1	0.57
(1,1613)	2:23:B:ASN:HB2	2:23:B:ASN:HD22	9	0.57
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD11	6	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD12	6	0.57
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD13	6	0.57
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD11	8	0.57
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD12	8	0.57
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD13	8	0.57
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD11	9	0.57
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD12	9	0.57
(1,1467)	2:45:C:LEU:HB2	2:45:C:LEU:HD13	9	0.57
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD11	9	0.57
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD12	9	0.57
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD13	9	0.57
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG21	10	0.57
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG22	10	0.57
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG23	10	0.57
(1,1242)	2:44:B:LEU:HD23	2:44:B:LEU:HB3	7	0.57
(1,1242)	2:44:C:LEU:HD13	2:44:C:LEU:HB3	8	0.57
(1,1204)	2:31:C:ILE:HD11	2:27:B:LEU:HG	3	0.57
(1,1204)	2:31:C:ILE:HD11	2:27:B:LEU:HG	9	0.57
(1,953)	2:31:B:ILE:HG21	2:24:C:PRO:HB2	3	0.57
(1,953)	2:31:B:ILE:HG22	2:24:C:PRO:HB2	3	0.57
(1,953)	2:31:B:ILE:HG23	2:24:C:PRO:HB2	3	0.57
(1,307)	1:14:A:ASN:HB3	1:14:A:ASN:HD22	3	0.57
(1,307)	1:14:A:ASN:HB3	1:14:A:ASN:HD22	4	0.57
(1,307)	1:14:A:ASN:HB3	1:14:A:ASN:HD22	5	0.57
(1,307)	1:14:A:ASN:HB3	1:14:A:ASN:HD22	9	0.57
(1,307)	1:14:A:ASN:HB3	1:14:A:ASN:HD22	10	0.57
(1,14)	1:17:A:VAL:H	1:16:A:LEU:HD23	9	0.57
(1,1791)	2:54:B:ALA:HB1	2:53:B:ASP:HB3	2	0.56
(1,1242)	2:44:B:LEU:HD22	2:44:B:LEU:HB3	1	0.56
(1,1242)	2:44:B:LEU:HD22	2:44:B:LEU:HB3	9	0.56
(1,1204)	2:31:C:ILE:HD12	2:27:B:LEU:HG	1	0.56
(1,1138)	2:24:B:PRO:HA	2:27:B:LEU:HB3	3	0.56
(1,307)	1:14:A:ASN:HB3	1:14:A:ASN:HD22	6	0.56
(1,307)	1:14:A:ASN:HB3	1:14:A:ASN:HD22	7	0.56
(1,63)	1:29:A:SER:H	1:29:A:SER:HB3	8	0.56
(1,14)	1:17:A:VAL:H	1:16:A:LEU:HD23	10	0.56
(1,1931)	2:19:B:LEU:HD21	2:48:B:ALA:HA	10	0.55
(1,1931)	2:19:B:LEU:HD22	2:48:B:ALA:HA	10	0.55
(1,1931)	2:19:B:LEU:HD23	2:48:B:ALA:HA	10	0.55
(1,1837)	2:19:C:LEU:HD11	2:22:C:LEU:HA	6	0.55
(1,1837)	2:19:C:LEU:HD12	2:22:C:LEU:HA	6	0.55
(1,1837)	2:19:C:LEU:HD13	2:22:C:LEU:HA	6	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1791)	2:54:B:ALA:HB3	2:53:B:ASP:HB3	5	0.55
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD11	6	0.55
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD12	6	0.55
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD13	6	0.55
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD11	10	0.55
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD12	10	0.55
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD13	10	0.55
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG21	2	0.55
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG22	2	0.55
(1,1326)	2:49:B:LYS:HD3	2:17:B:VAL:HG23	2	0.55
(1,1242)	2:44:B:LEU:HD23	2:44:B:LEU:HB3	6	0.55
(1,1204)	2:31:C:ILE:HD13	2:27:B:LEU:HG	5	0.55
(1,1204)	2:31:C:ILE:HD12	2:27:B:LEU:HG	7	0.55
(1,14)	1:17:A:VAL:H	1:16:A:LEU:HD23	6	0.55
(1,1829)	2:21:C:ASN:H	2:20:C:PRO:HG3	6	0.54
(1,1794)	2:23:C:ASN:HD22	2:26:C:GLN:HG2	9	0.54
(1,1794)	2:23:C:ASN:HD22	2:26:C:GLN:HG2	10	0.54
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	9	0.54
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	9	0.54
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	9	0.54
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	9	0.54
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	9	0.54
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	9	0.54
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	9	0.54
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	9	0.54
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	9	0.54
(1,1213)	2:31:B:ILE:HD11	2:27:C:LEU:HD21	2	0.54
(1,63)	1:29:A:SER:H	1:29:A:SER:HB3	5	0.54
(1,1895)	2:31:C:ILE:HG13	2:34:C:ILE:HD12	1	0.53
(1,1836)	2:19:B:LEU:HD21	2:22:B:LEU:HA	6	0.53
(1,1836)	2:19:B:LEU:HD22	2:22:B:LEU:HA	6	0.53
(1,1836)	2:19:B:LEU:HD23	2:22:B:LEU:HA	6	0.53
(1,1714)	2:44:C:LEU:HD11	2:40:C:GLN:HG3	3	0.53
(1,1714)	2:44:C:LEU:HD12	2:40:C:GLN:HG3	3	0.53
(1,1714)	2:44:C:LEU:HD13	2:40:C:GLN:HG3	3	0.53
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD11	3	0.53
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD12	3	0.53
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD13	3	0.53
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD11	10	0.53
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD12	10	0.53
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD13	10	0.53
(1,1619)	2:23:C:ASN:HB2	2:24:C:PRO:HD2	6	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1242)	2:44:B:LEU:HD21	2:44:B:LEU:HB3	4	0.53
(1,1204)	2:31:C:ILE:HD12	2:27:B:LEU:HG	8	0.53
(1,1873)	2:23:B:ASN:HD22	2:26:B:GLN:HG2	6	0.52
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	7	0.52
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	7	0.52
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	7	0.52
(1,1837)	2:19:C:LEU:HD11	2:22:C:LEU:HA	9	0.52
(1,1837)	2:19:C:LEU:HD12	2:22:C:LEU:HA	9	0.52
(1,1837)	2:19:C:LEU:HD13	2:22:C:LEU:HA	9	0.52
(1,1829)	2:21:C:ASN:H	2:20:C:PRO:HG3	9	0.52
(1,1791)	2:54:B:ALA:HB1	2:53:B:ASP:HB3	7	0.52
(1,1791)	2:54:B:ALA:HB2	2:53:B:ASP:HB3	10	0.52
(1,1752)	2:44:C:LEU:HD21	2:43:C:ASN:HB2	4	0.52
(1,1752)	2:44:C:LEU:HD21	2:43:C:ASN:HB3	4	0.52
(1,1752)	2:44:C:LEU:HD22	2:43:C:ASN:HB2	4	0.52
(1,1752)	2:44:C:LEU:HD22	2:43:C:ASN:HB3	4	0.52
(1,1752)	2:44:C:LEU:HD23	2:43:C:ASN:HB2	4	0.52
(1,1752)	2:44:C:LEU:HD23	2:43:C:ASN:HB3	4	0.52
(1,1714)	2:44:C:LEU:HD11	2:40:C:GLN:HG3	10	0.52
(1,1714)	2:44:C:LEU:HD12	2:40:C:GLN:HG3	10	0.52
(1,1714)	2:44:C:LEU:HD13	2:40:C:GLN:HG3	10	0.52
(1,1606)	2:19:B:LEU:HD21	2:52:B:ASN:HB2	8	0.52
(1,1606)	2:19:B:LEU:HD22	2:52:B:ASN:HB2	8	0.52
(1,1606)	2:19:B:LEU:HD23	2:52:B:ASN:HB2	8	0.52
(1,1204)	2:31:C:ILE:HD11	2:27:B:LEU:HG	2	0.52
(1,1204)	2:31:C:ILE:HD12	2:27:B:LEU:HG	6	0.52
(1,423)	1:28:A:SER:HB2	1:12:A:LEU:HB2	2	0.52
(1,423)	1:28:A:SER:HB2	1:12:A:LEU:HB3	2	0.52
(1,63)	1:29:A:SER:H	1:29:A:SER:HB3	2	0.52
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD11	2	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD12	2	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD13	2	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD11	4	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD12	4	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD13	4	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD11	5	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD12	5	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD13	5	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD11	7	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD12	7	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD13	7	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD11	8	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD12	8	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD13	8	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD11	9	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD12	9	0.51
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD13	9	0.51
(1,1591)	2:39:B:SER:H	2:38:B:PRO:HG3	5	0.51
(1,1083)	2:34:C:ILE:HG21	2:34:C:ILE:HG12	8	0.51
(1,1083)	2:34:C:ILE:HG22	2:34:C:ILE:HG12	8	0.51
(1,1083)	2:34:C:ILE:HG23	2:34:C:ILE:HG12	8	0.51
(1,1895)	2:31:C:ILE:HG13	2:34:C:ILE:HD12	3	0.5
(1,1873)	2:23:B:ASN:HD22	2:26:B:GLN:HG2	4	0.5
(1,1837)	2:19:C:LEU:HD11	2:22:C:LEU:HA	2	0.5
(1,1837)	2:19:C:LEU:HD12	2:22:C:LEU:HA	2	0.5
(1,1837)	2:19:C:LEU:HD13	2:22:C:LEU:HA	2	0.5
(1,1837)	2:19:C:LEU:HD11	2:22:C:LEU:HA	8	0.5
(1,1837)	2:19:C:LEU:HD12	2:22:C:LEU:HA	8	0.5
(1,1837)	2:19:C:LEU:HD13	2:22:C:LEU:HA	8	0.5
(1,1829)	2:21:C:ASN:H	2:20:C:PRO:HG3	2	0.5
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD11	1	0.5
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD12	1	0.5
(1,1685)	2:37:C:ASP:HB3	2:44:C:LEU:HD13	1	0.5
(1,1658)	2:35:B:HIS:HB2	2:36:B:ASP:H	1	0.5
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	3	0.5
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	3	0.5
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	3	0.5
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	3	0.5
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	3	0.5
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	3	0.5
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	3	0.5
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	3	0.5
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	3	0.5
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD11	8	0.5
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD12	8	0.5
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD13	8	0.5
(1,1083)	2:34:C:ILE:HG21	2:34:C:ILE:HG12	1	0.5
(1,1083)	2:34:C:ILE:HG22	2:34:C:ILE:HG12	1	0.5
(1,1083)	2:34:C:ILE:HG23	2:34:C:ILE:HG12	1	0.5
(1,1083)	2:34:C:ILE:HG21	2:34:C:ILE:HG12	2	0.5
(1,1083)	2:34:C:ILE:HG22	2:34:C:ILE:HG12	2	0.5
(1,1083)	2:34:C:ILE:HG23	2:34:C:ILE:HG12	2	0.5
(1,1083)	2:34:C:ILE:HG21	2:34:C:ILE:HG12	3	0.5
(1,1083)	2:34:C:ILE:HG22	2:34:C:ILE:HG12	3	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1083)	2:34:C:ILE:HG23	2:34:C:ILE:HG12	3	0.5
(1,1083)	2:34:C:ILE:HG21	2:34:C:ILE:HG12	4	0.5
(1,1083)	2:34:C:ILE:HG22	2:34:C:ILE:HG12	4	0.5
(1,1083)	2:34:C:ILE:HG23	2:34:C:ILE:HG12	4	0.5
(1,1083)	2:34:C:ILE:HG21	2:34:C:ILE:HG12	5	0.5
(1,1083)	2:34:C:ILE:HG22	2:34:C:ILE:HG12	5	0.5
(1,1083)	2:34:C:ILE:HG23	2:34:C:ILE:HG12	5	0.5
(1,1083)	2:34:C:ILE:HG21	2:34:C:ILE:HG12	6	0.5
(1,1083)	2:34:C:ILE:HG22	2:34:C:ILE:HG12	6	0.5
(1,1083)	2:34:C:ILE:HG23	2:34:C:ILE:HG12	6	0.5
(1,1083)	2:34:C:ILE:HG21	2:34:C:ILE:HG12	7	0.5
(1,1083)	2:34:C:ILE:HG22	2:34:C:ILE:HG12	7	0.5
(1,1083)	2:34:C:ILE:HG23	2:34:C:ILE:HG12	7	0.5
(1,1083)	2:34:C:ILE:HG21	2:34:C:ILE:HG12	9	0.5
(1,1083)	2:34:C:ILE:HG22	2:34:C:ILE:HG12	9	0.5
(1,1083)	2:34:C:ILE:HG23	2:34:C:ILE:HG12	9	0.5
(1,1083)	2:34:C:ILE:HG21	2:34:C:ILE:HG12	10	0.5
(1,1083)	2:34:C:ILE:HG22	2:34:C:ILE:HG12	10	0.5
(1,1083)	2:34:C:ILE:HG23	2:34:C:ILE:HG12	10	0.5
(1,953)	2:31:B:ILE:HG21	2:24:C:PRO:HB2	2	0.5
(1,953)	2:31:B:ILE:HG22	2:24:C:PRO:HB2	2	0.5
(1,953)	2:31:B:ILE:HG23	2:24:C:PRO:HB2	2	0.5
(1,175)	1:27:A:LEU:HD11	1:27:A:LEU:HA	6	0.5
(1,175)	1:27:A:LEU:HD12	1:27:A:LEU:HA	6	0.5
(1,175)	1:27:A:LEU:HD13	1:27:A:LEU:HA	6	0.5
(1,1836)	2:19:B:LEU:HD21	2:22:B:LEU:HA	2	0.49
(1,1836)	2:19:B:LEU:HD22	2:22:B:LEU:HA	2	0.49
(1,1836)	2:19:B:LEU:HD23	2:22:B:LEU:HA	2	0.49
(1,1714)	2:44:C:LEU:HD11	2:40:C:GLN:HG3	2	0.49
(1,1714)	2:44:C:LEU:HD12	2:40:C:GLN:HG3	2	0.49
(1,1714)	2:44:C:LEU:HD13	2:40:C:GLN:HG3	2	0.49
(1,1658)	2:35:B:HIS:HB2	2:36:B:ASP:H	4	0.49
(1,1658)	2:35:B:HIS:HB2	2:36:B:ASP:H	8	0.49
(1,175)	1:27:A:LEU:HD11	1:27:A:LEU:HA	4	0.49
(1,175)	1:27:A:LEU:HD12	1:27:A:LEU:HA	4	0.49
(1,175)	1:27:A:LEU:HD13	1:27:A:LEU:HA	4	0.49
(1,175)	1:27:A:LEU:HD11	1:27:A:LEU:HA	7	0.49
(1,175)	1:27:A:LEU:HD12	1:27:A:LEU:HA	7	0.49
(1,175)	1:27:A:LEU:HD13	1:27:A:LEU:HA	7	0.49
(1,175)	1:27:A:LEU:HD11	1:27:A:LEU:HA	10	0.49
(1,175)	1:27:A:LEU:HD12	1:27:A:LEU:HA	10	0.49
(1,175)	1:27:A:LEU:HD13	1:27:A:LEU:HA	10	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD11	3	0.48
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD12	3	0.48
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD13	3	0.48
(1,1658)	2:35:B:HIS:HB2	2:36:B:ASP:H	10	0.48
(1,1591)	2:39:B:SER:H	2:38:B:PRO:HG3	2	0.48
(1,1552)	2:17:B:VAL:HG21	2:15:B:GLU:HG2	10	0.48
(1,1552)	2:17:B:VAL:HG22	2:15:B:GLU:HG2	10	0.48
(1,1552)	2:17:B:VAL:HG23	2:15:B:GLU:HG2	10	0.48
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	1	0.48
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	1	0.48
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	1	0.48
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	1	0.48
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	1	0.48
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	1	0.48
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	1	0.48
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	1	0.48
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	1	0.48
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	8	0.48
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	8	0.48
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	8	0.48
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	8	0.48
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	8	0.48
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	8	0.48
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	8	0.48
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	8	0.48
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	8	0.48
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD11	3	0.48
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD12	3	0.48
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD13	3	0.48
(1,175)	1:27:A:LEU:HD11	1:27:A:LEU:HA	1	0.48
(1,175)	1:27:A:LEU:HD12	1:27:A:LEU:HA	1	0.48
(1,175)	1:27:A:LEU:HD13	1:27:A:LEU:HA	1	0.48
(1,175)	1:27:A:LEU:HD11	1:27:A:LEU:HA	2	0.48
(1,175)	1:27:A:LEU:HD12	1:27:A:LEU:HA	2	0.48
(1,175)	1:27:A:LEU:HD13	1:27:A:LEU:HA	2	0.48
(1,175)	1:27:A:LEU:HD11	1:27:A:LEU:HA	5	0.48
(1,175)	1:27:A:LEU:HD12	1:27:A:LEU:HA	5	0.48
(1,175)	1:27:A:LEU:HD13	1:27:A:LEU:HA	5	0.48
(1,1844)	2:19:C:LEU:HD11	2:22:C:LEU:HG	10	0.47
(1,1844)	2:19:C:LEU:HD12	2:22:C:LEU:HG	10	0.47
(1,1844)	2:19:C:LEU:HD13	2:22:C:LEU:HG	10	0.47
(1,1836)	2:19:B:LEU:HD21	2:22:B:LEU:HA	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1836)	2:19:B:LEU:HD22	2:22:B:LEU:HA	9	0.47
(1,1836)	2:19:B:LEU:HD23	2:22:B:LEU:HA	9	0.47
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD11	8	0.47
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD12	8	0.47
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD13	8	0.47
(1,1658)	2:35:B:HIS:HB2	2:36:B:ASP:H	3	0.47
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG21	3	0.47
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG22	3	0.47
(1,1324)	2:49:B:LYS:HD2	2:17:B:VAL:HG23	3	0.47
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	1	0.47
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	1	0.47
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	1	0.47
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	1	0.47
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	1	0.47
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	1	0.47
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	1	0.47
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	1	0.47
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	1	0.47
(1,276)	1:27:A:LEU:HD11	2:45:C:LEU:HG	2	0.47
(1,276)	1:27:A:LEU:HD12	2:45:C:LEU:HG	2	0.47
(1,276)	1:27:A:LEU:HD13	2:45:C:LEU:HG	2	0.47
(1,175)	1:27:A:LEU:HD11	1:27:A:LEU:HA	3	0.47
(1,175)	1:27:A:LEU:HD12	1:27:A:LEU:HA	3	0.47
(1,175)	1:27:A:LEU:HD13	1:27:A:LEU:HA	3	0.47
(1,175)	1:27:A:LEU:HD11	1:27:A:LEU:HA	9	0.47
(1,175)	1:27:A:LEU:HD12	1:27:A:LEU:HA	9	0.47
(1,175)	1:27:A:LEU:HD13	1:27:A:LEU:HA	9	0.47
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	8	0.46
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	8	0.46
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	8	0.46
(1,1837)	2:19:C:LEU:HD11	2:22:C:LEU:HA	5	0.46
(1,1837)	2:19:C:LEU:HD12	2:22:C:LEU:HA	5	0.46
(1,1837)	2:19:C:LEU:HD13	2:22:C:LEU:HA	5	0.46
(1,1829)	2:21:C:ASN:H	2:20:C:PRO:HG3	8	0.46
(1,1658)	2:35:B:HIS:HB2	2:36:B:ASP:H	6	0.46
(1,1658)	2:35:B:HIS:HB2	2:36:B:ASP:H	9	0.46
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD11	4	0.46
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD12	4	0.46
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD13	4	0.46
(1,962)	2:44:C:LEU:HD11	2:34:C:ILE:HB	9	0.46
(1,962)	2:44:C:LEU:HD12	2:34:C:ILE:HB	9	0.46
(1,962)	2:44:C:LEU:HD13	2:34:C:ILE:HB	9	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD11	8	0.46
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD12	8	0.46
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD13	8	0.46
(1,175)	1:27:A:LEU:HD11	1:27:A:LEU:HA	8	0.46
(1,175)	1:27:A:LEU:HD12	1:27:A:LEU:HA	8	0.46
(1,175)	1:27:A:LEU:HD13	1:27:A:LEU:HA	8	0.46
(1,1836)	2:19:B:LEU:HD21	2:22:B:LEU:HA	5	0.45
(1,1836)	2:19:B:LEU:HD22	2:22:B:LEU:HA	5	0.45
(1,1836)	2:19:B:LEU:HD23	2:22:B:LEU:HA	5	0.45
(1,1606)	2:19:B:LEU:HD21	2:52:B:ASN:HB2	1	0.45
(1,1606)	2:19:B:LEU:HD22	2:52:B:ASN:HB2	1	0.45
(1,1606)	2:19:B:LEU:HD23	2:52:B:ASN:HB2	1	0.45
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	10	0.45
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	10	0.45
(1,1352)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	10	0.45
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	10	0.45
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	10	0.45
(1,1352)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	10	0.45
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	10	0.45
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	10	0.45
(1,1352)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	10	0.45
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	5	0.45
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	5	0.45
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	5	0.45
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	5	0.45
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	5	0.45
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	5	0.45
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	5	0.45
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	5	0.45
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	5	0.45
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	8	0.45
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	8	0.45
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	8	0.45
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	8	0.45
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	8	0.45
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	8	0.45
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	8	0.45
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	8	0.45
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	8	0.45
(1,407)	1:12:A:LEU:HD21	2:38:C:PRO:HB3	4	0.45
(1,407)	1:12:A:LEU:HD22	2:38:C:PRO:HB3	4	0.45
(1,407)	1:12:A:LEU:HD23	2:38:C:PRO:HB3	4	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	1	0.44
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	1	0.44
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	1	0.44
(1,1790)	2:56:C:ALA:HB2	2:53:C:ASP:HB3	2	0.44
(1,1777)	2:47:C:GLU:HG2	2:47:C:GLU:HB3	4	0.44
(1,1658)	2:35:B:HIS:HB2	2:36:B:ASP:H	7	0.44
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	6	0.44
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	6	0.44
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	6	0.44
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	6	0.44
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	6	0.44
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	6	0.44
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	6	0.44
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	6	0.44
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	6	0.44
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD11	5	0.44
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD12	5	0.44
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD13	5	0.44
(1,407)	1:12:A:LEU:HD21	2:38:C:PRO:HB3	8	0.44
(1,407)	1:12:A:LEU:HD22	2:38:C:PRO:HB3	8	0.44
(1,407)	1:12:A:LEU:HD23	2:38:C:PRO:HB3	8	0.44
(1,350)	1:10:A:GLN:HG2	1:10:A:GLN:HE22	3	0.44
(1,350)	1:10:A:GLN:HG3	1:10:A:GLN:HE22	3	0.44
(1,350)	1:10:A:GLN:HG2	1:10:A:GLN:HE22	4	0.44
(1,350)	1:10:A:GLN:HG3	1:10:A:GLN:HE22	4	0.44
(1,350)	1:10:A:GLN:HG2	1:10:A:GLN:HE22	7	0.44
(1,350)	1:10:A:GLN:HG3	1:10:A:GLN:HE22	7	0.44
(1,350)	1:10:A:GLN:HG2	1:10:A:GLN:HE22	10	0.44
(1,350)	1:10:A:GLN:HG3	1:10:A:GLN:HE22	10	0.44
(1,63)	1:29:A:SER:H	1:29:A:SER:HB3	4	0.44
(1,1777)	2:47:C:GLU:HG2	2:47:C:GLU:HB3	6	0.43
(1,1752)	2:44:C:LEU:HD21	2:43:C:ASN:HB2	8	0.43
(1,1752)	2:44:C:LEU:HD21	2:43:C:ASN:HB3	8	0.43
(1,1752)	2:44:C:LEU:HD22	2:43:C:ASN:HB2	8	0.43
(1,1752)	2:44:C:LEU:HD22	2:43:C:ASN:HB3	8	0.43
(1,1752)	2:44:C:LEU:HD23	2:43:C:ASN:HB2	8	0.43
(1,1752)	2:44:C:LEU:HD23	2:43:C:ASN:HB3	8	0.43
(1,1605)	2:19:B:LEU:HD21	2:52:B:ASN:HB3	1	0.43
(1,1605)	2:19:B:LEU:HD22	2:52:B:ASN:HB3	1	0.43
(1,1605)	2:19:B:LEU:HD23	2:52:B:ASN:HB3	1	0.43
(1,1605)	2:19:B:LEU:HD21	2:52:B:ASN:HB3	8	0.43
(1,1605)	2:19:B:LEU:HD22	2:52:B:ASN:HB3	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1605)	2:19:B:LEU:HD23	2:52:B:ASN:HB3	8	0.43
(1,1591)	2:39:B:SER:H	2:38:B:PRO:HG3	3	0.43
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	7	0.43
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	7	0.43
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	7	0.43
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	7	0.43
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	7	0.43
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	7	0.43
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	7	0.43
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	7	0.43
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	7	0.43
(1,1242)	2:44:C:LEU:HD12	2:44:C:LEU:HB3	5	0.43
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	2	0.43
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	2	0.43
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	2	0.43
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	2	0.43
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	2	0.43
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	2	0.43
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	2	0.43
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	2	0.43
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	2	0.43
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	7	0.43
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	7	0.43
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	7	0.43
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	7	0.43
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	7	0.43
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	7	0.43
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	7	0.43
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	7	0.43
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	7	0.43
(1,407)	1:12:A:LEU:HD21	2:38:C:PRO:HB3	2	0.43
(1,407)	1:12:A:LEU:HD22	2:38:C:PRO:HB3	2	0.43
(1,407)	1:12:A:LEU:HD23	2:38:C:PRO:HB3	2	0.43
(1,350)	1:10:A:GLN:HG2	1:10:A:GLN:HE22	6	0.43
(1,350)	1:10:A:GLN:HG3	1:10:A:GLN:HE22	6	0.43
(1,100)	1:28:A:SER:HB2	1:12:A:LEU:H	2	0.43
(1,1930)	2:19:C:LEU:HD11	2:48:C:ALA:HA	10	0.42
(1,1930)	2:19:C:LEU:HD12	2:48:C:ALA:HA	10	0.42
(1,1930)	2:19:C:LEU:HD13	2:48:C:ALA:HA	10	0.42
(1,1605)	2:19:B:LEU:HD21	2:52:B:ASN:HB3	10	0.42
(1,1605)	2:19:B:LEU:HD22	2:52:B:ASN:HB3	10	0.42
(1,1605)	2:19:B:LEU:HD23	2:52:B:ASN:HB3	10	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	9	0.42
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	9	0.42
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	9	0.42
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	9	0.42
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	9	0.42
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	9	0.42
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	9	0.42
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	9	0.42
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	9	0.42
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD11	6	0.42
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD12	6	0.42
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD13	6	0.42
(1,407)	1:12:A:LEU:HD21	2:38:C:PRO:HB3	5	0.42
(1,407)	1:12:A:LEU:HD22	2:38:C:PRO:HB3	5	0.42
(1,407)	1:12:A:LEU:HD23	2:38:C:PRO:HB3	5	0.42
(1,276)	1:27:A:LEU:HD11	2:45:C:LEU:HG	3	0.42
(1,276)	1:27:A:LEU:HD12	2:45:C:LEU:HG	3	0.42
(1,276)	1:27:A:LEU:HD13	2:45:C:LEU:HG	3	0.42
(1,1777)	2:47:C:GLU:HG2	2:47:C:GLU:HB3	5	0.41
(1,1591)	2:39:B:SER:H	2:38:B:PRO:HG3	8	0.41
(1,1552)	2:17:B:VAL:HG21	2:15:B:GLU:HG2	9	0.41
(1,1552)	2:17:B:VAL:HG22	2:15:B:GLU:HG2	9	0.41
(1,1552)	2:17:B:VAL:HG23	2:15:B:GLU:HG2	9	0.41
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	6	0.41
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	6	0.41
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	6	0.41
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	6	0.41
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	6	0.41
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	6	0.41
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	6	0.41
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	6	0.41
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	6	0.41
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD11	7	0.41
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD12	7	0.41
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD13	7	0.41
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD11	6	0.41
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD12	6	0.41
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD13	6	0.41
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD11	6	0.41
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD12	6	0.41
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD13	6	0.41
(1,407)	1:12:A:LEU:HD21	2:38:C:PRO:HB3	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:12:A:LEU:HD22	2:38:C:PRO:HB3	1	0.41
(1,407)	1:12:A:LEU:HD23	2:38:C:PRO:HB3	1	0.41
(1,407)	1:12:A:LEU:HD21	2:38:C:PRO:HB3	7	0.41
(1,407)	1:12:A:LEU:HD22	2:38:C:PRO:HB3	7	0.41
(1,407)	1:12:A:LEU:HD23	2:38:C:PRO:HB3	7	0.41
(1,253)	1:27:A:LEU:H	1:27:A:LEU:HD21	7	0.41
(1,1895)	2:31:C:ILE:HG13	2:34:C:ILE:HD12	9	0.4
(1,1829)	2:21:C:ASN:H	2:20:C:PRO:HG3	1	0.4
(1,1829)	2:21:C:ASN:H	2:20:C:PRO:HG3	10	0.4
(1,1777)	2:47:C:GLU:HG2	2:47:C:GLU:HB3	1	0.4
(1,1777)	2:47:C:GLU:HG2	2:47:C:GLU:HB3	10	0.4
(1,1713)	2:44:C:LEU:HD11	2:40:C:GLN:HG2	5	0.4
(1,1713)	2:44:C:LEU:HD12	2:40:C:GLN:HG2	5	0.4
(1,1713)	2:44:C:LEU:HD13	2:40:C:GLN:HG2	5	0.4
(1,1628)	2:22:C:LEU:H	2:21:C:ASN:HB2	9	0.4
(1,1615)	2:23:B:ASN:HB3	2:23:B:ASN:HD22	6	0.4
(1,1393)	2:29:C:ALA:H	2:29:C:ALA:HB3	8	0.4
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD11	2	0.4
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD12	2	0.4
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD13	2	0.4
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD11	7	0.4
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD12	7	0.4
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD13	7	0.4
(1,46)	1:27:A:LEU:H	1:28:A:SER:H	6	0.4
(1,46)	1:27:A:LEU:H	1:28:A:SER:H	8	0.4
(1,46)	1:27:A:LEU:H	1:28:A:SER:H	9	0.4
(1,1829)	2:21:C:ASN:H	2:20:C:PRO:HG3	3	0.39
(1,1777)	2:47:C:GLU:HG2	2:47:C:GLU:HB3	3	0.39
(1,1777)	2:47:B:GLU:HG3	2:47:B:GLU:HB2	7	0.39
(1,1774)	2:47:B:GLU:HA	2:47:B:GLU:HG2	1	0.39
(1,1604)	2:19:C:LEU:HD11	2:52:C:ASN:HB3	5	0.39
(1,1604)	2:19:C:LEU:HD12	2:52:C:ASN:HB3	5	0.39
(1,1604)	2:19:C:LEU:HD13	2:52:C:ASN:HB3	5	0.39
(1,1604)	2:19:C:LEU:HD11	2:52:C:ASN:HB3	9	0.39
(1,1604)	2:19:C:LEU:HD12	2:52:C:ASN:HB3	9	0.39
(1,1604)	2:19:C:LEU:HD13	2:52:C:ASN:HB3	9	0.39
(1,1591)	2:39:B:SER:H	2:38:B:PRO:HG3	7	0.39
(1,1551)	2:17:B:VAL:HG21	2:15:B:GLU:HG3	3	0.39
(1,1551)	2:17:B:VAL:HG22	2:15:B:GLU:HG3	3	0.39
(1,1551)	2:17:B:VAL:HG23	2:15:B:GLU:HG3	3	0.39
(1,1393)	2:29:B:ALA:H	2:29:B:ALA:HB1	3	0.39
(1,1393)	2:29:C:ALA:H	2:29:C:ALA:HB1	4	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1393)	2:29:C:ALA:H	2:29:C:ALA:HB3	5	0.39
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD11	1	0.39
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD12	1	0.39
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD13	1	0.39
(1,1196)	2:27:B:LEU:H	2:27:B:LEU:HB3	5	0.39
(1,1128)	2:31:C:ILE:HG21	2:27:B:LEU:HB3	5	0.39
(1,1128)	2:31:C:ILE:HG22	2:27:B:LEU:HB3	5	0.39
(1,1128)	2:31:C:ILE:HG23	2:27:B:LEU:HB3	5	0.39
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	4	0.39
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	4	0.39
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	4	0.39
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	4	0.39
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	4	0.39
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	4	0.39
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	4	0.39
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	4	0.39
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	4	0.39
(1,407)	1:12:A:LEU:HD21	2:38:C:PRO:HB3	9	0.39
(1,407)	1:12:A:LEU:HD22	2:38:C:PRO:HB3	9	0.39
(1,407)	1:12:A:LEU:HD23	2:38:C:PRO:HB3	9	0.39
(1,46)	1:27:A:LEU:H	1:28:A:SER:H	7	0.39
(1,1777)	2:47:B:GLU:HG3	2:47:B:GLU:HB2	2	0.38
(1,1777)	2:47:B:GLU:HG3	2:47:B:GLU:HB2	9	0.38
(1,1774)	2:47:B:GLU:HA	2:47:B:GLU:HG2	2	0.38
(1,1533)	2:51:C:LEU:HA	2:54:C:ALA:HB2	9	0.38
(1,1393)	2:29:B:ALA:H	2:29:B:ALA:HB3	1	0.38
(1,1393)	2:29:B:ALA:H	2:29:B:ALA:HB1	6	0.38
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD11	4	0.38
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD12	4	0.38
(1,1387)	2:51:B:LEU:HD21	2:22:B:LEU:HD13	4	0.38
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD11	4	0.38
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD12	4	0.38
(1,1387)	2:51:B:LEU:HD22	2:22:B:LEU:HD13	4	0.38
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD11	4	0.38
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD12	4	0.38
(1,1387)	2:51:B:LEU:HD23	2:22:B:LEU:HD13	4	0.38
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD11	4	0.38
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD12	4	0.38
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD13	4	0.38
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD11	8	0.38
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD12	8	0.38
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD13	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1196)	2:27:B:LEU:H	2:27:B:LEU:HB3	2	0.38
(1,1196)	2:27:B:LEU:H	2:27:B:LEU:HB3	6	0.38
(1,1196)	2:27:B:LEU:H	2:27:B:LEU:HB3	8	0.38
(1,1196)	2:27:B:LEU:H	2:27:B:LEU:HB3	10	0.38
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	3	0.38
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	3	0.38
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	3	0.38
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	3	0.38
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	3	0.38
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	3	0.38
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	3	0.38
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	3	0.38
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	3	0.38
(1,362)	1:11:A:ARG:HA	1:11:A:ARG:HG2	9	0.38
(1,1777)	2:47:B:GLU:HG3	2:47:B:GLU:HB2	8	0.37
(1,1774)	2:47:B:GLU:HA	2:47:B:GLU:HG2	7	0.37
(1,1629)	2:22:B:LEU:H	2:21:B:ASN:HB2	7	0.37
(1,1353)	2:22:B:LEU:HD22	2:22:B:LEU:HD12	9	0.37
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD11	2	0.37
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD12	2	0.37
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD13	2	0.37
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD11	5	0.37
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD12	5	0.37
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD13	5	0.37
(1,1196)	2:27:B:LEU:H	2:27:B:LEU:HB3	1	0.37
(1,1196)	2:27:B:LEU:H	2:27:B:LEU:HB3	3	0.37
(1,1196)	2:27:B:LEU:H	2:27:B:LEU:HB3	4	0.37
(1,1196)	2:27:B:LEU:H	2:27:B:LEU:HB3	7	0.37
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB1	10	0.37
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB2	10	0.37
(1,1099)	1:27:A:LEU:HD21	2:42:C:ALA:HB3	10	0.37
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB1	10	0.37
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB2	10	0.37
(1,1099)	1:27:A:LEU:HD22	2:42:C:ALA:HB3	10	0.37
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB1	10	0.37
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB2	10	0.37
(1,1099)	1:27:A:LEU:HD23	2:42:C:ALA:HB3	10	0.37
(1,991)	2:16:C:ILE:HG23	1:26:A:ILE:HG13	6	0.37
(1,350)	1:10:A:GLN:HG2	1:10:A:GLN:HE22	2	0.37
(1,350)	1:10:A:GLN:HG3	1:10:A:GLN:HE22	2	0.37
(1,350)	1:10:A:GLN:HG2	1:10:A:GLN:HE22	5	0.37
(1,350)	1:10:A:GLN:HG3	1:10:A:GLN:HE22	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,350)	1:10:A:GLN:HG2	1:10:A:GLN:HE22	8	0.37
(1,350)	1:10:A:GLN:HG3	1:10:A:GLN:HE22	8	0.37
(1,350)	1:10:A:GLN:HG2	1:10:A:GLN:HE22	9	0.37
(1,350)	1:10:A:GLN:HG3	1:10:A:GLN:HE22	9	0.37
(1,1595)	2:38:B:PRO:HB2	2:38:B:PRO:HD2	1	0.36
(1,1534)	2:54:B:ALA:HA	2:54:B:ALA:HB3	10	0.36
(1,1393)	2:29:B:ALA:H	2:29:B:ALA:HB3	2	0.36
(1,1393)	2:29:C:ALA:H	2:29:C:ALA:HB3	7	0.36
(1,1393)	2:29:B:ALA:H	2:29:B:ALA:HB3	9	0.36
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD11	2	0.36
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD12	2	0.36
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD13	2	0.36
(1,1196)	2:27:B:LEU:H	2:27:B:LEU:HB3	9	0.36
(1,1128)	2:31:C:ILE:HG21	2:27:B:LEU:HB3	9	0.36
(1,1128)	2:31:C:ILE:HG22	2:27:B:LEU:HB3	9	0.36
(1,1128)	2:31:C:ILE:HG23	2:27:B:LEU:HB3	9	0.36
(1,350)	1:10:A:GLN:HG2	1:10:A:GLN:HE22	1	0.36
(1,350)	1:10:A:GLN:HG3	1:10:A:GLN:HE22	1	0.36
(1,253)	1:27:A:LEU:H	1:27:A:LEU:HD21	2	0.36
(1,1534)	2:54:B:ALA:HA	2:54:B:ALA:HB3	1	0.35
(1,1534)	2:54:B:ALA:HA	2:54:B:ALA:HB2	2	0.35
(1,1534)	2:54:C:ALA:HA	2:54:C:ALA:HB1	5	0.35
(1,1534)	2:54:C:ALA:HA	2:54:C:ALA:HB1	9	0.35
(1,1393)	2:29:B:ALA:H	2:29:B:ALA:HB3	10	0.35
(1,1353)	2:22:B:LEU:HD21	2:22:B:LEU:HD12	6	0.35
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD11	9	0.35
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD12	9	0.35
(1,1343)	2:22:B:LEU:H	2:22:B:LEU:HD13	9	0.35
(1,888)	2:21:C:ASN:H	2:20:C:PRO:HG3	7	0.35
(1,1812)	2:51:C:LEU:HD11	2:26:C:GLN:HG2	9	0.34
(1,1812)	2:51:C:LEU:HD12	2:26:C:GLN:HG2	9	0.34
(1,1812)	2:51:C:LEU:HD13	2:26:C:GLN:HG2	9	0.34
(1,1794)	2:23:C:ASN:HD22	2:26:C:GLN:HG2	6	0.34
(1,1774)	2:47:B:GLU:HA	2:47:B:GLU:HG2	8	0.34
(1,1643)	2:32:B:HIS:HA	2:24:C:PRO:HB2	2	0.34
(1,1618)	2:23:C:ASN:HB3	2:24:C:PRO:HD2	3	0.34
(1,1618)	2:23:C:ASN:HB3	2:24:C:PRO:HD2	5	0.34
(1,1595)	2:38:B:PRO:HB2	2:38:B:PRO:HD2	3	0.34
(1,1595)	2:38:B:PRO:HB2	2:38:B:PRO:HD2	4	0.34
(1,1595)	2:38:B:PRO:HB2	2:38:B:PRO:HD2	6	0.34
(1,1595)	2:38:B:PRO:HB2	2:38:B:PRO:HD2	8	0.34
(1,1534)	2:54:C:ALA:HA	2:54:C:ALA:HB1	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1534)	2:54:C:ALA:HA	2:54:C:ALA:HB3	6	0.34
(1,1532)	2:54:B:ALA:HA	2:54:B:ALA:HB2	2	0.34
(1,1532)	2:54:B:ALA:HA	2:54:B:ALA:HB3	10	0.34
(1,1427)	2:19:B:LEU:HD21	2:19:B:LEU:HB3	4	0.34
(1,1427)	2:19:B:LEU:HD22	2:19:B:LEU:HB3	4	0.34
(1,1427)	2:19:B:LEU:HD23	2:19:B:LEU:HB3	4	0.34
(1,1316)	2:17:B:VAL:HG21	2:49:B:LYS:HE2	1	0.34
(1,1316)	2:17:B:VAL:HG21	2:49:B:LYS:HE3	1	0.34
(1,1316)	2:17:B:VAL:HG22	2:49:B:LYS:HE2	1	0.34
(1,1316)	2:17:B:VAL:HG22	2:49:B:LYS:HE3	1	0.34
(1,1316)	2:17:B:VAL:HG23	2:49:B:LYS:HE2	1	0.34
(1,1316)	2:17:B:VAL:HG23	2:49:B:LYS:HE3	1	0.34
(1,253)	1:27:A:LEU:H	1:27:A:LEU:HD23	9	0.34
(1,252)	1:27:A:LEU:HD21	2:42:C:ALA:H	1	0.34
(1,252)	1:27:A:LEU:HD22	2:42:C:ALA:H	1	0.34
(1,252)	1:27:A:LEU:HD23	2:42:C:ALA:H	1	0.34
(1,46)	2:17:C:VAL:H	1:27:A:LEU:H	4	0.34
(1,1713)	2:44:C:LEU:HD11	2:40:C:GLN:HG2	6	0.33
(1,1713)	2:44:C:LEU:HD12	2:40:C:GLN:HG2	6	0.33
(1,1713)	2:44:C:LEU:HD13	2:40:C:GLN:HG2	6	0.33
(1,1619)	2:23:C:ASN:HB2	2:24:C:PRO:HD2	9	0.33
(1,1595)	2:38:B:PRO:HB2	2:38:B:PRO:HD2	7	0.33
(1,1595)	2:38:B:PRO:HB2	2:38:B:PRO:HD2	9	0.33
(1,1595)	2:38:B:PRO:HB2	2:38:B:PRO:HD2	10	0.33
(1,1534)	2:54:B:ALA:HA	2:54:B:ALA:HB2	8	0.33
(1,1532)	2:54:B:ALA:HA	2:54:B:ALA:HB3	1	0.33
(1,1532)	2:54:C:ALA:HA	2:54:C:ALA:HB1	5	0.33
(1,1532)	2:54:C:ALA:HA	2:54:C:ALA:HB1	9	0.33
(1,1523)	2:46:B:ALA:HB2	2:46:B:ALA:HA	2	0.33
(1,1523)	2:46:B:ALA:HB2	2:46:B:ALA:HA	7	0.33
(1,1427)	2:19:B:LEU:HD21	2:19:B:LEU:HB3	3	0.33
(1,1427)	2:19:B:LEU:HD22	2:19:B:LEU:HB3	3	0.33
(1,1427)	2:19:B:LEU:HD23	2:19:B:LEU:HB3	3	0.33
(1,1427)	2:19:B:LEU:HD21	2:19:B:LEU:HB3	6	0.33
(1,1427)	2:19:B:LEU:HD22	2:19:B:LEU:HB3	6	0.33
(1,1427)	2:19:B:LEU:HD23	2:19:B:LEU:HB3	6	0.33
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD11	9	0.33
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD12	9	0.33
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD13	9	0.33
(1,1128)	2:31:C:ILE:HG21	2:27:B:LEU:HB3	4	0.33
(1,1128)	2:31:C:ILE:HG22	2:27:B:LEU:HB3	4	0.33
(1,1128)	2:31:C:ILE:HG23	2:27:B:LEU:HB3	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD11	4	0.33
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD12	4	0.33
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD13	4	0.33
(1,797)	2:37:B:ASP:H	2:38:B:PRO:HD2	7	0.33
(1,46)	2:17:C:VAL:H	1:27:A:LEU:H	3	0.33
(1,46)	2:17:C:VAL:H	1:27:A:LEU:H	5	0.33
(1,1884)	2:51:C:LEU:HD21	2:26:C:GLN:HG2	6	0.32
(1,1884)	2:51:C:LEU:HD22	2:26:C:GLN:HG2	6	0.32
(1,1884)	2:51:C:LEU:HD23	2:26:C:GLN:HG2	6	0.32
(1,1774)	2:47:B:GLU:HA	2:47:B:GLU:HG2	9	0.32
(1,1752)	2:44:C:LEU:HD21	2:43:C:ASN:HB2	5	0.32
(1,1752)	2:44:C:LEU:HD21	2:43:C:ASN:HB3	5	0.32
(1,1752)	2:44:C:LEU:HD22	2:43:C:ASN:HB2	5	0.32
(1,1752)	2:44:C:LEU:HD22	2:43:C:ASN:HB3	5	0.32
(1,1752)	2:44:C:LEU:HD23	2:43:C:ASN:HB2	5	0.32
(1,1752)	2:44:C:LEU:HD23	2:43:C:ASN:HB3	5	0.32
(1,1595)	2:38:B:PRO:HB2	2:38:B:PRO:HD2	5	0.32
(1,1591)	2:39:B:SER:H	2:38:B:PRO:HG3	6	0.32
(1,1591)	2:39:B:SER:H	2:38:B:PRO:HG3	9	0.32
(1,1551)	2:17:B:VAL:HG21	2:15:B:GLU:HG3	4	0.32
(1,1551)	2:17:B:VAL:HG22	2:15:B:GLU:HG3	4	0.32
(1,1551)	2:17:B:VAL:HG23	2:15:B:GLU:HG3	4	0.32
(1,1533)	2:51:C:LEU:HA	2:54:C:ALA:HB2	10	0.32
(1,1532)	2:54:C:ALA:HA	2:54:C:ALA:HB1	4	0.32
(1,1532)	2:54:C:ALA:HA	2:54:C:ALA:HB3	6	0.32
(1,1532)	2:54:B:ALA:HA	2:54:B:ALA:HB2	8	0.32
(1,1523)	2:46:B:ALA:HB2	2:46:B:ALA:HA	1	0.32
(1,1523)	2:46:B:ALA:HB1	2:46:B:ALA:HA	3	0.32
(1,1523)	2:46:B:ALA:HB3	2:46:B:ALA:HA	5	0.32
(1,1523)	2:46:B:ALA:HB3	2:46:B:ALA:HA	6	0.32
(1,1523)	2:46:C:ALA:HA	2:46:C:ALA:HB1	8	0.32
(1,1523)	2:46:B:ALA:HB3	2:46:B:ALA:HA	9	0.32
(1,1427)	2:19:B:LEU:HD21	2:19:B:LEU:HB3	2	0.32
(1,1427)	2:19:B:LEU:HD22	2:19:B:LEU:HB3	2	0.32
(1,1427)	2:19:B:LEU:HD23	2:19:B:LEU:HB3	2	0.32
(1,1427)	2:19:B:LEU:HD21	2:19:B:LEU:HB3	5	0.32
(1,1427)	2:19:B:LEU:HD22	2:19:B:LEU:HB3	5	0.32
(1,1427)	2:19:B:LEU:HD23	2:19:B:LEU:HB3	5	0.32
(1,1427)	2:19:B:LEU:HD21	2:19:B:LEU:HB3	7	0.32
(1,1427)	2:19:B:LEU:HD22	2:19:B:LEU:HB3	7	0.32
(1,1427)	2:19:B:LEU:HD23	2:19:B:LEU:HB3	7	0.32
(1,1427)	2:19:B:LEU:HD21	2:19:B:LEU:HB3	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1427)	2:19:B:LEU:HD22	2:19:B:LEU:HB3	9	0.32
(1,1427)	2:19:B:LEU:HD23	2:19:B:LEU:HB3	9	0.32
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD11	8	0.32
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD12	8	0.32
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD13	8	0.32
(1,1353)	2:22:B:LEU:HD22	2:22:B:LEU:HD12	2	0.32
(1,1353)	2:22:B:LEU:HD23	2:22:B:LEU:HD11	3	0.32
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD11	3	0.32
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD12	3	0.32
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD13	3	0.32
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD11	6	0.32
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD12	6	0.32
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD13	6	0.32
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD11	2	0.32
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD12	2	0.32
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD13	2	0.32
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD11	1	0.32
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD12	1	0.32
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD13	1	0.32
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD11	8	0.32
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD12	8	0.32
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD13	8	0.32
(1,362)	1:11:A:ARG:HA	1:11:A:ARG:HG2	6	0.32
(1,268)	1:27:A:LEU:HD21	2:45:C:LEU:HB3	7	0.32
(1,268)	1:27:A:LEU:HD22	2:45:C:LEU:HB3	7	0.32
(1,268)	1:27:A:LEU:HD23	2:45:C:LEU:HB3	7	0.32
(1,46)	2:17:C:VAL:H	1:27:A:LEU:H	1	0.32
(1,1884)	2:51:C:LEU:HD21	2:26:C:GLN:HG2	9	0.31
(1,1884)	2:51:C:LEU:HD22	2:26:C:GLN:HG2	9	0.31
(1,1884)	2:51:C:LEU:HD23	2:26:C:GLN:HG2	9	0.31
(1,1884)	2:51:C:LEU:HD21	2:26:C:GLN:HG2	10	0.31
(1,1884)	2:51:C:LEU:HD22	2:26:C:GLN:HG2	10	0.31
(1,1884)	2:51:C:LEU:HD23	2:26:C:GLN:HG2	10	0.31
(1,1713)	2:44:C:LEU:HD11	2:40:C:GLN:HG2	9	0.31
(1,1713)	2:44:C:LEU:HD12	2:40:C:GLN:HG2	9	0.31
(1,1713)	2:44:C:LEU:HD13	2:40:C:GLN:HG2	9	0.31
(1,1595)	2:38:B:PRO:HB2	2:38:B:PRO:HD2	2	0.31
(1,1534)	2:54:C:ALA:HA	2:54:C:ALA:HB2	3	0.31
(1,1534)	2:54:C:ALA:HA	2:54:C:ALA:HB1	7	0.31
(1,1525)	2:55:B:GLN:H	2:54:B:ALA:HA	4	0.31
(1,1525)	2:55:B:GLN:H	2:54:B:ALA:HA	6	0.31
(1,1523)	2:46:B:ALA:HB3	2:46:B:ALA:HA	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1523)	2:46:B:ALA:HB3	2:46:B:ALA:HA	10	0.31
(1,1353)	2:22:B:LEU:HD22	2:22:B:LEU:HD12	1	0.31
(1,1353)	2:22:B:LEU:HD23	2:22:B:LEU:HD13	4	0.31
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD11	5	0.31
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD12	5	0.31
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD13	5	0.31
(1,1219)	2:31:B:ILE:HG21	2:27:C:LEU:HD11	9	0.31
(1,1219)	2:31:B:ILE:HG21	2:27:C:LEU:HD12	9	0.31
(1,1219)	2:31:B:ILE:HG21	2:27:C:LEU:HD13	9	0.31
(1,1219)	2:31:B:ILE:HG22	2:27:C:LEU:HD11	9	0.31
(1,1219)	2:31:B:ILE:HG22	2:27:C:LEU:HD12	9	0.31
(1,1219)	2:31:B:ILE:HG22	2:27:C:LEU:HD13	9	0.31
(1,1219)	2:31:B:ILE:HG23	2:27:C:LEU:HD11	9	0.31
(1,1219)	2:31:B:ILE:HG23	2:27:C:LEU:HD12	9	0.31
(1,1219)	2:31:B:ILE:HG23	2:27:C:LEU:HD13	9	0.31
(1,1216)	2:27:B:LEU:HD11	2:27:B:LEU:H	6	0.31
(1,1216)	2:27:B:LEU:HD12	2:27:B:LEU:H	6	0.31
(1,1216)	2:27:B:LEU:HD13	2:27:B:LEU:H	6	0.31
(1,46)	2:17:C:VAL:H	1:27:A:LEU:H	2	0.31
(1,1873)	2:23:B:ASN:HD22	2:26:B:GLN:HG2	3	0.3
(1,1551)	2:17:B:VAL:HG21	2:15:B:GLU:HG3	8	0.3
(1,1551)	2:17:B:VAL:HG22	2:15:B:GLU:HG3	8	0.3
(1,1551)	2:17:B:VAL:HG23	2:15:B:GLU:HG3	8	0.3
(1,1353)	2:22:B:LEU:HD22	2:22:B:LEU:HD12	5	0.3
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD11	4	0.3
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD12	4	0.3
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD13	4	0.3
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD11	10	0.3
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD12	10	0.3
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD13	10	0.3
(1,1213)	2:31:B:ILE:HD13	2:27:C:LEU:HD22	3	0.3
(1,1128)	2:31:C:ILE:HG21	2:27:B:LEU:HB3	1	0.3
(1,1128)	2:31:C:ILE:HG22	2:27:B:LEU:HB3	1	0.3
(1,1128)	2:31:C:ILE:HG23	2:27:B:LEU:HB3	1	0.3
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD11	9	0.3
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD12	9	0.3
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD13	9	0.3
(1,1884)	2:51:C:LEU:HD21	2:26:C:GLN:HG2	5	0.29
(1,1884)	2:51:C:LEU:HD22	2:26:C:GLN:HG2	5	0.29
(1,1884)	2:51:C:LEU:HD23	2:26:C:GLN:HG2	5	0.29
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD21	6	0.29
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD22	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD23	6	0.29
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD11	6	0.29
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD12	6	0.29
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD13	6	0.29
(1,1713)	2:44:C:LEU:HD11	2:40:C:GLN:HG2	8	0.29
(1,1713)	2:44:C:LEU:HD12	2:40:C:GLN:HG2	8	0.29
(1,1713)	2:44:C:LEU:HD13	2:40:C:GLN:HG2	8	0.29
(1,1532)	2:54:C:ALA:HA	2:54:C:ALA:HB2	3	0.29
(1,1532)	2:54:C:ALA:HA	2:54:C:ALA:HB1	7	0.29
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD11	6	0.29
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD12	6	0.29
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD13	6	0.29
(1,1404)	2:17:C:VAL:HG11	2:45:C:LEU:HG	4	0.29
(1,1404)	2:17:C:VAL:HG12	2:45:C:LEU:HG	4	0.29
(1,1404)	2:17:C:VAL:HG13	2:45:C:LEU:HG	4	0.29
(1,1404)	2:17:C:VAL:HG11	2:45:C:LEU:HG	10	0.29
(1,1404)	2:17:C:VAL:HG12	2:45:C:LEU:HG	10	0.29
(1,1404)	2:17:C:VAL:HG13	2:45:C:LEU:HG	10	0.29
(1,1353)	2:22:B:LEU:HD21	2:22:B:LEU:HD12	8	0.29
(1,1216)	2:27:B:LEU:HD11	2:27:B:LEU:H	3	0.29
(1,1216)	2:27:B:LEU:HD12	2:27:B:LEU:H	3	0.29
(1,1216)	2:27:B:LEU:HD13	2:27:B:LEU:H	3	0.29
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD11	7	0.29
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD12	7	0.29
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD13	7	0.29
(1,1884)	2:51:C:LEU:HD21	2:26:C:GLN:HG2	8	0.28
(1,1884)	2:51:C:LEU:HD22	2:26:C:GLN:HG2	8	0.28
(1,1884)	2:51:C:LEU:HD23	2:26:C:GLN:HG2	8	0.28
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD21	3	0.28
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD22	3	0.28
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD23	3	0.28
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	7	0.28
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	7	0.28
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	7	0.28
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD11	8	0.28
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD12	8	0.28
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD13	8	0.28
(1,1353)	2:22:B:LEU:HD22	2:22:B:LEU:HD13	7	0.28
(1,1353)	2:22:B:LEU:HD21	2:22:B:LEU:HD12	10	0.28
(1,1128)	2:31:C:ILE:HG21	2:27:B:LEU:HB3	2	0.28
(1,1128)	2:31:C:ILE:HG22	2:27:B:LEU:HB3	2	0.28
(1,1128)	2:31:C:ILE:HG23	2:27:B:LEU:HB3	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1128)	2:31:C:ILE:HG21	2:27:B:LEU:HB3	8	0.28
(1,1128)	2:31:C:ILE:HG22	2:27:B:LEU:HB3	8	0.28
(1,1128)	2:31:C:ILE:HG23	2:27:B:LEU:HB3	8	0.28
(1,268)	1:27:A:LEU:HD21	2:45:C:LEU:HB3	5	0.28
(1,268)	1:27:A:LEU:HD22	2:45:C:LEU:HB3	5	0.28
(1,268)	1:27:A:LEU:HD23	2:45:C:LEU:HB3	5	0.28
(1,268)	1:27:A:LEU:HD21	2:45:C:LEU:HB3	6	0.28
(1,268)	1:27:A:LEU:HD22	2:45:C:LEU:HB3	6	0.28
(1,268)	1:27:A:LEU:HD23	2:45:C:LEU:HB3	6	0.28
(1,1775)	2:47:C:GLU:HG3	2:47:C:GLU:HB3	3	0.27
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD11	7	0.27
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD12	7	0.27
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD13	7	0.27
(1,1525)	2:55:B:GLN:H	2:54:B:ALA:HA	1	0.27
(1,1525)	2:55:B:GLN:H	2:54:B:ALA:HA	8	0.27
(1,1469)	2:45:C:LEU:HB2	2:45:C:LEU:HD21	10	0.27
(1,1469)	2:45:C:LEU:HB2	2:45:C:LEU:HD22	10	0.27
(1,1469)	2:45:C:LEU:HB2	2:45:C:LEU:HD23	10	0.27
(1,1308)	2:49:B:LYS:H	2:49:B:LYS:HG2	1	0.27
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG21	2	0.27
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG22	2	0.27
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG23	2	0.27
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG21	3	0.27
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG22	3	0.27
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG23	3	0.27
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG21	5	0.27
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG22	5	0.27
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG23	5	0.27
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG21	7	0.27
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG22	7	0.27
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG23	7	0.27
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG21	8	0.27
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG22	8	0.27
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG23	8	0.27
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD11	7	0.27
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD12	7	0.27
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD13	7	0.27
(1,797)	2:37:B:ASP:H	2:38:B:PRO:HD2	8	0.27
(1,362)	1:11:A:ARG:HA	1:11:A:ARG:HG2	2	0.27
(1,362)	1:11:A:ARG:HA	1:11:A:ARG:HG2	3	0.27
(1,362)	1:11:A:ARG:HA	1:11:A:ARG:HG2	4	0.27
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD11	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD12	1	0.27
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD13	1	0.27
(1,1812)	2:51:C:LEU:HD11	2:26:C:GLN:HG2	10	0.26
(1,1812)	2:51:C:LEU:HD12	2:26:C:GLN:HG2	10	0.26
(1,1812)	2:51:C:LEU:HD13	2:26:C:GLN:HG2	10	0.26
(1,1776)	2:47:C:GLU:HG2	2:47:C:GLU:HB3	4	0.26
(1,1775)	2:47:C:GLU:HG3	2:47:C:GLU:HB3	8	0.26
(1,1775)	2:47:C:GLU:HG3	2:47:C:GLU:HB3	10	0.26
(1,1618)	2:23:C:ASN:HB3	2:24:C:PRO:HD2	1	0.26
(1,1613)	2:23:B:ASN:HB2	2:23:B:ASN:HD22	2	0.26
(1,1613)	2:23:B:ASN:HB2	2:23:B:ASN:HD22	7	0.26
(1,1591)	2:39:B:SER:H	2:38:B:PRO:HG3	10	0.26
(1,1525)	2:55:B:GLN:H	2:54:B:ALA:HA	2	0.26
(1,1525)	2:55:B:GLN:H	2:54:B:ALA:HA	7	0.26
(1,1517)	2:49:B:LYS:H	2:46:B:ALA:HA	1	0.26
(1,1469)	2:45:C:LEU:HB2	2:45:C:LEU:HD21	4	0.26
(1,1469)	2:45:C:LEU:HB2	2:45:C:LEU:HD22	4	0.26
(1,1469)	2:45:C:LEU:HB2	2:45:C:LEU:HD23	4	0.26
(1,1392)	2:29:C:ALA:HB3	2:29:C:ALA:HA	1	0.26
(1,1392)	2:29:C:ALA:HB3	2:29:C:ALA:HA	6	0.26
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG21	1	0.26
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG22	1	0.26
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG23	1	0.26
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG21	6	0.26
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG22	6	0.26
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG23	6	0.26
(1,962)	2:44:C:LEU:HD11	2:34:C:ILE:HB	2	0.26
(1,962)	2:44:C:LEU:HD12	2:34:C:ILE:HB	2	0.26
(1,962)	2:44:C:LEU:HD13	2:34:C:ILE:HB	2	0.26
(1,962)	2:44:C:LEU:HD11	2:34:C:ILE:HB	10	0.26
(1,962)	2:44:C:LEU:HD12	2:34:C:ILE:HB	10	0.26
(1,962)	2:44:C:LEU:HD13	2:34:C:ILE:HB	10	0.26
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD11	4	0.26
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD12	4	0.26
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD13	4	0.26
(1,501)	2:25:B:ASP:H	2:24:B:PRO:HD3	9	0.26
(1,268)	1:27:A:LEU:HD21	2:45:C:LEU:HB3	1	0.26
(1,268)	1:27:A:LEU:HD22	2:45:C:LEU:HB3	1	0.26
(1,268)	1:27:A:LEU:HD23	2:45:C:LEU:HB3	1	0.26
(1,253)	1:27:A:LEU:H	1:27:A:LEU:HD23	6	0.26
(1,1776)	2:47:C:GLU:HG2	2:47:C:GLU:HB3	6	0.25
(1,1775)	2:47:C:GLU:HG3	2:47:C:GLU:HB3	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB2	5	0.25
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB3	5	0.25
(1,1613)	2:23:B:ASN:HB2	2:23:B:ASN:HD22	1	0.25
(1,1613)	2:23:B:ASN:HB2	2:23:B:ASN:HD22	8	0.25
(1,1613)	2:23:B:ASN:HB2	2:23:B:ASN:HD22	10	0.25
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD11	9	0.25
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD12	9	0.25
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD13	9	0.25
(1,1424)	2:48:B:ALA:HB1	2:19:B:LEU:HB2	6	0.25
(1,1424)	2:48:B:ALA:HB2	2:19:B:LEU:HB2	6	0.25
(1,1424)	2:48:B:ALA:HB3	2:19:B:LEU:HB2	6	0.25
(1,1392)	2:29:C:ALA:HB3	2:29:C:ALA:HA	3	0.25
(1,1392)	2:29:C:ALA:HB2	2:29:C:ALA:HA	4	0.25
(1,1392)	2:29:B:ALA:HA	2:29:B:ALA:HB1	5	0.25
(1,1392)	2:29:C:ALA:HB1	2:29:C:ALA:HA	7	0.25
(1,1392)	2:29:C:ALA:HB2	2:29:C:ALA:HA	8	0.25
(1,1392)	2:29:C:ALA:HB1	2:29:C:ALA:HA	9	0.25
(1,1392)	2:29:B:ALA:HA	2:29:B:ALA:HB1	10	0.25
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD11	5	0.25
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD12	5	0.25
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD13	5	0.25
(1,1362)	2:51:B:LEU:H	2:51:B:LEU:HB3	2	0.25
(1,1362)	2:51:B:LEU:H	2:51:B:LEU:HB3	4	0.25
(1,421)	1:28:A:SER:HB2	1:14:A:ASN:HD21	2	0.25
(1,421)	1:28:A:SER:HB3	1:14:A:ASN:HD21	2	0.25
(1,396)	1:12:A:LEU:HA	1:12:A:LEU:HD11	10	0.25
(1,396)	1:12:A:LEU:HA	1:12:A:LEU:HD12	10	0.25
(1,396)	1:12:A:LEU:HA	1:12:A:LEU:HD13	10	0.25
(1,268)	1:27:A:LEU:HD21	2:45:C:LEU:HB3	9	0.25
(1,268)	1:27:A:LEU:HD22	2:45:C:LEU:HB3	9	0.25
(1,268)	1:27:A:LEU:HD23	2:45:C:LEU:HB3	9	0.25
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD11	10	0.25
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD12	10	0.25
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD13	10	0.25
(1,1916)	2:40:B:GLN:HA	2:40:B:GLN:HG3	5	0.24
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	3	0.24
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	3	0.24
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	3	0.24
(1,1776)	2:47:C:GLU:HG2	2:47:C:GLU:HB3	5	0.24
(1,1713)	2:44:C:LEU:HD11	2:40:C:GLN:HG2	7	0.24
(1,1713)	2:44:C:LEU:HD12	2:40:C:GLN:HG2	7	0.24
(1,1713)	2:44:C:LEU:HD13	2:40:C:GLN:HG2	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG21	8	0.24
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG22	8	0.24
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG23	8	0.24
(1,1628)	2:22:C:LEU:H	2:21:C:ASN:HB2	7	0.24
(1,1613)	2:23:B:ASN:HB2	2:23:B:ASN:HD22	3	0.24
(1,1613)	2:23:B:ASN:HB2	2:23:B:ASN:HD22	5	0.24
(1,1564)	2:19:C:LEU:HD21	2:49:C:LYS:HG2	4	0.24
(1,1564)	2:19:C:LEU:HD21	2:49:C:LYS:HG3	4	0.24
(1,1564)	2:19:C:LEU:HD22	2:49:C:LYS:HG2	4	0.24
(1,1564)	2:19:C:LEU:HD22	2:49:C:LYS:HG3	4	0.24
(1,1564)	2:19:C:LEU:HD23	2:49:C:LYS:HG2	4	0.24
(1,1564)	2:19:C:LEU:HD23	2:49:C:LYS:HG3	4	0.24
(1,1525)	2:55:B:GLN:H	2:54:B:ALA:HA	10	0.24
(1,1524)	2:46:B:ALA:HB2	2:46:B:ALA:HA	2	0.24
(1,1524)	2:46:B:ALA:HB3	2:46:B:ALA:HA	6	0.24
(1,1524)	2:46:B:ALA:HB2	2:46:B:ALA:HA	7	0.24
(1,1439)	2:19:B:LEU:HD21	2:48:B:ALA:HB1	3	0.24
(1,1439)	2:19:B:LEU:HD21	2:48:B:ALA:HB2	3	0.24
(1,1439)	2:19:B:LEU:HD21	2:48:B:ALA:HB3	3	0.24
(1,1439)	2:19:B:LEU:HD22	2:48:B:ALA:HB1	3	0.24
(1,1439)	2:19:B:LEU:HD22	2:48:B:ALA:HB2	3	0.24
(1,1439)	2:19:B:LEU:HD22	2:48:B:ALA:HB3	3	0.24
(1,1439)	2:19:B:LEU:HD23	2:48:B:ALA:HB1	3	0.24
(1,1439)	2:19:B:LEU:HD23	2:48:B:ALA:HB2	3	0.24
(1,1439)	2:19:B:LEU:HD23	2:48:B:ALA:HB3	3	0.24
(1,1424)	2:48:B:ALA:HB1	2:19:B:LEU:HB2	3	0.24
(1,1424)	2:48:B:ALA:HB2	2:19:B:LEU:HB2	3	0.24
(1,1424)	2:48:B:ALA:HB3	2:19:B:LEU:HB2	3	0.24
(1,1424)	2:48:B:ALA:HB1	2:19:B:LEU:HB2	5	0.24
(1,1424)	2:48:B:ALA:HB2	2:19:B:LEU:HB2	5	0.24
(1,1424)	2:48:B:ALA:HB3	2:19:B:LEU:HB2	5	0.24
(1,1392)	2:29:B:ALA:HA	2:29:B:ALA:HB1	2	0.24
(1,1362)	2:51:B:LEU:H	2:51:B:LEU:HB3	5	0.24
(1,1362)	2:51:B:LEU:H	2:51:B:LEU:HB3	6	0.24
(1,1362)	2:51:B:LEU:H	2:51:B:LEU:HB3	7	0.24
(1,1362)	2:51:B:LEU:H	2:51:B:LEU:HB3	9	0.24
(1,1211)	2:27:C:LEU:HD21	2:27:C:LEU:HG	1	0.24
(1,1211)	2:27:B:LEU:HD23	2:27:B:LEU:HG	5	0.24
(1,1211)	2:27:B:LEU:HD21	2:27:B:LEU:HG	7	0.24
(1,1211)	2:27:C:LEU:HD21	2:27:C:LEU:HG	10	0.24
(1,1145)	2:17:B:VAL:HG21	2:15:B:GLU:HB2	3	0.24
(1,1145)	2:17:B:VAL:HG22	2:15:B:GLU:HB2	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1145)	2:17:B:VAL:HG23	2:15:B:GLU:HB2	3	0.24
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG21	4	0.24
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG22	4	0.24
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG23	4	0.24
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG21	9	0.24
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG22	9	0.24
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG23	9	0.24
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG21	10	0.24
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG22	10	0.24
(1,1025)	2:17:B:VAL:HA	2:17:B:VAL:HG23	10	0.24
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD11	2	0.24
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD12	2	0.24
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD13	2	0.24
(1,423)	1:28:A:SER:HB3	1:12:A:LEU:HB3	9	0.24
(1,362)	1:11:A:ARG:HA	1:11:A:ARG:HG2	5	0.24
(1,362)	1:11:A:ARG:HA	1:11:A:ARG:HG2	8	0.24
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD11	7	0.24
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD12	7	0.24
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD13	7	0.24
(1,46)	2:17:C:VAL:H	1:27:A:LEU:H	10	0.24
(1,1775)	2:47:C:GLU:HG3	2:47:C:GLU:HB3	4	0.23
(1,1775)	2:47:C:GLU:HG3	2:47:C:GLU:HB3	6	0.23
(1,1775)	2:47:C:GLU:HG3	2:47:C:GLU:HB3	7	0.23
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG21	4	0.23
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG22	4	0.23
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG23	4	0.23
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG21	5	0.23
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG22	5	0.23
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG23	5	0.23
(1,1612)	2:23:C:ASN:HB2	2:23:C:ASN:HD21	8	0.23
(1,1591)	2:39:B:SER:H	2:38:B:PRO:HG3	1	0.23
(1,1564)	2:19:C:LEU:HD21	2:49:C:LYS:HG2	5	0.23
(1,1564)	2:19:C:LEU:HD21	2:49:C:LYS:HG3	5	0.23
(1,1564)	2:19:C:LEU:HD22	2:49:C:LYS:HG2	5	0.23
(1,1564)	2:19:C:LEU:HD22	2:49:C:LYS:HG3	5	0.23
(1,1564)	2:19:C:LEU:HD23	2:49:C:LYS:HG2	5	0.23
(1,1564)	2:19:C:LEU:HD23	2:49:C:LYS:HG3	5	0.23
(1,1525)	2:55:B:GLN:H	2:54:B:ALA:HA	3	0.23
(1,1524)	2:46:B:ALA:HB2	2:46:B:ALA:HA	1	0.23
(1,1524)	2:46:B:ALA:HB1	2:46:B:ALA:HA	3	0.23
(1,1524)	2:46:B:ALA:HB3	2:46:B:ALA:HA	5	0.23
(1,1524)	2:46:C:ALA:HA	2:46:C:ALA:HB1	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1524)	2:46:B:ALA:HB3	2:46:B:ALA:HA	9	0.23
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD11	7	0.23
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD12	7	0.23
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD13	7	0.23
(1,1424)	2:48:B:ALA:HB1	2:19:B:LEU:HB2	7	0.23
(1,1424)	2:48:B:ALA:HB2	2:19:B:LEU:HB2	7	0.23
(1,1424)	2:48:B:ALA:HB3	2:19:B:LEU:HB2	7	0.23
(1,1362)	2:51:B:LEU:H	2:51:B:LEU:HB3	8	0.23
(1,1211)	2:27:C:LEU:HD21	2:27:C:LEU:HG	2	0.23
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD11	9	0.23
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD12	9	0.23
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD13	9	0.23
(1,253)	1:27:A:LEU:H	1:27:A:LEU:HD21	3	0.23
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD11	4	0.23
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD12	4	0.23
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD13	4	0.23
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD11	5	0.23
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD12	5	0.23
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD13	5	0.23
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD11	6	0.23
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD12	6	0.23
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD13	6	0.23
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD11	9	0.23
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD12	9	0.23
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD13	9	0.23
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD21	4	0.22
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD22	4	0.22
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD23	4	0.22
(1,1795)	2:26:B:GLN:H	2:26:B:GLN:HG2	1	0.22
(1,1776)	2:47:C:GLU:HG2	2:47:C:GLU:HB3	1	0.22
(1,1776)	2:47:C:GLU:HG2	2:47:C:GLU:HB3	10	0.22
(1,1775)	2:47:B:GLU:HG2	2:47:B:GLU:HB2	1	0.22
(1,1775)	2:47:C:GLU:HG3	2:47:C:GLU:HB3	2	0.22
(1,1775)	2:47:C:GLU:HG3	2:47:C:GLU:HB3	9	0.22
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD11	5	0.22
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD12	5	0.22
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD13	5	0.22
(1,1713)	2:44:C:LEU:HD11	2:40:C:GLN:HG2	4	0.22
(1,1713)	2:44:C:LEU:HD12	2:40:C:GLN:HG2	4	0.22
(1,1713)	2:44:C:LEU:HD13	2:40:C:GLN:HG2	4	0.22
(1,1615)	2:23:B:ASN:HB3	2:23:B:ASN:HD22	3	0.22
(1,1612)	2:23:C:ASN:HB2	2:23:C:ASN:HD21	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	8	0.22
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	8	0.22
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	8	0.22
(1,1591)	2:39:B:SER:H	2:38:B:PRO:HG3	4	0.22
(1,1525)	2:55:B:GLN:H	2:54:B:ALA:HA	9	0.22
(1,1524)	2:46:B:ALA:HB3	2:46:B:ALA:HA	4	0.22
(1,1524)	2:46:B:ALA:HB3	2:46:B:ALA:HA	10	0.22
(1,1362)	2:51:B:LEU:H	2:51:B:LEU:HB3	3	0.22
(1,1362)	2:51:B:LEU:H	2:51:B:LEU:HB3	10	0.22
(1,1216)	2:27:B:LEU:HD11	2:27:B:LEU:H	4	0.22
(1,1216)	2:27:B:LEU:HD12	2:27:B:LEU:H	4	0.22
(1,1216)	2:27:B:LEU:HD13	2:27:B:LEU:H	4	0.22
(1,1216)	2:27:B:LEU:HD11	2:27:B:LEU:H	9	0.22
(1,1216)	2:27:B:LEU:HD12	2:27:B:LEU:H	9	0.22
(1,1216)	2:27:B:LEU:HD13	2:27:B:LEU:H	9	0.22
(1,1211)	2:27:C:LEU:HD23	2:27:C:LEU:HG	3	0.22
(1,1211)	2:27:B:LEU:HD21	2:27:B:LEU:HG	8	0.22
(1,1206)	2:27:B:LEU:HB3	2:27:B:LEU:HG	2	0.22
(1,1206)	2:27:B:LEU:HB3	2:27:B:LEU:HG	4	0.22
(1,1206)	2:27:B:LEU:HB3	2:27:B:LEU:HG	5	0.22
(1,1206)	2:27:B:LEU:HB3	2:27:B:LEU:HG	6	0.22
(1,1206)	2:27:B:LEU:HB3	2:27:B:LEU:HG	7	0.22
(1,1206)	2:27:B:LEU:HB3	2:27:B:LEU:HG	8	0.22
(1,1206)	2:27:B:LEU:HB3	2:27:B:LEU:HG	9	0.22
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD11	3	0.22
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD12	3	0.22
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD13	3	0.22
(1,797)	2:37:B:ASP:H	2:38:B:PRO:HD2	6	0.22
(1,797)	2:37:B:ASP:H	2:38:B:PRO:HD2	10	0.22
(1,362)	1:11:A:ARG:HA	1:11:A:ARG:HG2	10	0.22
(1,253)	1:27:A:LEU:H	1:27:A:LEU:HD22	4	0.22
(1,66)	1:29:A:SER:HB2	1:30:A:THR:H	6	0.22
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD11	2	0.22
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD12	2	0.22
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD13	2	0.22
(1,1895)	2:31:C:ILE:HG13	2:34:C:ILE:HD12	7	0.21
(1,1776)	2:47:C:GLU:HG2	2:47:C:GLU:HB3	3	0.21
(1,1776)	2:47:B:GLU:HG3	2:47:B:GLU:HB2	7	0.21
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG21	1	0.21
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG22	1	0.21
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG23	1	0.21
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG21	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG22	2	0.21
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG23	2	0.21
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG21	3	0.21
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG22	3	0.21
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG23	3	0.21
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG21	7	0.21
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG22	7	0.21
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG23	7	0.21
(1,1615)	2:23:B:ASN:HB3	2:23:B:ASN:HD22	4	0.21
(1,1615)	2:23:B:ASN:HB3	2:23:B:ASN:HD22	5	0.21
(1,1615)	2:23:B:ASN:HB3	2:23:B:ASN:HD22	8	0.21
(1,1613)	2:23:B:ASN:HB2	2:23:B:ASN:HD22	4	0.21
(1,1612)	2:23:C:ASN:HB2	2:23:C:ASN:HD21	3	0.21
(1,1424)	2:48:B:ALA:HB1	2:19:B:LEU:HB2	9	0.21
(1,1424)	2:48:B:ALA:HB2	2:19:B:LEU:HB2	9	0.21
(1,1424)	2:48:B:ALA:HB3	2:19:B:LEU:HB2	9	0.21
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD11	10	0.21
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD12	10	0.21
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD13	10	0.21
(1,1362)	2:51:B:LEU:H	2:51:B:LEU:HB3	1	0.21
(1,1319)	2:49:B:LYS:HG2	2:17:B:VAL:HG11	3	0.21
(1,1319)	2:49:B:LYS:HG2	2:17:B:VAL:HG12	3	0.21
(1,1319)	2:49:B:LYS:HG2	2:17:B:VAL:HG13	3	0.21
(1,1211)	2:27:C:LEU:HD21	2:27:C:LEU:HG	4	0.21
(1,1211)	2:27:B:LEU:HD22	2:27:B:LEU:HG	6	0.21
(1,1211)	2:27:B:LEU:HD21	2:27:B:LEU:HG	9	0.21
(1,1206)	2:27:B:LEU:HB3	2:27:B:LEU:HG	1	0.21
(1,1206)	2:27:B:LEU:HB3	2:27:B:LEU:HG	3	0.21
(1,1206)	2:27:B:LEU:HB3	2:27:B:LEU:HG	10	0.21
(1,1105)	2:31:C:ILE:HD11	2:31:C:ILE:HA	8	0.21
(1,1105)	2:31:C:ILE:HD12	2:31:C:ILE:HA	8	0.21
(1,1105)	2:31:C:ILE:HD13	2:31:C:ILE:HA	8	0.21
(1,1105)	2:31:C:ILE:HD11	2:31:C:ILE:HA	9	0.21
(1,1105)	2:31:C:ILE:HD12	2:31:C:ILE:HA	9	0.21
(1,1105)	2:31:C:ILE:HD13	2:31:C:ILE:HA	9	0.21
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD11	1	0.21
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD12	1	0.21
(1,829)	2:40:C:GLN:H	2:44:C:LEU:HD13	1	0.21
(1,797)	2:37:B:ASP:H	2:38:B:PRO:HD2	9	0.21
(1,413)	1:11:A:ARG:HG2	1:12:A:LEU:HD11	6	0.21
(1,413)	1:11:A:ARG:HG2	1:12:A:LEU:HD12	6	0.21
(1,413)	1:11:A:ARG:HG2	1:12:A:LEU:HD13	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:12:A:LEU:HA	1:12:A:LEU:HD11	6	0.21
(1,396)	1:12:A:LEU:HA	1:12:A:LEU:HD12	6	0.21
(1,396)	1:12:A:LEU:HA	1:12:A:LEU:HD13	6	0.21
(1,362)	1:11:A:ARG:HA	1:11:A:ARG:HG2	1	0.21
(1,356)	1:10:A:GLN:HG2	1:12:A:LEU:HD21	3	0.21
(1,356)	1:10:A:GLN:HG2	1:12:A:LEU:HD22	3	0.21
(1,356)	1:10:A:GLN:HG2	1:12:A:LEU:HD23	3	0.21
(1,356)	1:10:A:GLN:HG3	1:12:A:LEU:HD21	3	0.21
(1,356)	1:10:A:GLN:HG3	1:12:A:LEU:HD22	3	0.21
(1,356)	1:10:A:GLN:HG3	1:12:A:LEU:HD23	3	0.21
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD11	3	0.21
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD12	3	0.21
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD13	3	0.21
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD11	8	0.21
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD12	8	0.21
(1,58)	1:28:A:SER:H	1:27:A:LEU:HD13	8	0.21
(1,1776)	2:47:B:GLU:HG3	2:47:B:GLU:HB2	2	0.2
(1,1776)	2:47:B:GLU:HG3	2:47:B:GLU:HB2	9	0.2
(1,1675)	2:37:B:ASP:H	2:37:B:ASP:HB3	1	0.2
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	1	0.2
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	1	0.2
(1,1607)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	1	0.2
(1,1470)	2:45:C:LEU:HA	2:45:C:LEU:HD21	5	0.2
(1,1470)	2:45:C:LEU:HA	2:45:C:LEU:HD22	5	0.2
(1,1470)	2:45:C:LEU:HA	2:45:C:LEU:HD23	5	0.2
(1,1426)	2:19:B:LEU:HD21	2:19:B:LEU:HB2	1	0.2
(1,1426)	2:19:B:LEU:HD22	2:19:B:LEU:HB2	1	0.2
(1,1426)	2:19:B:LEU:HD23	2:19:B:LEU:HB2	1	0.2
(1,1424)	2:48:B:ALA:HB1	2:19:B:LEU:HB2	2	0.2
(1,1424)	2:48:B:ALA:HB2	2:19:B:LEU:HB2	2	0.2
(1,1424)	2:48:B:ALA:HB3	2:19:B:LEU:HB2	2	0.2
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD11	6	0.2
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD12	6	0.2
(1,1374)	2:51:C:LEU:HB3	2:22:C:LEU:HD13	6	0.2
(1,1216)	2:27:B:LEU:HD11	2:27:B:LEU:H	8	0.2
(1,1216)	2:27:B:LEU:HD12	2:27:B:LEU:H	8	0.2
(1,1216)	2:27:B:LEU:HD13	2:27:B:LEU:H	8	0.2
(1,1193)	2:31:C:ILE:HG21	2:27:B:LEU:HB3	5	0.2
(1,1193)	2:31:C:ILE:HG22	2:27:B:LEU:HB3	5	0.2
(1,1193)	2:31:C:ILE:HG23	2:27:B:LEU:HB3	5	0.2
(1,1128)	2:31:C:ILE:HG21	2:27:B:LEU:HB3	6	0.2
(1,1128)	2:31:C:ILE:HG22	2:27:B:LEU:HB3	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1128)	2:31:C:ILE:HG23	2:27:B:LEU:HB3	6	0.2
(1,1105)	2:31:C:ILE:HD11	2:31:C:ILE:HA	1	0.2
(1,1105)	2:31:C:ILE:HD12	2:31:C:ILE:HA	1	0.2
(1,1105)	2:31:C:ILE:HD13	2:31:C:ILE:HA	1	0.2
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD11	3	0.2
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD12	3	0.2
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD13	3	0.2
(1,307)	1:14:A:ASN:HB3	1:14:A:ASN:HD22	1	0.2
(1,66)	1:29:A:SER:HB2	1:30:A:THR:H	1	0.2
(1,1776)	2:47:B:GLU:HG3	2:47:B:GLU:HB2	8	0.19
(1,1713)	2:44:C:LEU:HD11	2:40:C:GLN:HG2	1	0.19
(1,1713)	2:44:C:LEU:HD12	2:40:C:GLN:HG2	1	0.19
(1,1713)	2:44:C:LEU:HD13	2:40:C:GLN:HG2	1	0.19
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG21	9	0.19
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG22	9	0.19
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG23	9	0.19
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG21	10	0.19
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG22	10	0.19
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG23	10	0.19
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB2	2	0.19
(1,1661)	2:35:B:HIS:HB2	2:36:B:ASP:HB3	2	0.19
(1,1615)	2:23:B:ASN:HB3	2:23:B:ASN:HD22	1	0.19
(1,1615)	2:23:B:ASN:HB3	2:23:B:ASN:HD22	7	0.19
(1,1615)	2:23:B:ASN:HB3	2:23:B:ASN:HD22	10	0.19
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB2	2	0.19
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB3	2	0.19
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB2	2	0.19
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB3	2	0.19
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB2	2	0.19
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB3	2	0.19
(1,1533)	2:51:C:LEU:HA	2:54:C:ALA:HB2	4	0.19
(1,1470)	2:45:C:LEU:HA	2:45:C:LEU:HD21	1	0.19
(1,1470)	2:45:C:LEU:HA	2:45:C:LEU:HD22	1	0.19
(1,1470)	2:45:C:LEU:HA	2:45:C:LEU:HD23	1	0.19
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD11	7	0.19
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD12	7	0.19
(1,1342)	2:22:C:LEU:H	2:22:C:LEU:HD13	7	0.19
(1,1273)	2:27:C:LEU:H	2:27:C:LEU:HB2	2	0.19
(1,1273)	2:27:C:LEU:H	2:27:C:LEU:HB2	5	0.19
(1,1265)	2:31:B:ILE:HG21	2:24:C:PRO:HG2	5	0.19
(1,1265)	2:31:B:ILE:HG22	2:24:C:PRO:HG2	5	0.19
(1,1265)	2:31:B:ILE:HG23	2:24:C:PRO:HG2	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1265)	2:31:B:ILE:HG21	2:24:C:PRO:HG2	6	0.19
(1,1265)	2:31:B:ILE:HG22	2:24:C:PRO:HG2	6	0.19
(1,1265)	2:31:B:ILE:HG23	2:24:C:PRO:HG2	6	0.19
(1,1265)	2:31:B:ILE:HG21	2:24:C:PRO:HG2	7	0.19
(1,1265)	2:31:B:ILE:HG22	2:24:C:PRO:HG2	7	0.19
(1,1265)	2:31:B:ILE:HG23	2:24:C:PRO:HG2	7	0.19
(1,1265)	2:31:B:ILE:HG21	2:24:C:PRO:HG2	10	0.19
(1,1265)	2:31:B:ILE:HG22	2:24:C:PRO:HG2	10	0.19
(1,1265)	2:31:B:ILE:HG23	2:24:C:PRO:HG2	10	0.19
(1,1210)	2:27:B:LEU:HD21	2:27:B:LEU:HB3	3	0.19
(1,1210)	2:27:B:LEU:HD22	2:27:B:LEU:HB3	3	0.19
(1,1210)	2:27:B:LEU:HD23	2:27:B:LEU:HB3	3	0.19
(1,1128)	2:31:C:ILE:HG21	2:27:B:LEU:HB3	10	0.19
(1,1128)	2:31:C:ILE:HG22	2:27:B:LEU:HB3	10	0.19
(1,1128)	2:31:C:ILE:HG23	2:27:B:LEU:HB3	10	0.19
(1,1105)	2:31:C:ILE:HD11	2:31:C:ILE:HA	4	0.19
(1,1105)	2:31:C:ILE:HD12	2:31:C:ILE:HA	4	0.19
(1,1105)	2:31:C:ILE:HD13	2:31:C:ILE:HA	4	0.19
(1,962)	2:44:C:LEU:HD11	2:34:C:ILE:HB	3	0.19
(1,962)	2:44:C:LEU:HD12	2:34:C:ILE:HB	3	0.19
(1,962)	2:44:C:LEU:HD13	2:34:C:ILE:HB	3	0.19
(1,888)	2:21:C:ASN:H	2:20:C:PRO:HG3	4	0.19
(1,809)	2:37:C:ASP:H	2:38:C:PRO:HG2	3	0.19
(1,809)	2:37:C:ASP:H	2:38:C:PRO:HG3	3	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG21	1	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG22	1	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG23	1	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG21	3	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG22	3	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG23	3	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG21	4	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG22	4	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG23	4	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG21	5	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG22	5	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG23	5	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG21	7	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG22	7	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG23	7	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG21	9	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG22	9	0.19
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG23	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,253)	1:27:A:LEU:H	1:27:A:LEU:HD22	8	0.19
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD11	8	0.19
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD12	8	0.19
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD13	8	0.19
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG21	1	0.19
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG22	1	0.19
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG23	1	0.19
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG21	4	0.19
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG22	4	0.19
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG23	4	0.19
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG21	7	0.19
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG22	7	0.19
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG23	7	0.19
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG21	9	0.19
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG22	9	0.19
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG23	9	0.19
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	6	0.18
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	6	0.18
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	6	0.18
(1,1798)	2:26:C:GLN:H	2:26:C:GLN:HG3	3	0.18
(1,1798)	2:26:C:GLN:H	2:26:C:GLN:HG3	5	0.18
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG21	6	0.18
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG22	6	0.18
(1,1692)	2:38:C:PRO:HB2	2:34:C:ILE:HG23	6	0.18
(1,1675)	2:37:B:ASP:H	2:37:B:ASP:HB3	4	0.18
(1,1615)	2:23:B:ASN:HB3	2:23:B:ASN:HD22	2	0.18
(1,1613)	2:23:B:ASN:HB2	2:23:B:ASN:HD22	6	0.18
(1,1424)	2:48:B:ALA:HB1	2:19:B:LEU:HB2	4	0.18
(1,1424)	2:48:B:ALA:HB2	2:19:B:LEU:HB2	4	0.18
(1,1424)	2:48:B:ALA:HB3	2:19:B:LEU:HB2	4	0.18
(1,1419)	2:25:C:ASP:H	2:24:C:PRO:HB3	5	0.18
(1,1300)	2:39:B:SER:H	2:38:B:PRO:HB3	5	0.18
(1,1273)	2:27:C:LEU:H	2:27:C:LEU:HB2	3	0.18
(1,1265)	2:31:B:ILE:HG21	2:24:C:PRO:HG2	1	0.18
(1,1265)	2:31:B:ILE:HG22	2:24:C:PRO:HG2	1	0.18
(1,1265)	2:31:B:ILE:HG23	2:24:C:PRO:HG2	1	0.18
(1,1265)	2:31:B:ILE:HG21	2:24:C:PRO:HG2	9	0.18
(1,1265)	2:31:B:ILE:HG22	2:24:C:PRO:HG2	9	0.18
(1,1265)	2:31:B:ILE:HG23	2:24:C:PRO:HG2	9	0.18
(1,1216)	2:27:B:LEU:HD11	2:27:B:LEU:H	7	0.18
(1,1216)	2:27:B:LEU:HD12	2:27:B:LEU:H	7	0.18
(1,1216)	2:27:B:LEU:HD13	2:27:B:LEU:H	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1210)	2:27:B:LEU:HD21	2:27:B:LEU:HB3	8	0.18
(1,1210)	2:27:B:LEU:HD22	2:27:B:LEU:HB3	8	0.18
(1,1210)	2:27:B:LEU:HD23	2:27:B:LEU:HB3	8	0.18
(1,1193)	2:31:C:ILE:HG21	2:27:B:LEU:HB3	9	0.18
(1,1193)	2:31:C:ILE:HG22	2:27:B:LEU:HB3	9	0.18
(1,1193)	2:31:C:ILE:HG23	2:27:B:LEU:HB3	9	0.18
(1,1105)	2:31:C:ILE:HD11	2:31:C:ILE:HA	5	0.18
(1,1105)	2:31:C:ILE:HD12	2:31:C:ILE:HA	5	0.18
(1,1105)	2:31:C:ILE:HD13	2:31:C:ILE:HA	5	0.18
(1,1105)	2:31:C:ILE:HD11	2:31:C:ILE:HA	6	0.18
(1,1105)	2:31:C:ILE:HD12	2:31:C:ILE:HA	6	0.18
(1,1105)	2:31:C:ILE:HD13	2:31:C:ILE:HA	6	0.18
(1,1105)	2:31:C:ILE:HD11	2:31:C:ILE:HA	10	0.18
(1,1105)	2:31:C:ILE:HD12	2:31:C:ILE:HA	10	0.18
(1,1105)	2:31:C:ILE:HD13	2:31:C:ILE:HA	10	0.18
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD11	10	0.18
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD12	10	0.18
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD13	10	0.18
(1,809)	2:37:C:ASP:H	2:38:C:PRO:HG2	5	0.18
(1,809)	2:37:C:ASP:H	2:38:C:PRO:HG3	5	0.18
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG21	2	0.18
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG22	2	0.18
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG23	2	0.18
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG21	8	0.18
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG22	8	0.18
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG23	8	0.18
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG21	10	0.18
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG22	10	0.18
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG23	10	0.18
(1,253)	1:27:A:LEU:H	1:27:A:LEU:HD23	1	0.18
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD11	1	0.18
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD12	1	0.18
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD13	1	0.18
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD11	5	0.18
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD12	5	0.18
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD13	5	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG21	2	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG22	2	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG23	2	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG21	3	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG22	3	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG23	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG21	5	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG22	5	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG23	5	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG21	8	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG22	8	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG23	8	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG21	10	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG22	10	0.18
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG23	10	0.18
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	2	0.17
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	2	0.17
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	2	0.17
(1,1795)	2:26:B:GLN:H	2:26:B:GLN:HG2	8	0.17
(1,1658)	2:35:B:HIS:HB2	2:36:B:ASP:H	5	0.17
(1,1564)	2:19:C:LEU:HD21	2:49:C:LYS:HG2	8	0.17
(1,1564)	2:19:C:LEU:HD21	2:49:C:LYS:HG3	8	0.17
(1,1564)	2:19:C:LEU:HD22	2:49:C:LYS:HG2	8	0.17
(1,1564)	2:19:C:LEU:HD22	2:49:C:LYS:HG3	8	0.17
(1,1564)	2:19:C:LEU:HD23	2:49:C:LYS:HG2	8	0.17
(1,1564)	2:19:C:LEU:HD23	2:49:C:LYS:HG3	8	0.17
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB2	1	0.17
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB3	1	0.17
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB2	1	0.17
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB3	1	0.17
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB2	1	0.17
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB3	1	0.17
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB2	8	0.17
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB3	8	0.17
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB2	8	0.17
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB3	8	0.17
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB2	8	0.17
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB3	8	0.17
(1,1554)	2:18:B:TYR:HE1	2:16:B:ILE:HG21	5	0.17
(1,1554)	2:18:B:TYR:HE1	2:16:B:ILE:HG22	5	0.17
(1,1554)	2:18:B:TYR:HE1	2:16:B:ILE:HG23	5	0.17
(1,1554)	2:18:B:TYR:HE2	2:16:B:ILE:HG21	5	0.17
(1,1554)	2:18:B:TYR:HE2	2:16:B:ILE:HG22	5	0.17
(1,1554)	2:18:B:TYR:HE2	2:16:B:ILE:HG23	5	0.17
(1,1426)	2:19:B:LEU:HD21	2:19:B:LEU:HB2	8	0.17
(1,1426)	2:19:B:LEU:HD22	2:19:B:LEU:HB2	8	0.17
(1,1426)	2:19:B:LEU:HD23	2:19:B:LEU:HB2	8	0.17
(1,1419)	2:25:C:ASP:H	2:24:C:PRO:HB3	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1419)	2:25:C:ASP:H	2:24:C:PRO:HB3	8	0.17
(1,1419)	2:25:C:ASP:H	2:24:C:PRO:HB3	9	0.17
(1,1391)	2:29:C:ALA:HB3	2:29:C:ALA:HA	1	0.17
(1,1300)	2:39:B:SER:H	2:38:B:PRO:HB3	2	0.17
(1,1273)	2:27:C:LEU:H	2:27:C:LEU:HB2	1	0.17
(1,1273)	2:27:C:LEU:H	2:27:C:LEU:HB2	7	0.17
(1,1213)	2:31:B:ILE:HD13	2:27:C:LEU:HD22	7	0.17
(1,1128)	2:31:C:ILE:HG21	2:27:B:LEU:HB3	7	0.17
(1,1128)	2:31:C:ILE:HG22	2:27:B:LEU:HB3	7	0.17
(1,1128)	2:31:C:ILE:HG23	2:27:B:LEU:HB3	7	0.17
(1,1105)	2:31:C:ILE:HD11	2:31:C:ILE:HA	3	0.17
(1,1105)	2:31:C:ILE:HD12	2:31:C:ILE:HA	3	0.17
(1,1105)	2:31:C:ILE:HD13	2:31:C:ILE:HA	3	0.17
(1,1105)	2:31:C:ILE:HD11	2:31:C:ILE:HA	7	0.17
(1,1105)	2:31:C:ILE:HD12	2:31:C:ILE:HA	7	0.17
(1,1105)	2:31:C:ILE:HD13	2:31:C:ILE:HA	7	0.17
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD11	5	0.17
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD12	5	0.17
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD13	5	0.17
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD11	6	0.17
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD12	6	0.17
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD13	6	0.17
(1,888)	2:21:C:ASN:H	2:20:C:PRO:HG3	5	0.17
(1,809)	2:37:C:ASP:H	2:38:C:PRO:HG2	4	0.17
(1,809)	2:37:C:ASP:H	2:38:C:PRO:HG3	4	0.17
(1,809)	2:37:C:ASP:H	2:38:C:PRO:HG2	8	0.17
(1,809)	2:37:C:ASP:H	2:38:C:PRO:HG3	8	0.17
(1,797)	2:37:B:ASP:H	2:38:B:PRO:HD2	4	0.17
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG21	6	0.17
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG22	6	0.17
(1,272)	1:17:A:VAL:H	1:17:A:VAL:HG23	6	0.17
(1,252)	1:27:A:LEU:HD21	2:42:C:ALA:H	5	0.17
(1,252)	1:27:A:LEU:HD22	2:42:C:ALA:H	5	0.17
(1,252)	1:27:A:LEU:HD23	2:42:C:ALA:H	5	0.17
(1,164)	2:17:C:VAL:H	1:25:A:ALA:HA	6	0.17
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG21	6	0.17
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG22	6	0.17
(1,13)	1:17:A:VAL:H	1:17:A:VAL:HG23	6	0.17
(1,1675)	2:37:B:ASP:H	2:37:B:ASP:HB3	10	0.16
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB2	4	0.16
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB3	4	0.16
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB2	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB3	4	0.16
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB2	4	0.16
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB3	4	0.16
(1,1551)	2:17:B:VAL:HG21	2:15:B:GLU:HG3	7	0.16
(1,1551)	2:17:B:VAL:HG22	2:15:B:GLU:HG3	7	0.16
(1,1551)	2:17:B:VAL:HG23	2:15:B:GLU:HG3	7	0.16
(1,1525)	2:55:B:GLN:H	2:54:B:ALA:HA	5	0.16
(1,1439)	2:19:B:LEU:HD21	2:48:B:ALA:HB1	1	0.16
(1,1439)	2:19:B:LEU:HD21	2:48:B:ALA:HB2	1	0.16
(1,1439)	2:19:B:LEU:HD21	2:48:B:ALA:HB3	1	0.16
(1,1439)	2:19:B:LEU:HD22	2:48:B:ALA:HB1	1	0.16
(1,1439)	2:19:B:LEU:HD22	2:48:B:ALA:HB2	1	0.16
(1,1439)	2:19:B:LEU:HD22	2:48:B:ALA:HB3	1	0.16
(1,1439)	2:19:B:LEU:HD23	2:48:B:ALA:HB1	1	0.16
(1,1439)	2:19:B:LEU:HD23	2:48:B:ALA:HB2	1	0.16
(1,1439)	2:19:B:LEU:HD23	2:48:B:ALA:HB3	1	0.16
(1,1419)	2:25:C:ASP:H	2:24:C:PRO:HB3	1	0.16
(1,1419)	2:25:C:ASP:H	2:24:C:PRO:HB3	3	0.16
(1,1419)	2:25:C:ASP:H	2:24:C:PRO:HB3	10	0.16
(1,1391)	2:29:B:ALA:HA	2:29:B:ALA:HB1	5	0.16
(1,1391)	2:29:C:ALA:HB3	2:29:C:ALA:HA	6	0.16
(1,1391)	2:29:C:ALA:HB1	2:29:C:ALA:HA	7	0.16
(1,1273)	2:27:C:LEU:H	2:27:C:LEU:HB2	4	0.16
(1,1210)	2:27:B:LEU:HD21	2:27:B:LEU:HB3	6	0.16
(1,1210)	2:27:B:LEU:HD22	2:27:B:LEU:HB3	6	0.16
(1,1210)	2:27:B:LEU:HD23	2:27:B:LEU:HB3	6	0.16
(1,1105)	2:31:C:ILE:HD11	2:31:C:ILE:HA	2	0.16
(1,1105)	2:31:C:ILE:HD12	2:31:C:ILE:HA	2	0.16
(1,1105)	2:31:C:ILE:HD13	2:31:C:ILE:HA	2	0.16
(1,501)	2:25:B:ASP:H	2:24:B:PRO:HD3	3	0.16
(1,372)	1:11:A:ARG:HG2	1:12:A:LEU:H	7	0.16
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD11	6	0.16
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD12	6	0.16
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD13	6	0.16
(1,164)	2:17:C:VAL:H	1:25:A:ALA:HA	5	0.16
(1,164)	2:17:C:VAL:H	1:25:A:ALA:HA	9	0.16
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD11	9	0.16
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD12	9	0.16
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD13	9	0.16
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD11	4	0.15
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD12	4	0.15
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD13	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD11	9	0.15
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD12	9	0.15
(1,1717)	2:41:C:SER:HA	2:44:C:LEU:HD13	9	0.15
(1,1658)	2:35:B:HIS:HB2	2:36:B:ASP:H	2	0.15
(1,1619)	2:23:C:ASN:HB2	2:24:C:PRO:HD2	4	0.15
(1,1618)	2:23:C:ASN:HB3	2:24:C:PRO:HD2	8	0.15
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB2	3	0.15
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB3	3	0.15
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB2	3	0.15
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB3	3	0.15
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB2	3	0.15
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB3	3	0.15
(1,1439)	2:19:B:LEU:HD21	2:48:B:ALA:HB1	6	0.15
(1,1439)	2:19:B:LEU:HD21	2:48:B:ALA:HB2	6	0.15
(1,1439)	2:19:B:LEU:HD21	2:48:B:ALA:HB3	6	0.15
(1,1439)	2:19:B:LEU:HD22	2:48:B:ALA:HB1	6	0.15
(1,1439)	2:19:B:LEU:HD22	2:48:B:ALA:HB2	6	0.15
(1,1439)	2:19:B:LEU:HD22	2:48:B:ALA:HB3	6	0.15
(1,1439)	2:19:B:LEU:HD23	2:48:B:ALA:HB1	6	0.15
(1,1439)	2:19:B:LEU:HD23	2:48:B:ALA:HB2	6	0.15
(1,1439)	2:19:B:LEU:HD23	2:48:B:ALA:HB3	6	0.15
(1,1426)	2:19:B:LEU:HD21	2:19:B:LEU:HB2	10	0.15
(1,1426)	2:19:B:LEU:HD22	2:19:B:LEU:HB2	10	0.15
(1,1426)	2:19:B:LEU:HD23	2:19:B:LEU:HB2	10	0.15
(1,1419)	2:25:C:ASP:H	2:24:C:PRO:HB3	7	0.15
(1,1391)	2:29:C:ALA:HB3	2:29:C:ALA:HA	3	0.15
(1,1391)	2:29:C:ALA:HB2	2:29:C:ALA:HA	4	0.15
(1,1391)	2:29:C:ALA:HB2	2:29:C:ALA:HA	8	0.15
(1,1391)	2:29:C:ALA:HB1	2:29:C:ALA:HA	9	0.15
(1,1391)	2:29:B:ALA:HA	2:29:B:ALA:HB1	10	0.15
(1,1327)	2:49:B:LYS:HD3	2:17:B:VAL:HG13	1	0.15
(1,1273)	2:27:C:LEU:H	2:27:C:LEU:HB2	6	0.15
(1,1273)	2:27:C:LEU:H	2:27:C:LEU:HB2	10	0.15
(1,1216)	2:27:B:LEU:HD11	2:27:B:LEU:H	2	0.15
(1,1216)	2:27:B:LEU:HD12	2:27:B:LEU:H	2	0.15
(1,1216)	2:27:B:LEU:HD13	2:27:B:LEU:H	2	0.15
(1,1210)	2:27:B:LEU:HD21	2:27:B:LEU:HB3	1	0.15
(1,1210)	2:27:B:LEU:HD22	2:27:B:LEU:HB3	1	0.15
(1,1210)	2:27:B:LEU:HD23	2:27:B:LEU:HB3	1	0.15
(1,1193)	2:31:C:ILE:HG21	2:27:B:LEU:HB3	4	0.15
(1,1193)	2:31:C:ILE:HG22	2:27:B:LEU:HB3	4	0.15
(1,1193)	2:31:C:ILE:HG23	2:27:B:LEU:HB3	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1145)	2:17:B:VAL:HG21	2:15:B:GLU:HB2	8	0.15
(1,1145)	2:17:B:VAL:HG22	2:15:B:GLU:HB2	8	0.15
(1,1145)	2:17:B:VAL:HG23	2:15:B:GLU:HB2	8	0.15
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD21	1	0.15
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD22	1	0.15
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD23	1	0.15
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD21	4	0.15
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD22	4	0.15
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD23	4	0.15
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD21	5	0.15
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD22	5	0.15
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD23	5	0.15
(1,274)	1:17:A:VAL:HB	2:17:B:VAL:HB	6	0.15
(1,253)	1:27:A:LEU:H	1:27:A:LEU:HD21	5	0.15
(1,252)	1:27:A:LEU:HD21	2:42:C:ALA:H	7	0.15
(1,252)	1:27:A:LEU:HD22	2:42:C:ALA:H	7	0.15
(1,252)	1:27:A:LEU:HD23	2:42:C:ALA:H	7	0.15
(1,237)	1:26:A:ILE:HG23	1:26:A:ILE:HD13	3	0.15
(1,164)	2:17:C:VAL:H	1:25:A:ALA:HA	7	0.15
(1,164)	2:17:C:VAL:H	1:25:A:ALA:HA	8	0.15
(1,93)	1:11:A:ARG:H	1:11:A:ARG:HG2	7	0.15
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD11	2	0.15
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD12	2	0.15
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD13	2	0.15
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD11	3	0.15
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD12	3	0.15
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD13	3	0.15
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD11	6	0.15
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD12	6	0.15
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD13	6	0.15
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD21	8	0.14
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD22	8	0.14
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD23	8	0.14
(1,1780)	2:51:B:LEU:HD11	2:47:B:GLU:HG2	1	0.14
(1,1780)	2:51:B:LEU:HD11	2:47:B:GLU:HG3	1	0.14
(1,1780)	2:51:B:LEU:HD12	2:47:B:GLU:HG2	1	0.14
(1,1780)	2:51:B:LEU:HD12	2:47:B:GLU:HG3	1	0.14
(1,1780)	2:51:B:LEU:HD13	2:47:B:GLU:HG2	1	0.14
(1,1780)	2:51:B:LEU:HD13	2:47:B:GLU:HG3	1	0.14
(1,1780)	2:51:B:LEU:HD11	2:47:B:GLU:HG2	2	0.14
(1,1780)	2:51:B:LEU:HD11	2:47:B:GLU:HG3	2	0.14
(1,1780)	2:51:B:LEU:HD12	2:47:B:GLU:HG2	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1780)	2:51:B:LEU:HD12	2:47:B:GLU:HG3	2	0.14
(1,1780)	2:51:B:LEU:HD13	2:47:B:GLU:HG2	2	0.14
(1,1780)	2:51:B:LEU:HD13	2:47:B:GLU:HG3	2	0.14
(1,1780)	2:51:B:LEU:HD11	2:47:B:GLU:HG2	7	0.14
(1,1780)	2:51:B:LEU:HD11	2:47:B:GLU:HG3	7	0.14
(1,1780)	2:51:B:LEU:HD12	2:47:B:GLU:HG2	7	0.14
(1,1780)	2:51:B:LEU:HD12	2:47:B:GLU:HG3	7	0.14
(1,1780)	2:51:B:LEU:HD13	2:47:B:GLU:HG2	7	0.14
(1,1780)	2:51:B:LEU:HD13	2:47:B:GLU:HG3	7	0.14
(1,1772)	2:48:B:ALA:H	2:47:B:GLU:HG2	10	0.14
(1,1772)	2:48:B:ALA:H	2:47:B:GLU:HG3	10	0.14
(1,1710)	2:40:C:GLN:H	2:40:C:GLN:HG3	9	0.14
(1,1675)	2:37:B:ASP:H	2:37:B:ASP:HB3	6	0.14
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB2	9	0.14
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB3	9	0.14
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB2	9	0.14
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB3	9	0.14
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB2	9	0.14
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB3	9	0.14
(1,1537)	1:15:A:PHE:HD1	2:27:B:LEU:HD21	4	0.14
(1,1537)	1:15:A:PHE:HD1	2:27:B:LEU:HD22	4	0.14
(1,1537)	1:15:A:PHE:HD1	2:27:B:LEU:HD23	4	0.14
(1,1537)	1:15:A:PHE:HD2	2:27:B:LEU:HD21	4	0.14
(1,1537)	1:15:A:PHE:HD2	2:27:B:LEU:HD22	4	0.14
(1,1537)	1:15:A:PHE:HD2	2:27:B:LEU:HD23	4	0.14
(1,1391)	2:29:B:ALA:HA	2:29:B:ALA:HB1	2	0.14
(1,1273)	2:27:C:LEU:H	2:27:C:LEU:HB2	8	0.14
(1,1273)	2:27:C:LEU:H	2:27:C:LEU:HB2	9	0.14
(1,1210)	2:27:B:LEU:HD21	2:27:B:LEU:HB3	7	0.14
(1,1210)	2:27:B:LEU:HD22	2:27:B:LEU:HB3	7	0.14
(1,1210)	2:27:B:LEU:HD23	2:27:B:LEU:HB3	7	0.14
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD11	10	0.14
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD12	10	0.14
(1,911)	2:23:B:ASN:H	2:22:B:LEU:HD13	10	0.14
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD11	4	0.14
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD12	4	0.14
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD13	4	0.14
(1,809)	2:37:C:ASP:H	2:38:C:PRO:HG2	7	0.14
(1,809)	2:37:C:ASP:H	2:38:C:PRO:HG3	7	0.14
(1,504)	2:51:B:LEU:H	2:51:B:LEU:HB3	2	0.14
(1,323)	1:23:A:PHE:H	1:23:A:PHE:HB2	9	0.14
(1,237)	1:26:A:ILE:HG13	1:26:A:ILE:HD12	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,237)	1:26:A:ILE:HG13	1:26:A:ILE:HD12	9	0.14
(1,164)	2:17:C:VAL:H	1:25:A:ALA:HA	1	0.14
(1,164)	2:17:C:VAL:H	1:25:A:ALA:HA	3	0.14
(1,164)	2:17:C:VAL:H	1:25:A:ALA:HA	10	0.14
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD11	1	0.14
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD12	1	0.14
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD13	1	0.14
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD11	7	0.14
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD12	7	0.14
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD13	7	0.14
(1,1798)	2:26:C:GLN:H	2:26:C:GLN:HG3	10	0.13
(1,1795)	2:26:B:GLN:H	2:26:B:GLN:HG2	3	0.13
(1,1780)	2:51:B:LEU:HD11	2:47:B:GLU:HG2	8	0.13
(1,1780)	2:51:B:LEU:HD11	2:47:B:GLU:HG3	8	0.13
(1,1780)	2:51:B:LEU:HD12	2:47:B:GLU:HG2	8	0.13
(1,1780)	2:51:B:LEU:HD12	2:47:B:GLU:HG3	8	0.13
(1,1780)	2:51:B:LEU:HD13	2:47:B:GLU:HG2	8	0.13
(1,1780)	2:51:B:LEU:HD13	2:47:B:GLU:HG3	8	0.13
(1,1780)	2:51:B:LEU:HD11	2:47:B:GLU:HG2	10	0.13
(1,1780)	2:51:B:LEU:HD11	2:47:B:GLU:HG3	10	0.13
(1,1780)	2:51:B:LEU:HD12	2:47:B:GLU:HG2	10	0.13
(1,1780)	2:51:B:LEU:HD12	2:47:B:GLU:HG3	10	0.13
(1,1780)	2:51:B:LEU:HD13	2:47:B:GLU:HG2	10	0.13
(1,1780)	2:51:B:LEU:HD13	2:47:B:GLU:HG3	10	0.13
(1,1710)	2:40:C:GLN:H	2:40:C:GLN:HG3	10	0.13
(1,1628)	2:22:C:LEU:H	2:21:C:ASN:HB2	4	0.13
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB2	7	0.13
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB3	7	0.13
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB2	7	0.13
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB3	7	0.13
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB2	7	0.13
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB3	7	0.13
(1,1533)	2:51:C:LEU:HA	2:54:C:ALA:HB3	7	0.13
(1,1517)	2:49:B:LYS:H	2:46:B:ALA:HA	10	0.13
(1,1432)	1:24:A:GLY:HA3	2:19:C:LEU:HB2	10	0.13
(1,1312)	2:49:B:LYS:HB2	2:49:B:LYS:HG2	1	0.13
(1,1312)	2:49:B:LYS:HB2	2:49:B:LYS:HG2	2	0.13
(1,1312)	2:49:B:LYS:HB2	2:49:B:LYS:HG2	5	0.13
(1,1312)	2:49:B:LYS:HB2	2:49:B:LYS:HG2	6	0.13
(1,1312)	2:49:B:LYS:HB2	2:49:B:LYS:HG2	9	0.13
(1,1312)	2:49:B:LYS:HB2	2:49:B:LYS:HG2	10	0.13
(1,1265)	2:31:B:ILE:HG21	2:24:C:PRO:HG2	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1265)	2:31:B:ILE:HG22	2:24:C:PRO:HG2	8	0.13
(1,1265)	2:31:B:ILE:HG23	2:24:C:PRO:HG2	8	0.13
(1,1216)	2:27:B:LEU:HD11	2:27:B:LEU:H	1	0.13
(1,1216)	2:27:B:LEU:HD12	2:27:B:LEU:H	1	0.13
(1,1216)	2:27:B:LEU:HD13	2:27:B:LEU:H	1	0.13
(1,1216)	2:27:B:LEU:HD11	2:27:B:LEU:H	5	0.13
(1,1216)	2:27:B:LEU:HD12	2:27:B:LEU:H	5	0.13
(1,1216)	2:27:B:LEU:HD13	2:27:B:LEU:H	5	0.13
(1,1216)	2:27:B:LEU:HD11	2:27:B:LEU:H	10	0.13
(1,1216)	2:27:B:LEU:HD12	2:27:B:LEU:H	10	0.13
(1,1216)	2:27:B:LEU:HD13	2:27:B:LEU:H	10	0.13
(1,1210)	2:27:B:LEU:HD21	2:27:B:LEU:HB3	4	0.13
(1,1210)	2:27:B:LEU:HD22	2:27:B:LEU:HB3	4	0.13
(1,1210)	2:27:B:LEU:HD23	2:27:B:LEU:HB3	4	0.13
(1,1210)	2:27:B:LEU:HD21	2:27:B:LEU:HB3	9	0.13
(1,1210)	2:27:B:LEU:HD22	2:27:B:LEU:HB3	9	0.13
(1,1210)	2:27:B:LEU:HD23	2:27:B:LEU:HB3	9	0.13
(1,1210)	2:27:B:LEU:HD21	2:27:B:LEU:HB3	10	0.13
(1,1210)	2:27:B:LEU:HD22	2:27:B:LEU:HB3	10	0.13
(1,1210)	2:27:B:LEU:HD23	2:27:B:LEU:HB3	10	0.13
(1,1149)	2:35:B:HIS:HB3	2:34:B:ILE:HB	5	0.13
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB1	2	0.13
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB2	2	0.13
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB3	2	0.13
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB1	7	0.13
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB2	7	0.13
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB3	7	0.13
(1,964)	2:45:C:LEU:H	2:45:C:LEU:HB3	10	0.13
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD11	5	0.13
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD12	5	0.13
(1,891)	2:21:C:ASN:H	2:22:C:LEU:HD13	5	0.13
(1,809)	2:37:C:ASP:H	2:38:C:PRO:HG2	2	0.13
(1,809)	2:37:C:ASP:H	2:38:C:PRO:HG3	2	0.13
(1,504)	2:51:B:LEU:H	2:51:B:LEU:HB3	4	0.13
(1,504)	2:51:B:LEU:H	2:51:B:LEU:HB3	5	0.13
(1,323)	1:23:A:PHE:H	1:23:A:PHE:HB2	5	0.13
(1,323)	1:23:A:PHE:H	1:23:A:PHE:HB2	10	0.13
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD21	7	0.13
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD22	7	0.13
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD23	7	0.13
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD21	8	0.13
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD22	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD23	8	0.13
(1,274)	1:17:A:VAL:HB	2:17:B:VAL:HB	2	0.13
(1,274)	1:17:A:VAL:HB	2:17:B:VAL:HB	3	0.13
(1,274)	1:17:A:VAL:HB	2:17:B:VAL:HB	5	0.13
(1,274)	1:17:A:VAL:HB	2:17:B:VAL:HB	7	0.13
(1,274)	1:17:A:VAL:HB	2:17:B:VAL:HB	8	0.13
(1,241)	2:18:B:TYR:HD1	1:26:A:ILE:HD11	5	0.13
(1,241)	2:18:B:TYR:HD1	1:26:A:ILE:HD12	5	0.13
(1,241)	2:18:B:TYR:HD1	1:26:A:ILE:HD13	5	0.13
(1,241)	2:18:B:TYR:HD2	1:26:A:ILE:HD11	5	0.13
(1,241)	2:18:B:TYR:HD2	1:26:A:ILE:HD12	5	0.13
(1,241)	2:18:B:TYR:HD2	1:26:A:ILE:HD13	5	0.13
(1,237)	1:26:A:ILE:HG13	1:26:A:ILE:HD11	1	0.13
(1,237)	1:26:A:ILE:HG23	1:26:A:ILE:HD13	4	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD11	2	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD12	2	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD13	2	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD11	3	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD12	3	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD13	3	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD11	4	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD12	4	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD13	4	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD11	7	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD12	7	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD13	7	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD11	8	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD12	8	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD13	8	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD11	9	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD12	9	0.13
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD13	9	0.13
(1,164)	2:17:C:VAL:H	1:25:A:ALA:HA	2	0.13
(1,164)	2:17:C:VAL:H	1:25:A:ALA:HA	4	0.13
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD11	4	0.13
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD12	4	0.13
(1,49)	1:27:A:LEU:H	1:27:A:LEU:HD13	4	0.13
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD21	7	0.12
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD22	7	0.12
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD23	7	0.12
(1,1812)	2:51:C:LEU:HD11	2:26:C:GLN:HG2	6	0.12
(1,1812)	2:51:C:LEU:HD12	2:26:C:GLN:HG2	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1812)	2:51:C:LEU:HD13	2:26:C:GLN:HG2	6	0.12
(1,1799)	2:23:B:ASN:HD21	2:26:B:GLN:HG2	8	0.12
(1,1798)	2:26:C:GLN:H	2:26:C:GLN:HG3	1	0.12
(1,1798)	2:26:C:GLN:H	2:26:C:GLN:HG3	4	0.12
(1,1772)	2:48:B:ALA:H	2:47:B:GLU:HG2	4	0.12
(1,1772)	2:48:B:ALA:H	2:47:B:GLU:HG3	4	0.12
(1,1772)	2:48:B:ALA:H	2:47:B:GLU:HG2	5	0.12
(1,1772)	2:48:B:ALA:H	2:47:B:GLU:HG3	5	0.12
(1,1710)	2:40:C:GLN:H	2:40:C:GLN:HG3	4	0.12
(1,1710)	2:40:C:GLN:H	2:40:C:GLN:HG3	6	0.12
(1,1675)	2:37:B:ASP:H	2:37:B:ASP:HB3	8	0.12
(1,1596)	2:38:C:PRO:HB2	2:38:C:PRO:HD3	10	0.12
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB2	5	0.12
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB3	5	0.12
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB2	5	0.12
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB3	5	0.12
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB2	5	0.12
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB3	5	0.12
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB2	6	0.12
(1,1560)	2:48:C:ALA:HB1	2:19:C:LEU:HB3	6	0.12
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB2	6	0.12
(1,1560)	2:48:C:ALA:HB2	2:19:C:LEU:HB3	6	0.12
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB2	6	0.12
(1,1560)	2:48:C:ALA:HB3	2:19:C:LEU:HB3	6	0.12
(1,1537)	1:15:A:PHE:HD1	2:27:B:LEU:HD21	6	0.12
(1,1537)	1:15:A:PHE:HD1	2:27:B:LEU:HD22	6	0.12
(1,1537)	1:15:A:PHE:HD1	2:27:B:LEU:HD23	6	0.12
(1,1537)	1:15:A:PHE:HD2	2:27:B:LEU:HD21	6	0.12
(1,1537)	1:15:A:PHE:HD2	2:27:B:LEU:HD22	6	0.12
(1,1537)	1:15:A:PHE:HD2	2:27:B:LEU:HD23	6	0.12
(1,1526)	2:56:B:ALA:H	2:54:B:ALA:HA	9	0.12
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD11	4	0.12
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD12	4	0.12
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD13	4	0.12
(1,1424)	2:48:B:ALA:HB1	2:19:B:LEU:HB2	1	0.12
(1,1424)	2:48:B:ALA:HB2	2:19:B:LEU:HB2	1	0.12
(1,1424)	2:48:B:ALA:HB3	2:19:B:LEU:HB2	1	0.12
(1,1388)	2:51:C:LEU:H	2:51:C:LEU:HD11	8	0.12
(1,1388)	2:51:C:LEU:H	2:51:C:LEU:HD12	8	0.12
(1,1388)	2:51:C:LEU:H	2:51:C:LEU:HD13	8	0.12
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD11	1	0.12
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD12	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1384)	2:51:B:LEU:HB3	2:22:B:LEU:HD13	1	0.12
(1,1312)	2:49:B:LYS:HB2	2:49:B:LYS:HG2	4	0.12
(1,1312)	2:49:B:LYS:HB2	2:49:B:LYS:HG2	8	0.12
(1,1230)	2:44:B:LEU:H	2:44:B:LEU:HB3	8	0.12
(1,1179)	2:15:C:GLU:HB3	2:16:C:ILE:H	1	0.12
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB1	5	0.12
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB2	5	0.12
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB3	5	0.12
(1,504)	2:51:B:LEU:H	2:51:B:LEU:HB3	6	0.12
(1,504)	2:51:B:LEU:H	2:51:B:LEU:HB3	7	0.12
(1,504)	2:51:B:LEU:H	2:51:B:LEU:HB3	9	0.12
(1,368)	1:27:A:LEU:HD21	1:11:A:ARG:HB2	10	0.12
(1,368)	1:27:A:LEU:HD21	1:11:A:ARG:HB3	10	0.12
(1,368)	1:27:A:LEU:HD22	1:11:A:ARG:HB2	10	0.12
(1,368)	1:27:A:LEU:HD22	1:11:A:ARG:HB3	10	0.12
(1,368)	1:27:A:LEU:HD23	1:11:A:ARG:HB2	10	0.12
(1,368)	1:27:A:LEU:HD23	1:11:A:ARG:HB3	10	0.12
(1,323)	1:23:A:PHE:H	1:23:A:PHE:HB2	4	0.12
(1,323)	1:23:A:PHE:H	1:23:A:PHE:HB2	6	0.12
(1,323)	1:23:A:PHE:H	1:23:A:PHE:HB2	7	0.12
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD21	2	0.12
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD22	2	0.12
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD23	2	0.12
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD21	3	0.12
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD22	3	0.12
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD23	3	0.12
(1,274)	1:17:A:VAL:HB	2:17:B:VAL:HB	9	0.12
(1,237)	1:26:A:ILE:HG13	1:26:A:ILE:HD11	8	0.12
(1,237)	1:26:A:ILE:HG21	1:26:A:ILE:HD13	10	0.12
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD11	10	0.12
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD12	10	0.12
(1,217)	1:26:A:ILE:HA	1:26:A:ILE:HD13	10	0.12
(1,94)	1:11:A:ARG:H	1:11:A:ARG:HB2	4	0.12
(1,94)	1:11:A:ARG:H	1:11:A:ARG:HB3	4	0.12
(1,94)	1:11:A:ARG:H	1:11:A:ARG:HB2	9	0.12
(1,94)	1:11:A:ARG:H	1:11:A:ARG:HB3	9	0.12
(1,83)	1:17:A:VAL:H	2:18:B:TYR:H	4	0.12
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD21	9	0.11
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD22	9	0.11
(1,1878)	2:52:C:ASN:HB3	2:22:C:LEU:HD23	9	0.11
(1,1798)	2:26:C:GLN:H	2:26:C:GLN:HG3	8	0.11
(1,1711)	2:40:B:GLN:H	2:40:B:GLN:HG2	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1710)	2:40:C:GLN:H	2:40:C:GLN:HG3	2	0.11
(1,1710)	2:40:C:GLN:H	2:40:C:GLN:HG3	3	0.11
(1,1710)	2:40:C:GLN:H	2:40:C:GLN:HG3	7	0.11
(1,1618)	2:23:C:ASN:HB3	2:24:C:PRO:HD2	2	0.11
(1,1596)	2:38:C:PRO:HB2	2:38:C:PRO:HD3	4	0.11
(1,1596)	2:38:C:PRO:HB2	2:38:C:PRO:HD3	6	0.11
(1,1533)	2:51:C:LEU:HA	2:54:C:ALA:HB3	5	0.11
(1,1529)	2:55:C:GLN:H	2:54:C:ALA:HB3	8	0.11
(1,1517)	2:49:C:LYS:H	2:46:C:ALA:HA	5	0.11
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD11	10	0.11
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD12	10	0.11
(1,1464)	2:45:C:LEU:H	2:45:C:LEU:HD13	10	0.11
(1,1439)	2:19:B:LEU:HD21	2:48:B:ALA:HB1	4	0.11
(1,1439)	2:19:B:LEU:HD21	2:48:B:ALA:HB2	4	0.11
(1,1439)	2:19:B:LEU:HD21	2:48:B:ALA:HB3	4	0.11
(1,1439)	2:19:B:LEU:HD22	2:48:B:ALA:HB1	4	0.11
(1,1439)	2:19:B:LEU:HD22	2:48:B:ALA:HB2	4	0.11
(1,1439)	2:19:B:LEU:HD22	2:48:B:ALA:HB3	4	0.11
(1,1439)	2:19:B:LEU:HD23	2:48:B:ALA:HB1	4	0.11
(1,1439)	2:19:B:LEU:HD23	2:48:B:ALA:HB2	4	0.11
(1,1439)	2:19:B:LEU:HD23	2:48:B:ALA:HB3	4	0.11
(1,1419)	2:25:C:ASP:H	2:24:C:PRO:HB3	4	0.11
(1,1388)	2:51:C:LEU:H	2:51:C:LEU:HD11	10	0.11
(1,1388)	2:51:C:LEU:H	2:51:C:LEU:HD12	10	0.11
(1,1388)	2:51:C:LEU:H	2:51:C:LEU:HD13	10	0.11
(1,1230)	2:44:B:LEU:H	2:44:B:LEU:HB3	6	0.11
(1,1230)	2:44:B:LEU:H	2:44:B:LEU:HB3	9	0.11
(1,1230)	2:44:B:LEU:H	2:44:B:LEU:HB3	10	0.11
(1,1210)	2:27:B:LEU:HD21	2:27:B:LEU:HB3	2	0.11
(1,1210)	2:27:B:LEU:HD22	2:27:B:LEU:HB3	2	0.11
(1,1210)	2:27:B:LEU:HD23	2:27:B:LEU:HB3	2	0.11
(1,1210)	2:27:B:LEU:HD21	2:27:B:LEU:HB3	5	0.11
(1,1210)	2:27:B:LEU:HD22	2:27:B:LEU:HB3	5	0.11
(1,1210)	2:27:B:LEU:HD23	2:27:B:LEU:HB3	5	0.11
(1,1193)	2:31:C:ILE:HG21	2:27:B:LEU:HB3	1	0.11
(1,1193)	2:31:C:ILE:HG22	2:27:B:LEU:HB3	1	0.11
(1,1193)	2:31:C:ILE:HG23	2:27:B:LEU:HB3	1	0.11
(1,1179)	2:15:C:GLU:HB3	2:16:C:ILE:H	6	0.11
(1,1179)	2:15:C:GLU:HB3	2:16:C:ILE:H	7	0.11
(1,1179)	2:15:C:GLU:HB3	2:16:C:ILE:H	9	0.11
(1,1149)	2:35:B:HIS:HB3	2:34:B:ILE:HB	2	0.11
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB1	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB2	4	0.11
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB3	4	0.11
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB1	9	0.11
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB2	9	0.11
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB3	9	0.11
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB1	10	0.11
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB2	10	0.11
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB3	10	0.11
(1,964)	2:45:C:LEU:H	2:45:C:LEU:HB3	2	0.11
(1,964)	2:45:C:LEU:H	2:45:C:LEU:HB3	3	0.11
(1,888)	2:21:C:ASN:H	2:20:C:PRO:HG3	6	0.11
(1,877)	2:21:B:ASN:H	2:20:B:PRO:HD2	7	0.11
(1,504)	2:51:B:LEU:H	2:51:B:LEU:HB3	8	0.11
(1,501)	2:25:B:ASP:H	2:24:B:PRO:HD3	7	0.11
(1,381)	1:27:A:LEU:HD11	1:11:A:ARG:HG2	7	0.11
(1,381)	1:27:A:LEU:HD12	1:11:A:ARG:HG2	7	0.11
(1,381)	1:27:A:LEU:HD13	1:11:A:ARG:HG2	7	0.11
(1,357)	1:10:A:GLN:HG2	1:12:A:LEU:HD11	4	0.11
(1,357)	1:10:A:GLN:HG2	1:12:A:LEU:HD12	4	0.11
(1,357)	1:10:A:GLN:HG2	1:12:A:LEU:HD13	4	0.11
(1,357)	1:10:A:GLN:HG3	1:12:A:LEU:HD11	4	0.11
(1,357)	1:10:A:GLN:HG3	1:12:A:LEU:HD12	4	0.11
(1,357)	1:10:A:GLN:HG3	1:12:A:LEU:HD13	4	0.11
(1,352)	1:10:A:GLN:HA	1:10:A:GLN:HG2	2	0.11
(1,352)	1:10:A:GLN:HA	1:10:A:GLN:HG3	2	0.11
(1,352)	1:10:A:GLN:HA	1:10:A:GLN:HG2	5	0.11
(1,352)	1:10:A:GLN:HA	1:10:A:GLN:HG3	5	0.11
(1,352)	1:10:A:GLN:HA	1:10:A:GLN:HG2	8	0.11
(1,352)	1:10:A:GLN:HA	1:10:A:GLN:HG3	8	0.11
(1,352)	1:10:A:GLN:HA	1:10:A:GLN:HG2	10	0.11
(1,352)	1:10:A:GLN:HA	1:10:A:GLN:HG3	10	0.11
(1,345)	1:10:A:GLN:HA	1:10:A:GLN:HG2	2	0.11
(1,345)	1:10:A:GLN:HA	1:10:A:GLN:HG3	2	0.11
(1,345)	1:10:A:GLN:HA	1:10:A:GLN:HG2	5	0.11
(1,345)	1:10:A:GLN:HA	1:10:A:GLN:HG3	5	0.11
(1,345)	1:10:A:GLN:HA	1:10:A:GLN:HG2	8	0.11
(1,345)	1:10:A:GLN:HA	1:10:A:GLN:HG3	8	0.11
(1,345)	1:10:A:GLN:HA	1:10:A:GLN:HG2	10	0.11
(1,345)	1:10:A:GLN:HA	1:10:A:GLN:HG3	10	0.11
(1,335)	1:14:A:ASN:HB2	1:13:A:ALA:HB1	7	0.11
(1,335)	1:14:A:ASN:HB2	1:13:A:ALA:HB2	7	0.11
(1,335)	1:14:A:ASN:HB2	1:13:A:ALA:HB3	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,335)	1:14:A:ASN:HB3	1:13:A:ALA:HB1	7	0.11
(1,335)	1:14:A:ASN:HB3	1:13:A:ALA:HB2	7	0.11
(1,335)	1:14:A:ASN:HB3	1:13:A:ALA:HB3	7	0.11
(1,323)	1:23:A:PHE:H	1:23:A:PHE:HB2	1	0.11
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD21	9	0.11
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD22	9	0.11
(1,289)	1:17:A:VAL:H	1:16:A:LEU:HD23	9	0.11
(1,274)	1:17:A:VAL:HB	2:17:B:VAL:HB	1	0.11
(1,252)	1:27:A:LEU:HD21	2:42:C:ALA:H	8	0.11
(1,252)	1:27:A:LEU:HD22	2:42:C:ALA:H	8	0.11
(1,252)	1:27:A:LEU:HD23	2:42:C:ALA:H	8	0.11
(1,170)	1:25:A:ALA:HB1	2:17:C:VAL:HG11	6	0.11
(1,170)	1:25:A:ALA:HB1	2:17:C:VAL:HG12	6	0.11
(1,170)	1:25:A:ALA:HB1	2:17:C:VAL:HG13	6	0.11
(1,170)	1:25:A:ALA:HB2	2:17:C:VAL:HG11	6	0.11
(1,170)	1:25:A:ALA:HB2	2:17:C:VAL:HG12	6	0.11
(1,170)	1:25:A:ALA:HB2	2:17:C:VAL:HG13	6	0.11
(1,170)	1:25:A:ALA:HB3	2:17:C:VAL:HG11	6	0.11
(1,170)	1:25:A:ALA:HB3	2:17:C:VAL:HG12	6	0.11
(1,170)	1:25:A:ALA:HB3	2:17:C:VAL:HG13	6	0.11
(1,94)	1:11:A:ARG:H	1:11:A:ARG:HB2	6	0.11
(1,94)	1:11:A:ARG:H	1:11:A:ARG:HB3	6	0.11
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD11	9	0.1
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD12	9	0.1
(1,1845)	2:52:B:ASN:HB3	2:22:B:LEU:HD13	9	0.1
(1,1800)	2:23:C:ASN:HD22	2:26:C:GLN:HG3	7	0.1
(1,1780)	2:51:B:LEU:HD11	2:47:B:GLU:HG2	9	0.1
(1,1780)	2:51:B:LEU:HD11	2:47:B:GLU:HG3	9	0.1
(1,1780)	2:51:B:LEU:HD12	2:47:B:GLU:HG2	9	0.1
(1,1780)	2:51:B:LEU:HD12	2:47:B:GLU:HG3	9	0.1
(1,1780)	2:51:B:LEU:HD13	2:47:B:GLU:HG2	9	0.1
(1,1780)	2:51:B:LEU:HD13	2:47:B:GLU:HG3	9	0.1
(1,1710)	2:40:C:GLN:H	2:40:C:GLN:HG3	1	0.1
(1,1596)	2:38:C:PRO:HB2	2:38:C:PRO:HD3	1	0.1
(1,1596)	2:38:C:PRO:HB2	2:38:C:PRO:HD3	2	0.1
(1,1564)	2:19:C:LEU:HD21	2:49:C:LYS:HG2	3	0.1
(1,1564)	2:19:C:LEU:HD21	2:49:C:LYS:HG3	3	0.1
(1,1564)	2:19:C:LEU:HD22	2:49:C:LYS:HG2	3	0.1
(1,1564)	2:19:C:LEU:HD22	2:49:C:LYS:HG3	3	0.1
(1,1564)	2:19:C:LEU:HD23	2:49:C:LYS:HG2	3	0.1
(1,1564)	2:19:C:LEU:HD23	2:49:C:LYS:HG3	3	0.1
(1,1564)	2:19:C:LEU:HD21	2:49:C:LYS:HG2	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1564)	2:19:C:LEU:HD21	2:49:C:LYS:HG3	7	0.1
(1,1564)	2:19:C:LEU:HD22	2:49:C:LYS:HG2	7	0.1
(1,1564)	2:19:C:LEU:HD22	2:49:C:LYS:HG3	7	0.1
(1,1564)	2:19:C:LEU:HD23	2:49:C:LYS:HG2	7	0.1
(1,1564)	2:19:C:LEU:HD23	2:49:C:LYS:HG3	7	0.1
(1,1535)	2:56:B:ALA:H	2:55:B:GLN:HA	7	0.1
(1,1517)	2:49:B:LYS:H	2:46:B:ALA:HA	4	0.1
(1,1300)	2:39:B:SER:H	2:38:B:PRO:HB3	3	0.1
(1,1289)	2:45:C:LEU:HB2	2:46:C:ALA:H	7	0.1
(1,1230)	2:44:B:LEU:H	2:44:B:LEU:HB3	1	0.1
(1,1230)	2:44:B:LEU:H	2:44:B:LEU:HB3	2	0.1
(1,1230)	2:44:B:LEU:H	2:44:B:LEU:HB3	3	0.1
(1,1230)	2:44:B:LEU:H	2:44:B:LEU:HB3	4	0.1
(1,1230)	2:44:B:LEU:H	2:44:B:LEU:HB3	5	0.1
(1,1179)	2:15:C:GLU:HB3	2:16:C:ILE:H	4	0.1
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB1	1	0.1
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB2	1	0.1
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB3	1	0.1
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB1	3	0.1
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB2	3	0.1
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB3	3	0.1
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB1	8	0.1
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB2	8	0.1
(1,1103)	2:56:B:ALA:H	2:56:B:ALA:HB3	8	0.1
(1,809)	2:37:C:ASP:H	2:38:C:PRO:HG2	1	0.1
(1,809)	2:37:C:ASP:H	2:38:C:PRO:HG3	1	0.1
(1,504)	2:51:B:LEU:H	2:51:B:LEU:HB3	3	0.1
(1,504)	2:51:B:LEU:H	2:51:B:LEU:HB3	10	0.1
(1,404)	1:12:A:LEU:H	1:12:A:LEU:HD11	7	0.1
(1,404)	1:12:A:LEU:H	1:12:A:LEU:HD12	7	0.1
(1,404)	1:12:A:LEU:H	1:12:A:LEU:HD13	7	0.1
(1,323)	1:23:A:PHE:H	1:23:A:PHE:HB2	8	0.1
(1,237)	1:26:A:ILE:HG13	1:26:A:ILE:HD13	7	0.1
(1,83)	1:17:A:VAL:H	2:18:B:TYR:H	9	0.1

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

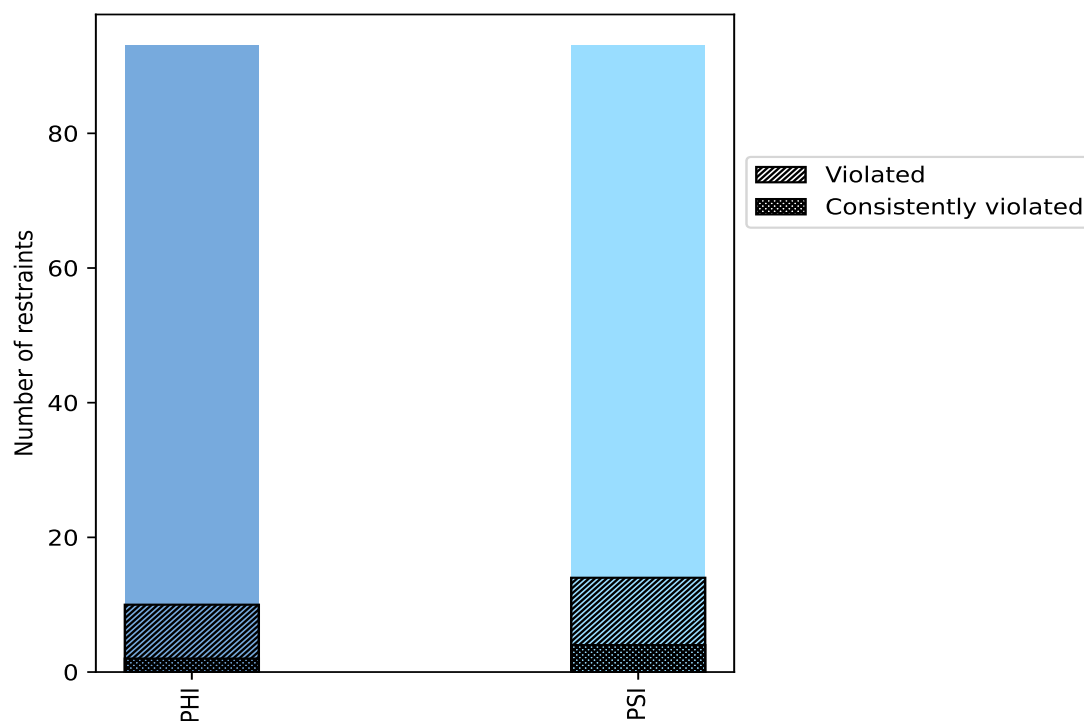
10.1 Summary of dihedral-angle violations [i](#)

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	93	50.0	10	10.8	5.4	2	2.2	1.1
PSI	93	50.0	14	15.1	7.5	4	4.3	2.2
Total	186	100.0	24	12.9	12.9	6	3.2	3.2

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](#)



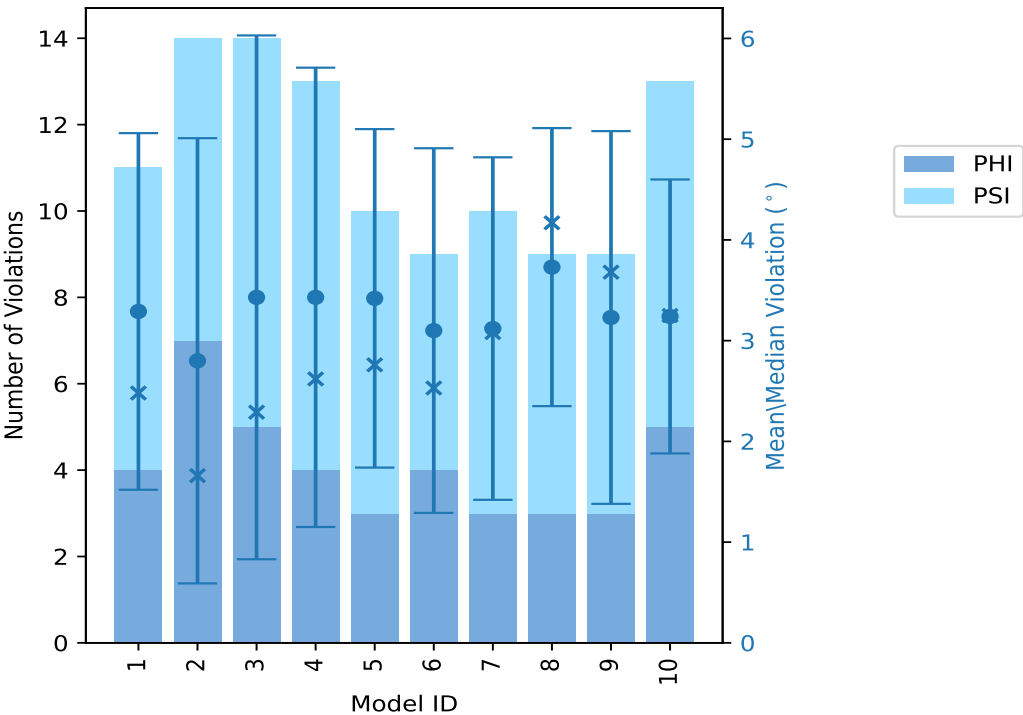
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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	4	7	11	3.29	7.0	1.77	2.48
2	7	7	14	2.8	8.2	2.21	1.66
3	5	9	14	3.43	9.57	2.6	2.29
4	4	9	13	3.43	8.45	2.28	2.62
5	3	7	10	3.42	6.48	1.68	2.76
6	4	5	9	3.1	6.42	1.81	2.53
7	3	7	10	3.12	6.06	1.7	3.08
8	3	6	9	3.73	5.55	1.38	4.17
9	3	6	9	3.23	5.69	1.85	3.68
10	5	8	13	3.24	5.77	1.36	3.25

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

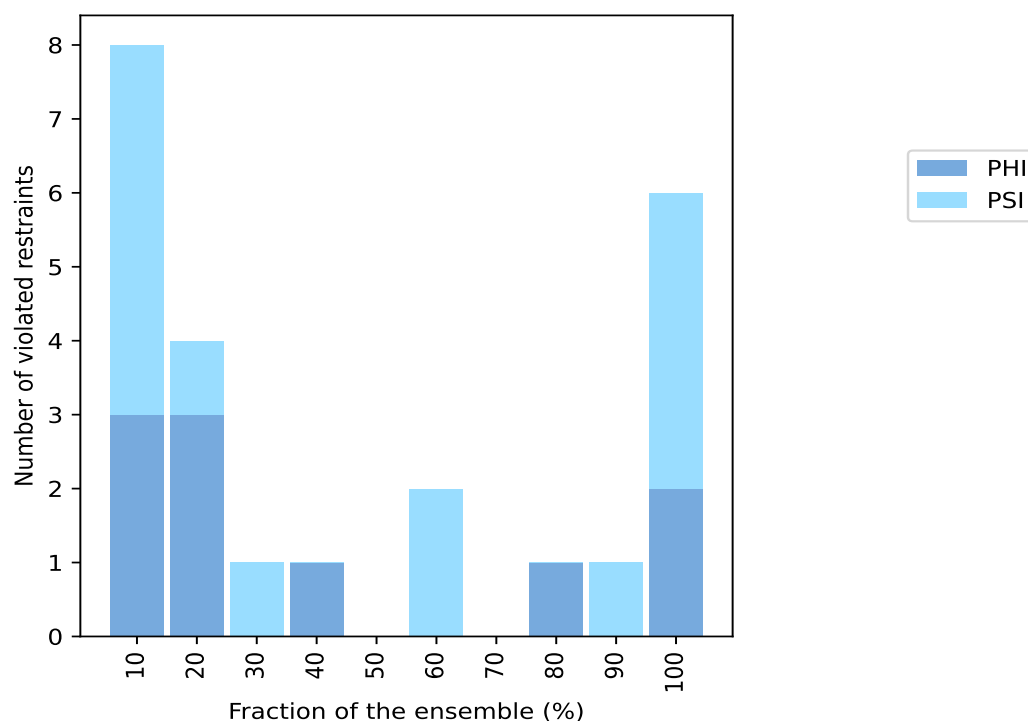
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
3	5	8	1	10.0
3	1	4	2	20.0
0	1	1	3	30.0
1	0	1	4	40.0
0	0	0	5	50.0
0	2	2	6	60.0
0	0	0	7	70.0
1	0	1	8	80.0
0	1	1	9	90.0
2	4	6	10	100.0

¹ Number of models with violations

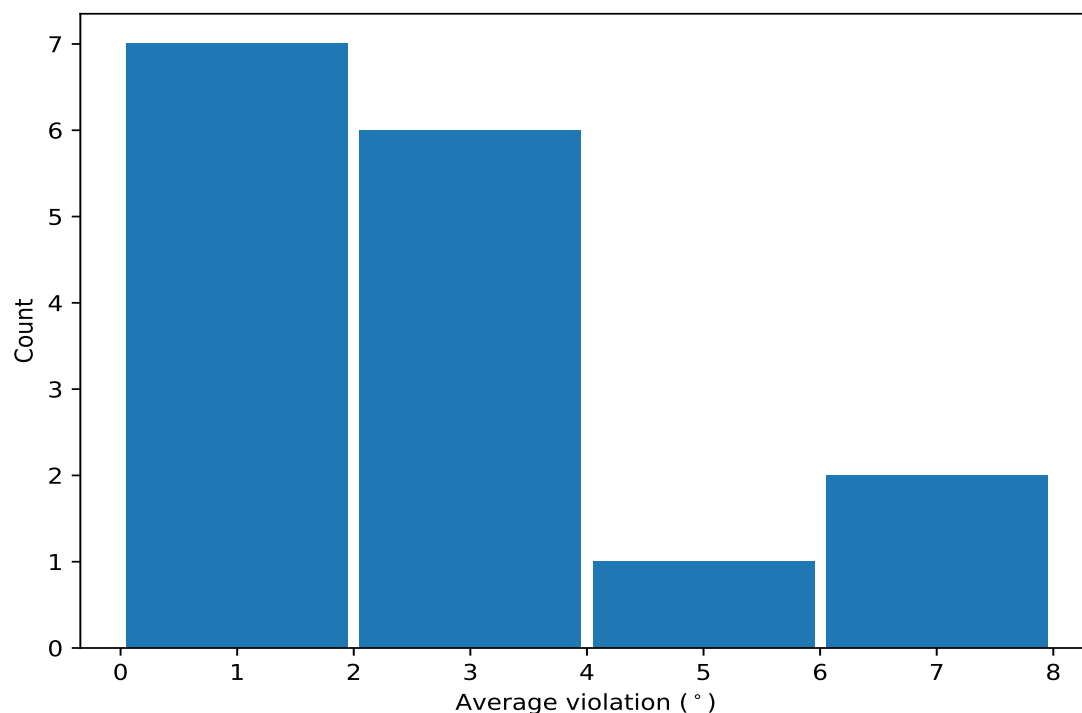
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,19)	1:20:A:SER:C	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	10	6.37	1.59	6.02
(1,18)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ASN:N	10	6.14	1.46	6.01
(1,30)	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	1:28:A:SER:N	10	4.39	1.31	4.48
(2,50)	2:40:B:GLN:N	2:40:B:GLN:CA	2:40:B:GLN:C	2:41:B:SER:N	10	3.67	1.15	3.8
(1,29)	1:26:A:ILE:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	10	2.35	0.93	2.28
(1,20)	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	1:22:A:ASN:N	10	2.08	0.82	1.64
(3,48)	2:40:C:GLN:N	2:40:C:GLN:CA	2:40:C:GLN:C	2:41:C:SER:N	9	3.21	1.02	3.64
(1,7)	1:14:A:ASN:C	1:15:A:PHE:N	1:15:A:PHE:CA	1:15:A:PHE:C	8	1.88	0.61	1.77
(2,10)	2:19:B:LEU:N	2:19:B:LEU:CA	2:19:B:LEU:C	2:20:B:PRO:N	6	3.72	0.98	3.52
(3,6)	2:17:C:VAL:N	2:17:C:VAL:CA	2:17:C:VAL:C	2:18:C:TYR:N	6	2.04	0.72	1.95
(1,27)	1:25:A:ALA:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	4	1.37	0.25	1.29
(1,6)	1:14:A:ASN:N	1:14:A:ASN:CA	1:14:A:ASN:C	1:15:A:PHE:N	3	1.57	0.2	1.46
(2,11)	2:19:B:LEU:C	2:20:B:PRO:N	2:20:B:PRO:CA	2:20:B:PRO:C	2	1.86	0.45	1.86

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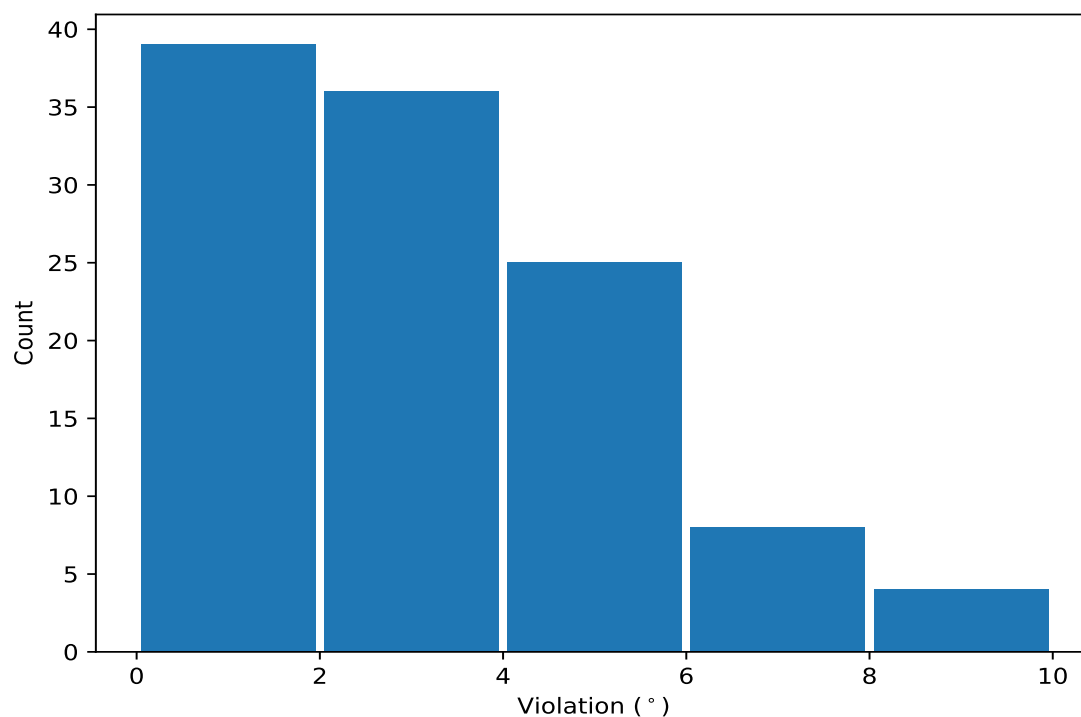
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(2,48)	2:39:B:SER:N	2:39:B:SER:CA	2:39:B:SER:C	2:40:B:GLN:N	2	1.74	0.55	1.74
(1,1)	1:11:A:ARG:C	1:12:A:LEU:N	1:12:A:LEU:CA	1:12:A:LEU:C	2	1.35	0.08	1.35
(2,51)	2:40:B:GLN:C	2:41:B:SER:N	2:41:B:SER:CA	2:41:B:SER:C	2	1.05	0.02	1.05

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 (°)
(1,19)	1:20:A:SER:C	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	3	9.57
(1,18)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ASN:N	3	8.63
(1,18)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ASN:N	4	8.45
(1,19)	1:20:A:SER:C	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	2	8.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,19)	1:20:A:SER:C	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	4	7.53
(1,19)	1:20:A:SER:C	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	1	7.0
(1,18)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ASN:N	2	6.81
(1,19)	1:20:A:SER:C	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	5	6.48
(1,30)	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	1:28:A:SER:N	6	6.42
(1,18)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ASN:N	1	6.26
(1,18)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ASN:N	5	6.25
(1,30)	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	1:28:A:SER:N	7	6.06
(1,18)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ASN:N	10	5.77
(2,50)	2:40:B:GLN:N	2:40:B:GLN:CA	2:40:B:GLN:C	2:41:B:SER:N	9	5.69
(1,19)	1:20:A:SER:C	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	8	5.55
(1,18)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ASN:N	9	5.43
(2,10)	2:19:B:LEU:N	2:19:B:LEU:CA	2:19:B:LEU:C	2:20:B:PRO:N	8	5.4
(1,18)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ASN:N	6	5.32
(2,50)	2:40:B:GLN:N	2:40:B:GLN:CA	2:40:B:GLN:C	2:41:B:SER:N	7	5.12
(1,19)	1:20:A:SER:C	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	10	5.06
(1,19)	1:20:A:SER:C	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	6	4.85
(1,18)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ASN:N	8	4.83
(1,19)	1:20:A:SER:C	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	7	4.77
(1,19)	1:20:A:SER:C	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	9	4.69
(1,30)	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	1:28:A:SER:N	8	4.63
(1,30)	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	1:28:A:SER:N	9	4.58
(1,30)	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	1:28:A:SER:N	4	4.56
(2,10)	2:19:B:LEU:N	2:19:B:LEU:CA	2:19:B:LEU:C	2:20:B:PRO:N	4	4.45
(1,30)	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	1:28:A:SER:N	10	4.41
(1,29)	1:26:A:ILE:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	1	4.41
(3,48)	2:40:C:GLN:N	2:40:C:GLN:CA	2:40:C:GLN:C	2:41:C:SER:N	2	4.32
(3,48)	2:40:C:GLN:N	2:40:C:GLN:CA	2:40:C:GLN:C	2:41:C:SER:N	3	4.32
(1,30)	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	1:28:A:SER:N	3	4.31
(1,20)	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	1:22:A:ASN:N	8	4.17
(3,48)	2:40:C:GLN:N	2:40:C:GLN:CA	2:40:C:GLN:C	2:41:C:SER:N	10	4.14
(2,50)	2:40:B:GLN:N	2:40:B:GLN:CA	2:40:B:GLN:C	2:41:B:SER:N	3	4.11
(1,30)	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	1:28:A:SER:N	5	4.01
(2,50)	2:40:B:GLN:N	2:40:B:GLN:CA	2:40:B:GLN:C	2:41:B:SER:N	5	3.95
(1,2)	1:12:A:LEU:N	1:12:A:LEU:CA	1:12:A:LEU:C	1:13:A:ALA:N	3	3.89
(2,50)	2:40:B:GLN:N	2:40:B:GLN:CA	2:40:B:GLN:C	2:41:B:SER:N	4	3.85
(3,24)	2:27:C:LEU:N	2:27:C:LEU:CA	2:27:C:LEU:C	2:28:C:CYS:N	4	3.83
(2,10)	2:19:B:LEU:N	2:19:B:LEU:CA	2:19:B:LEU:C	2:20:B:PRO:N	10	3.79
(2,50)	2:40:B:GLN:N	2:40:B:GLN:CA	2:40:B:GLN:C	2:41:B:SER:N	2	3.76
(3,48)	2:40:C:GLN:N	2:40:C:GLN:CA	2:40:C:GLN:C	2:41:C:SER:N	9	3.68
(1,18)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ASN:N	7	3.66
(3,48)	2:40:C:GLN:N	2:40:C:GLN:CA	2:40:C:GLN:C	2:41:C:SER:N	7	3.64
(1,30)	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	1:28:A:SER:N	2	3.51
(1,29)	1:26:A:ILE:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	10	3.35
(2,50)	2:40:B:GLN:N	2:40:B:GLN:CA	2:40:B:GLN:C	2:41:B:SER:N	1	3.27
(3,6)	2:17:C:VAL:N	2:17:C:VAL:CA	2:17:C:VAL:C	2:18:C:TYR:N	10	3.25
(2,10)	2:19:B:LEU:N	2:19:B:LEU:CA	2:19:B:LEU:C	2:20:B:PRO:N	1	3.24
(2,50)	2:40:B:GLN:N	2:40:B:GLN:CA	2:40:B:GLN:C	2:41:B:SER:N	10	3.2
(1,7)	1:14:A:ASN:C	1:15:A:PHE:N	1:15:A:PHE:CA	1:15:A:PHE:C	10	3.0
(2,10)	2:19:B:LEU:N	2:19:B:LEU:CA	2:19:B:LEU:C	2:20:B:PRO:N	5	2.88
(1,20)	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	1:22:A:ASN:N	6	2.73

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(3,48)	2:40:C:GLN:N	2:40:C:GLN:CA	2:40:C:GLN:C	2:41:C:SER:N	5	2.63
(1,29)	1:26:A:ILE:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	4	2.62
(3,6)	2:17:C:VAL:N	2:17:C:VAL:CA	2:17:C:VAL:C	2:18:C:TYR:N	5	2.6
(3,48)	2:40:C:GLN:N	2:40:C:GLN:CA	2:40:C:GLN:C	2:41:C:SER:N	8	2.53
(2,10)	2:19:B:LEU:N	2:19:B:LEU:CA	2:19:B:LEU:C	2:20:B:PRO:N	7	2.53
(1,7)	1:14:A:ASN:C	1:15:A:PHE:N	1:15:A:PHE:CA	1:15:A:PHE:C	6	2.53
(1,29)	1:26:A:ILE:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	5	2.52
(3,48)	2:40:C:GLN:N	2:40:C:GLN:CA	2:40:C:GLN:C	2:41:C:SER:N	1	2.48
(1,20)	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	1:22:A:ASN:N	1	2.47
(2,11)	2:19:B:LEU:C	2:20:B:PRO:N	2:20:B:PRO:CA	2:20:B:PRO:C	8	2.32
(2,48)	2:39:B:SER:N	2:39:B:SER:CA	2:39:B:SER:C	2:40:B:GLN:N	3	2.29
(1,29)	1:26:A:ILE:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	3	2.29
(1,29)	1:26:A:ILE:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	2	2.28
(1,7)	1:14:A:ASN:C	1:15:A:PHE:N	1:15:A:PHE:CA	1:15:A:PHE:C	3	2.19
(2,50)	2:40:B:GLN:N	2:40:B:GLN:CA	2:40:B:GLN:C	2:41:B:SER:N	8	2.15
(1,20)	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	1:22:A:ASN:N	4	2.14
(3,6)	2:17:C:VAL:N	2:17:C:VAL:CA	2:17:C:VAL:C	2:18:C:TYR:N	1	2.03
(1,29)	1:26:A:ILE:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	8	2.0
(1,7)	1:14:A:ASN:C	1:15:A:PHE:N	1:15:A:PHE:CA	1:15:A:PHE:C	1	1.92
(3,6)	2:17:C:VAL:N	2:17:C:VAL:CA	2:17:C:VAL:C	2:18:C:TYR:N	2	1.88
(1,6)	1:14:A:ASN:N	1:14:A:ASN:CA	1:14:A:ASN:C	1:15:A:PHE:N	10	1.85
(1,8)	1:15:A:PHE:N	1:15:A:PHE:CA	1:15:A:PHE:C	1:16:A:LEU:N	4	1.81
(1,27)	1:25:A:ALA:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1	1.77
(1,20)	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	1:22:A:ASN:N	3	1.66
(2,50)	2:40:B:GLN:N	2:40:B:GLN:CA	2:40:B:GLN:C	2:41:B:SER:N	6	1.64
(1,20)	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	1:22:A:ASN:N	7	1.63
(1,7)	1:14:A:ASN:C	1:15:A:PHE:N	1:15:A:PHE:CA	1:15:A:PHE:C	4	1.62
(1,20)	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	1:22:A:ASN:N	10	1.61
(1,29)	1:26:A:ILE:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	6	1.56
(1,20)	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	1:22:A:ASN:N	5	1.51
(1,6)	1:14:A:ASN:N	1:14:A:ASN:CA	1:14:A:ASN:C	1:15:A:PHE:N	6	1.46
(1,20)	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	1:22:A:ASN:N	9	1.45
(1,20)	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	1:22:A:ASN:N	2	1.44
(1,29)	1:26:A:ILE:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	7	1.43
(1,1)	1:11:A:ARG:C	1:12:A:LEU:N	1:12:A:LEU:CA	1:12:A:LEU:C	6	1.43
(2,43)	2:35:B:HIS:C	2:36:B:ASP:N	2:36:B:ASP:CA	2:36:B:ASP:C	2	1.42
(2,11)	2:19:B:LEU:C	2:20:B:PRO:N	2:20:B:PRO:CA	2:20:B:PRO:C	10	1.41
(1,27)	1:25:A:ALA:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	7	1.39
(1,6)	1:14:A:ASN:N	1:14:A:ASN:CA	1:14:A:ASN:C	1:15:A:PHE:N	3	1.39
(1,30)	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	1:28:A:SER:N	1	1.37
(1,7)	1:14:A:ASN:C	1:15:A:PHE:N	1:15:A:PHE:CA	1:15:A:PHE:C	5	1.37
(2,73)	2:51:B:LEU:C	2:52:B:ASN:N	2:52:B:ASN:CA	2:52:B:ASN:C	10	1.32
(1,7)	1:14:A:ASN:C	1:15:A:PHE:N	1:15:A:PHE:CA	1:15:A:PHE:C	9	1.31
(3,6)	2:17:C:VAL:N	2:17:C:VAL:CA	2:17:C:VAL:C	2:18:C:TYR:N	4	1.29
(1,1)	1:11:A:ARG:C	1:12:A:LEU:N	1:12:A:LEU:CA	1:12:A:LEU:C	4	1.27
(3,6)	2:17:C:VAL:N	2:17:C:VAL:CA	2:17:C:VAL:C	2:18:C:TYR:N	3	1.19
(2,48)	2:39:B:SER:N	2:39:B:SER:CA	2:39:B:SER:C	2:40:B:GLN:N	9	1.19
(1,27)	1:25:A:ALA:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	2	1.19
(3,48)	2:40:C:GLN:N	2:40:C:GLN:CA	2:40:C:GLN:C	2:41:C:SER:N	4	1.15
(1,7)	1:14:A:ASN:C	1:15:A:PHE:N	1:15:A:PHE:CA	1:15:A:PHE:C	2	1.14
(2,60)	2:45:B:LEU:N	2:45:B:LEU:CA	2:45:B:LEU:C	2:46:B:ALA:N	2	1.13

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,27)	1:25:A:ALA:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	3	1.12
(2,51)	2:40:B:GLN:C	2:41:B:SER:N	2:41:B:SER:CA	2:41:B:SER:C	3	1.07
(1,29)	1:26:A:ILE:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	9	1.06
(2,51)	2:40:B:GLN:C	2:41:B:SER:N	2:41:B:SER:CA	2:41:B:SER:C	2	1.03
(2,49)	2:39:B:SER:C	2:40:B:GLN:N	2:40:B:GLN:CA	2:40:B:GLN:C	2	1.02
(1,32)	1:28:A:SER:N	1:28:A:SER:CA	1:28:A:SER:C	1:29:A:SER:N	7	1.02