



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 10:39 PM UTC

PDB ID : 2MKZ / pdb_00002mkz
BMRB ID : 19801
Title : solution structure of a protein C-terminal domain
Authors : Feng, Y.; Jiao, L.
Deposited on : 2014-02-17

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

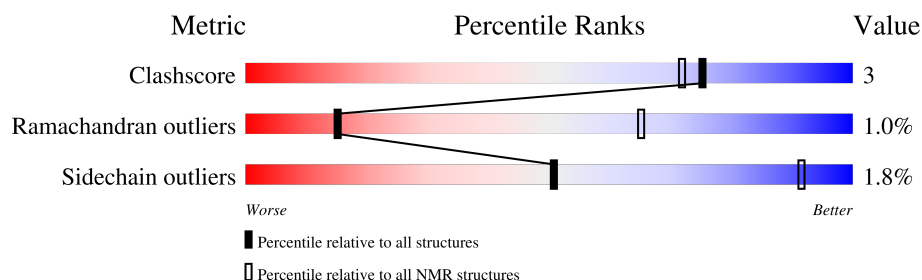
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 95%.

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	141	

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:21-A:115 (95)	0.43	11

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 9 single-model clusters were found.

Cluster number	Models
1	3, 11, 12, 13, 17, 19
2	1, 5, 15
3	4, 16
Single-model clusters	2; 6; 7; 8; 9; 10; 14; 18; 20

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2048 atoms, of which 1013 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Proteasomal ubiquitin receptor ADRM1.

Mol	Chain	Residues	Atoms						Trace
1	A	141	Total	C	H	N	O	S	0
			2048	640	1013	170	218	7	

There are 3 discrepancies between the modelled and reference sequences:

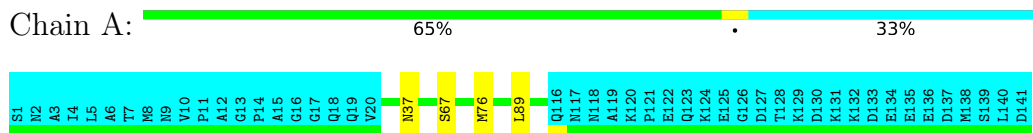
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q16186
A	2	ASN	-	expression tag	UNP Q16186
A	3	ALA	-	expression tag	UNP Q16186

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Proteasomal ubiquitin receptor ADRM1

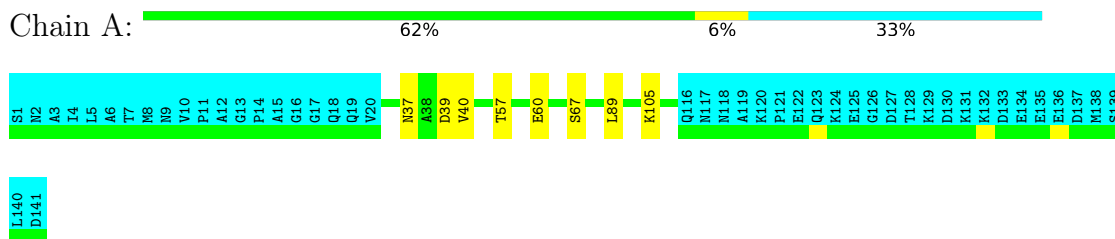


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

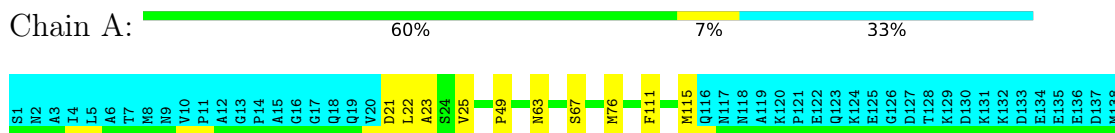
4.2.1 Score per residue for model 1

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.2 Score per residue for model 2

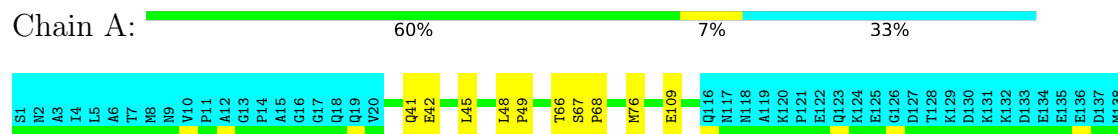
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



S139
L140
D141

4.2.3 Score per residue for model 3

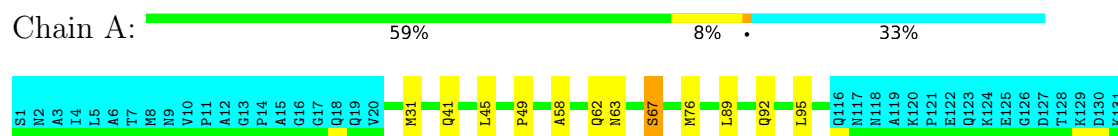
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



S139
L140
D141

4.2.4 Score per residue for model 4

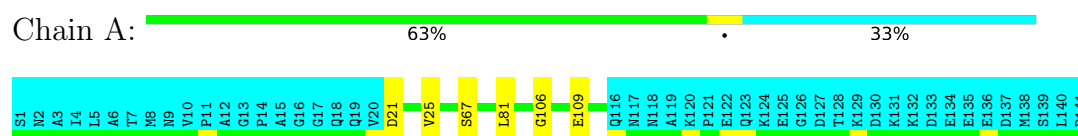
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



K132
D133
E134
E135
E136
D137
M138
L140
D141

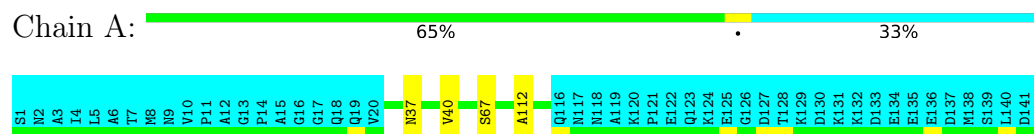
4.2.5 Score per residue for model 5

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



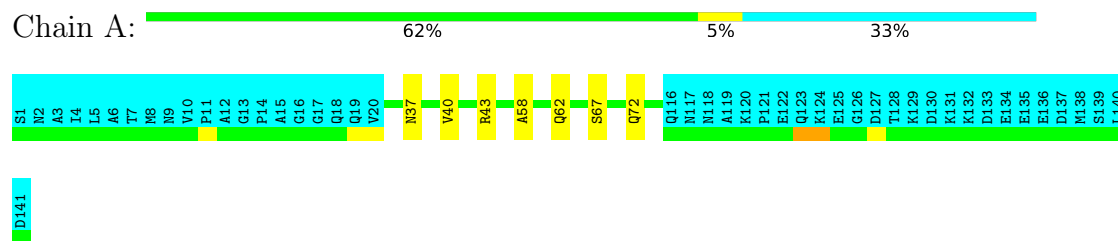
4.2.6 Score per residue for model 6

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



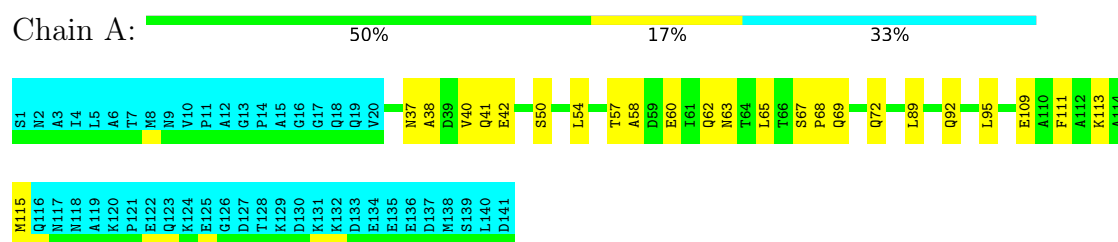
4.2.7 Score per residue for model 7

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



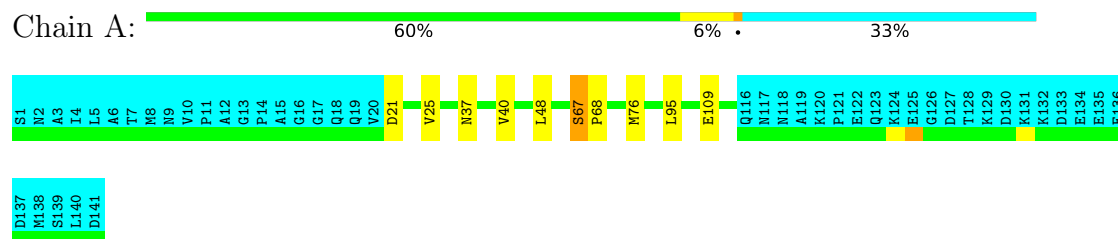
4.2.8 Score per residue for model 8

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



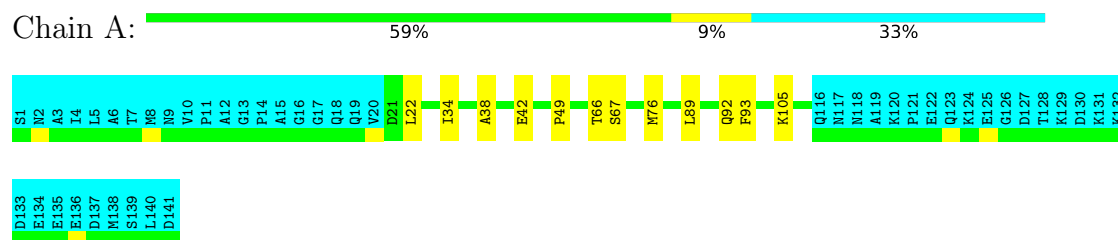
4.2.9 Score per residue for model 9

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



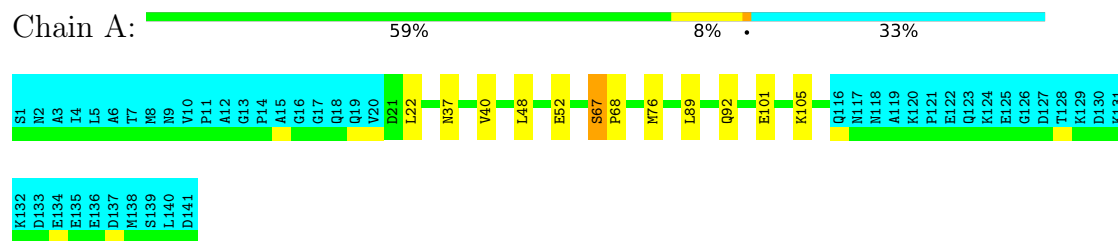
4.2.10 Score per residue for model 10

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



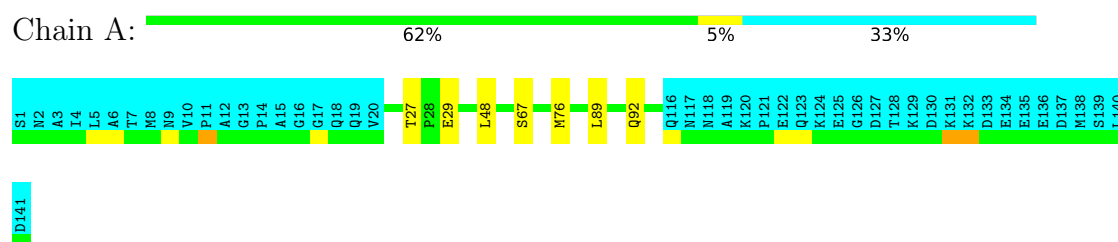
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



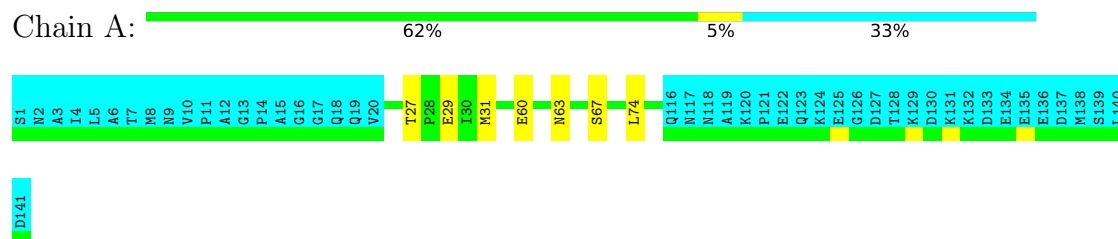
4.2.12 Score per residue for model 12

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



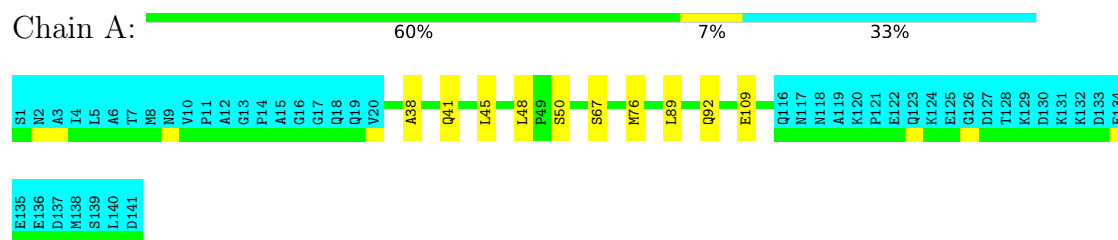
4.2.13 Score per residue for model 13

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



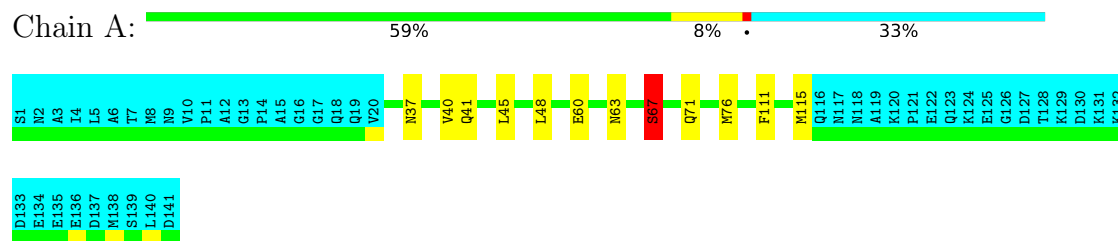
4.2.14 Score per residue for model 14

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



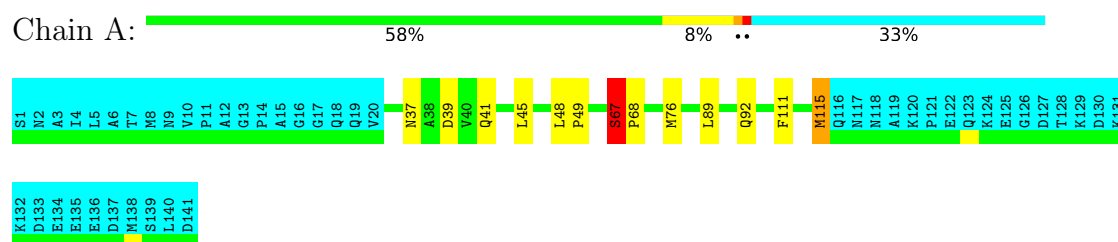
4.2.15 Score per residue for model 15

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



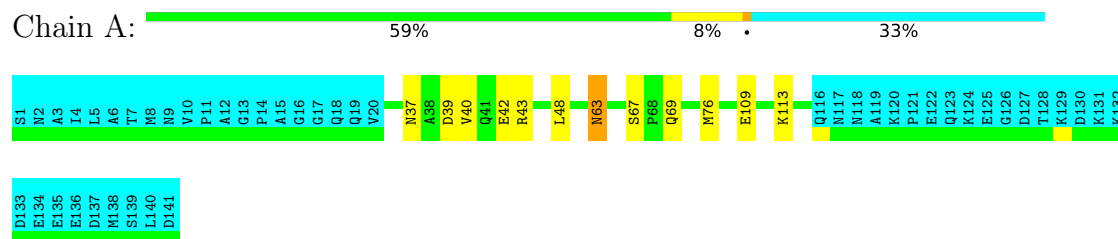
4.2.16 Score per residue for model 16

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



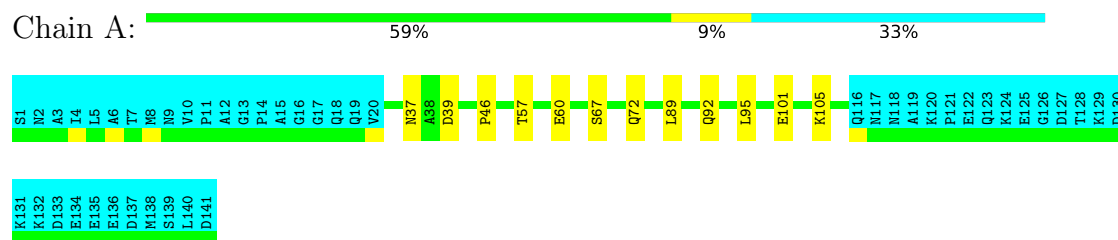
4.2.17 Score per residue for model 17

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



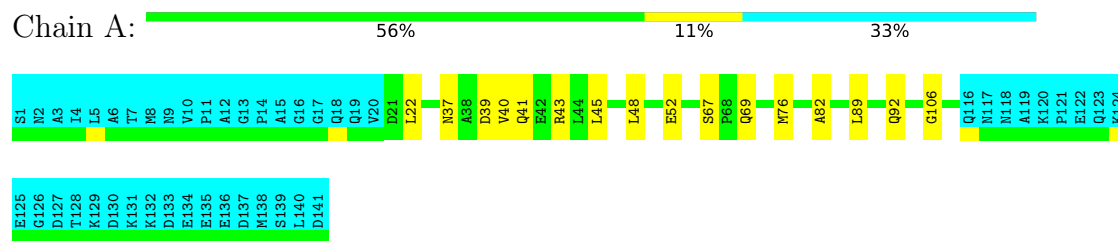
4.2.18 Score per residue for model 18

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



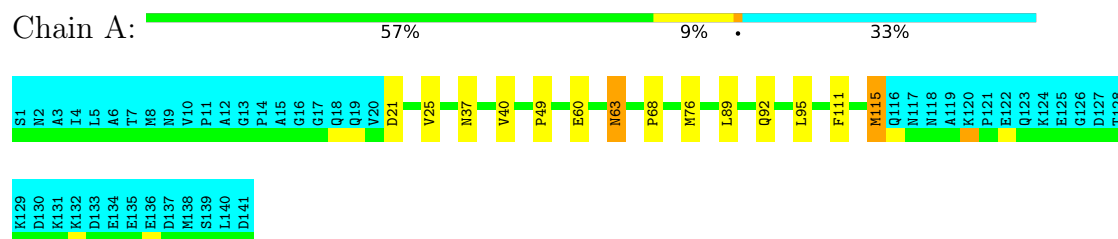
4.2.19 Score per residue for model 19

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.20 Score per residue for model 20

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
CYANA	structure solution	
SANE	refinement	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1665
Number of shifts mapped to atoms	1665
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	95%

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	0.91±0.02	0±0/707 (0.0± 0.1%)	0.98±0.03	0±0/965 (0.0± 0.0%)
All	All	0.91	3/14140 (0.0%)	0.98	5/19300 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
All	All	0	2

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	67	SER	C-N	5.28	1.40	1.34	16	3

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	63	ASN	CA-CB-CG	6.87	119.47	112.60	20	5

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	43	ARG	Sidechain	2

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	694	689	689	4±2
All	All	13880	13780	13780	85

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:GLU:HA	1:A:63:ASN:ND2	0.69	2.02	13	3
1:A:89:LEU:O	1:A:92:GLN:HG2	0.58	1.98	16	10
1:A:48:LEU:HA	1:A:76:MET:SD	0.58	2.37	14	9
1:A:49:PRO:HD3	1:A:76:MET:SD	0.57	2.39	3	6
1:A:39:ASP:O	1:A:43:ARG:HD3	0.56	2.01	19	1
1:A:41:GLN:O	1:A:45:LEU:HG	0.53	2.04	14	6
1:A:111:PHE:O	1:A:115:MET:HB2	0.50	2.07	20	2
1:A:67:SER:HB2	1:A:68:PRO:HD3	0.49	1.82	11	2
1:A:27:THR:HB	1:A:29:GLU:OE1	0.49	2.08	13	2
1:A:67:SER:HB2	1:A:68:PRO:HD2	0.48	1.85	8	1
1:A:67:SER:OG	1:A:68:PRO:HD3	0.48	2.08	9	1
1:A:57:THR:OG1	1:A:60:GLU:HG2	0.48	2.09	18	2
1:A:111:PHE:O	1:A:115:MET:HG2	0.47	2.09	2	1
1:A:31:MET:SD	1:A:74:LEU:HD13	0.46	2.51	13	1
1:A:101:GLU:O	1:A:105:LYS:HG2	0.45	2.10	11	2
1:A:37:ASN:O	1:A:40:VAL:HG22	0.45	2.11	9	10
1:A:21:ASP:O	1:A:25:VAL:HG12	0.45	2.12	9	4
1:A:39:ASP:OD1	1:A:89:LEU:HD11	0.45	2.12	1	1
1:A:41:GLN:HB3	1:A:54:LEU:HD13	0.44	1.88	8	1
1:A:69:GLN:HA	1:A:72:GLN:CD	0.44	2.38	8	1
1:A:52:GLU:OE1	1:A:69:GLN:HB3	0.43	2.12	19	1
1:A:65:LEU:HD12	1:A:69:GLN:C	0.43	2.38	8	1
1:A:82:ALA:HA	1:A:106:GLY:CA	0.42	2.45	19	1
1:A:81:LEU:O	1:A:106:GLY:HA2	0.42	2.15	5	1
1:A:38:ALA:O	1:A:42:GLU:HG3	0.42	2.15	8	2
1:A:111:PHE:O	1:A:115:MET:HG3	0.42	2.15	8	2
1:A:37:ASN:OD1	1:A:39:ASP:HB3	0.42	2.14	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:LEU:HD12	1:A:23:ALA:N	0.42	2.30	2	1
1:A:66:THR:O	1:A:68:PRO:HD2	0.41	2.15	3	1
1:A:39:ASP:O	1:A:42:GLU:HB3	0.41	2.15	17	1
1:A:67:SER:O	1:A:71:GLN:HG3	0.41	2.15	15	1
1:A:58:ALA:O	1:A:62:GLN:HG2	0.41	2.16	8	3
1:A:37:ASN:ND2	1:A:39:ASP:HB3	0.40	2.31	16	1
1:A:57:THR:O	1:A:60:GLU:HG2	0.40	2.16	1	1
1:A:34:ILE:HG23	1:A:93:PHE:CE2	0.40	2.52	10	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	95/141 (67%)	92±1 (97±1%)	2±1 (2±1%)	1±0 (1±0%)	15	65
All	All	1900/2820 (67%)	1844 (97%)	37 (2%)	19 (1%)	15	65

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	67	SER	18
1	A	66	THR	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	73/110 (66%)	72±1 (98±2%)	1±1 (2±2%)	51	91
All	All	1460/2200 (66%)	1433 (98%)	27 (2%)	51	91

All 14 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	109	GLU	6
1	A	95	LEU	5
1	A	22	LEU	3
1	A	105	LYS	2
1	A	115	MET	2
1	A	42	GLU	1
1	A	31	MET	1
1	A	50	SER	1
1	A	113	LYS	1
1	A	52	GLU	1
1	A	63	ASN	1
1	A	69	GLN	1
1	A	72	GLN	1
1	A	68	PRO	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 95% for the well-defined parts and 94% 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	1665
Number of shifts mapped to atoms	1665
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	138	-0.28 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	128	0.16 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}'$	138	-0.13 ± 0.11	None needed (< 0.5 ppm)
^{15}N	126	0.00 ± 0.18	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 95%, i.e. 1152 atoms were assigned a chemical shift out of a possible 1208. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	455/465 (98%)	184/188 (98%)	186/190 (98%)	85/87 (98%)
Sidechain	651/694 (94%)	447/459 (97%)	192/219 (88%)	12/16 (75%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	46/49 (94%)	23/24 (96%)	23/25 (92%)	0/0 (—%)
Overall	1152/1208 (95%)	654/671 (97%)	401/434 (92%)	97/103 (94%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 94%, i.e. 1665 atoms were assigned a chemical shift out of a possible 1768. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	676/693 (98%)	274/281 (98%)	276/282 (98%)	126/130 (97%)
Sidechain	943/1026 (92%)	645/669 (96%)	278/328 (85%)	20/29 (69%)
Aromatic	46/49 (94%)	23/24 (96%)	23/25 (92%)	0/0 (—%)
Overall	1665/1768 (94%)	942/974 (97%)	577/635 (91%)	146/159 (92%)

7.1.4 Statistically unusual chemical shifts [i](#)

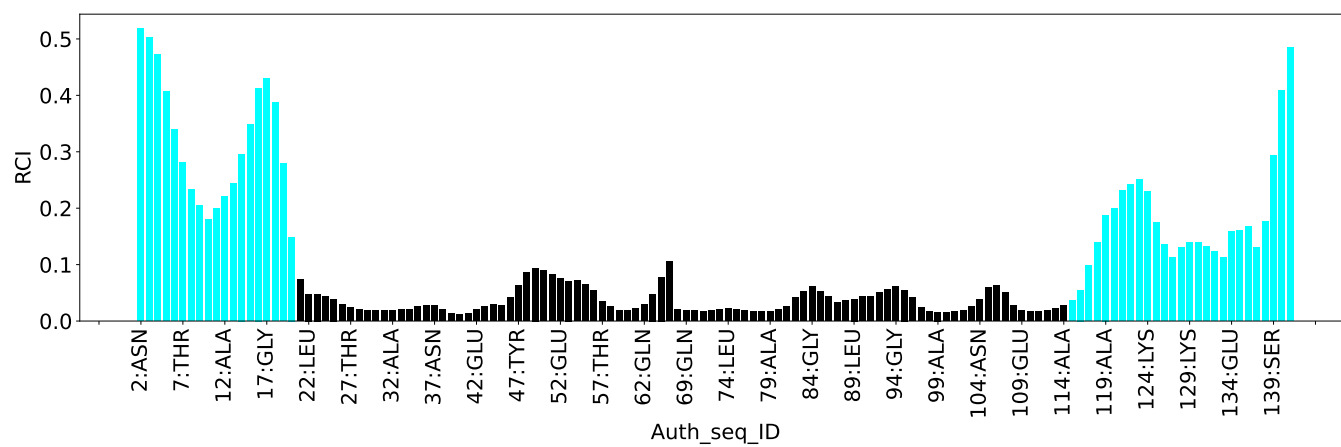
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	28	PRO	HG2	0.32	0.41 – 3.45	-5.3

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3888
Intra-residue ($ i-j =0$)	1216
Sequential ($ i-j =1$)	977
Medium range ($ i-j >1$ and $ i-j <5$)	803
Long range ($ i-j \geq 5$)	806
Inter-chain	0
Hydrogen bond restraints	86
Disulfide bond restraints	0
Total dihedral-angle restraints	176
Number of unmapped restraints	0
Number of restraints per residue	28.8
Number of long range restraints per residue ¹	5.7

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)	71.3	0.2
0.2-0.5 (Medium)	133.3	0.5
>0.5 (Large)	111.6	1.62

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)	0.6	1.88
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

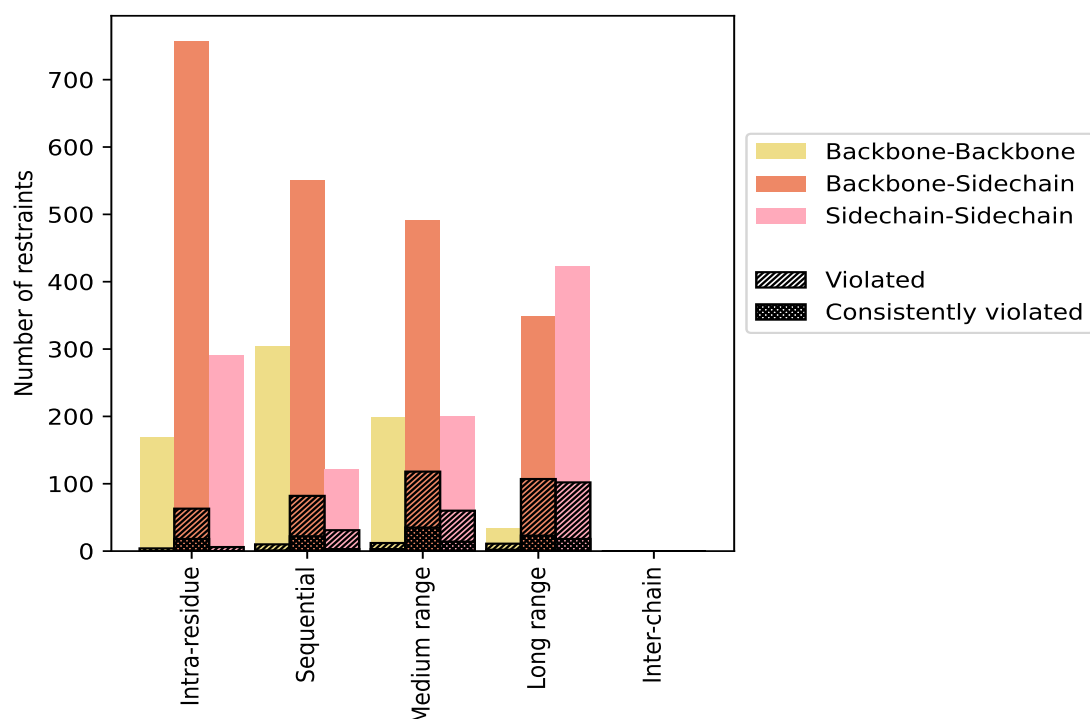
9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1216	31.3	73	6.0	1.9	18	1.5	0.5
Backbone-Backbone	169	4.3	4	2.4	0.1	0	0.0	0.0
Backbone-Sidechain	757	19.5	63	8.3	1.6	18	2.4	0.5
Sidechain-Sidechain	290	7.5	6	2.1	0.2	0	0.0	0.0
Sequential ($i-j =1$)	977	25.1	123	12.6	3.2	26	2.7	0.7
Backbone-Backbone	304	7.8	10	3.3	0.3	1	0.3	0.0
Backbone-Sidechain	551	14.2	82	14.9	2.1	22	4.0	0.6
Sidechain-Sidechain	122	3.1	31	25.4	0.8	3	2.5	0.1
Medium range ($i-j >1$ & $i-j <5$)	803	20.7	189	23.5	4.9	52	6.5	1.3
Backbone-Backbone	198	5.1	12	6.1	0.3	3	1.5	0.1
Backbone-Sidechain	405	10.4	117	28.9	3.0	35	8.6	0.9
Sidechain-Sidechain	200	5.1	60	30.0	1.5	14	7.0	0.4
Long range ($i-j \geq 5$)	806	20.7	220	27.3	5.7	43	5.3	1.1
Backbone-Backbone	34	0.9	11	32.4	0.3	2	5.9	0.1
Backbone-Sidechain	349	9.0	107	30.7	2.8	23	6.6	0.6
Sidechain-Sidechain	423	10.9	102	24.1	2.6	18	4.3	0.5
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	86	2.2	1	1.2	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3888	100.0	606	15.6	15.6	139	3.6	3.6
Backbone-Backbone	705	18.1	37	5.2	1.0	6	0.9	0.2
Backbone-Sidechain	2148	55.2	370	17.2	9.5	98	4.6	2.5
Sidechain-Sidechain	1035	26.6	199	19.2	5.1	35	3.4	0.9

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	45	61	101	112	0	319	0.45	1.46	0.28	0.39
2	42	60	103	102	0	307	0.45	1.58	0.29	0.39
3	44	61	106	102	0	313	0.46	1.43	0.29	0.38
4	44	53	106	126	0	329	0.46	1.54	0.29	0.39
5	45	62	105	108	0	320	0.45	1.52	0.29	0.37
6	50	56	117	109	0	332	0.42	1.3	0.27	0.36
7	47	66	107	100	0	320	0.45	1.44	0.27	0.39
8	38	68	115	104	0	325	0.44	1.49	0.28	0.37
9	43	57	110	104	0	314	0.44	1.52	0.29	0.38
10	44	58	105	101	0	308	0.43	1.38	0.28	0.38

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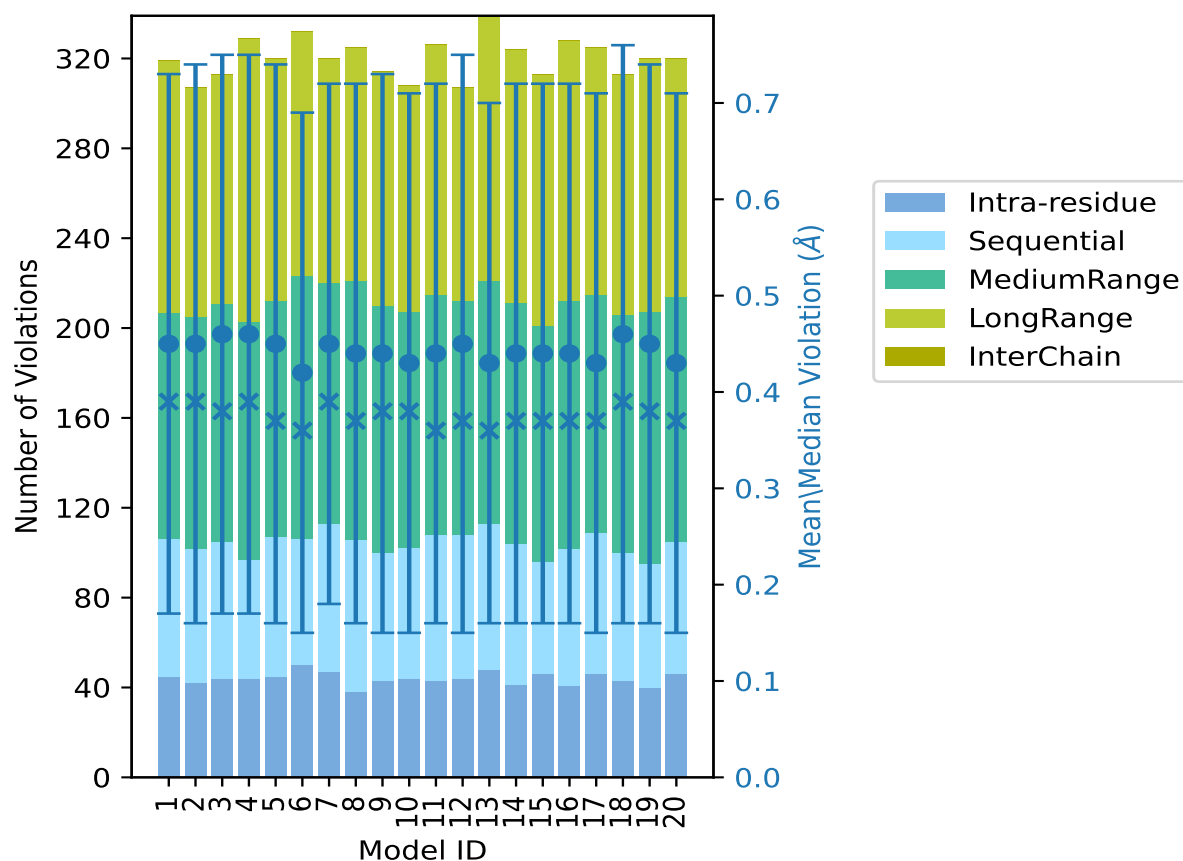
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	43	65	107	111	0	326	0.44	1.53	0.28	0.36
12	44	64	104	95	0	307	0.45	1.61	0.3	0.37
13	48	65	108	118	0	339	0.43	1.3	0.27	0.36
14	41	63	107	113	0	324	0.44	1.5	0.28	0.37
15	46	50	105	112	0	313	0.44	1.46	0.28	0.37
16	41	61	110	116	0	328	0.44	1.43	0.28	0.37
17	46	63	106	110	0	325	0.43	1.42	0.28	0.37
18	43	57	106	107	0	313	0.46	1.51	0.3	0.39
19	40	55	112	113	0	320	0.45	1.62	0.29	0.38
20	46	59	109	106	0	320	0.43	1.5	0.28	0.37

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 ⓘ



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

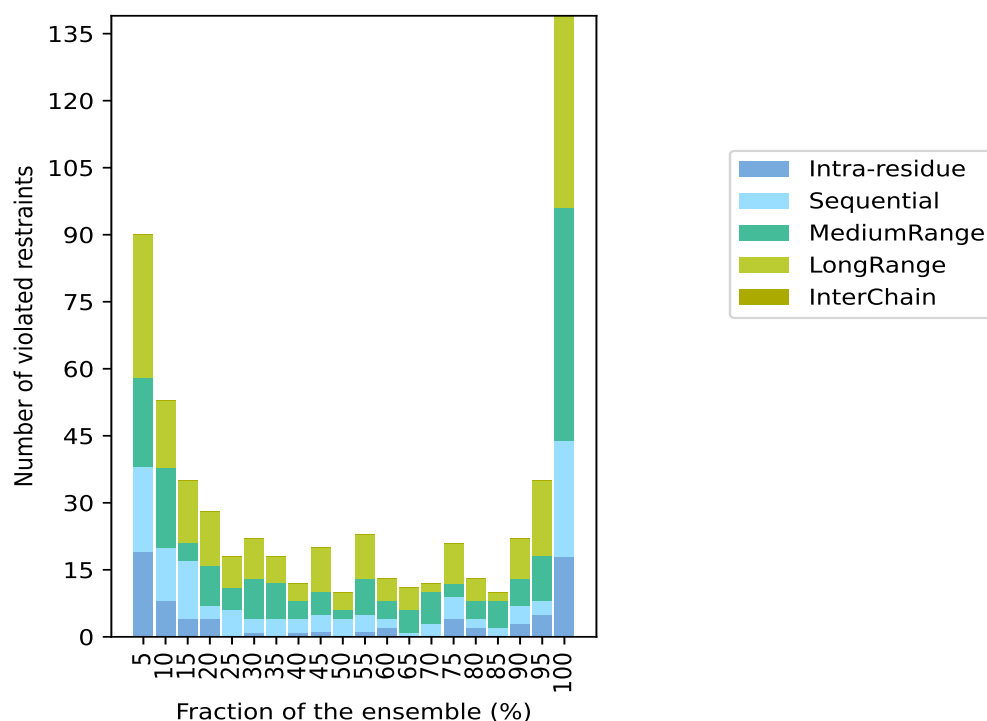
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3197(IR:1143, SQ:854, MR:614, LR:586, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
19	19	20	32	0	90	1	5.0
8	12	18	15	0	53	2	10.0
4	13	4	14	0	35	3	15.0
4	3	9	12	0	28	4	20.0
0	6	5	7	0	18	5	25.0
1	3	9	9	0	22	6	30.0
0	4	8	6	0	18	7	35.0
1	3	4	4	0	12	8	40.0
1	4	5	10	0	20	9	45.0
0	4	2	4	0	10	10	50.0
1	4	8	10	0	23	11	55.0
2	2	4	5	0	13	12	60.0
0	1	5	5	0	11	13	65.0
0	3	7	2	0	12	14	70.0
4	5	3	9	0	21	15	75.0
2	2	4	5	0	13	16	80.0
0	2	6	2	0	10	17	85.0
3	4	6	9	0	22	18	90.0
5	3	10	17	0	35	19	95.0
18	26	52	43	0	139	20	100.0

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

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

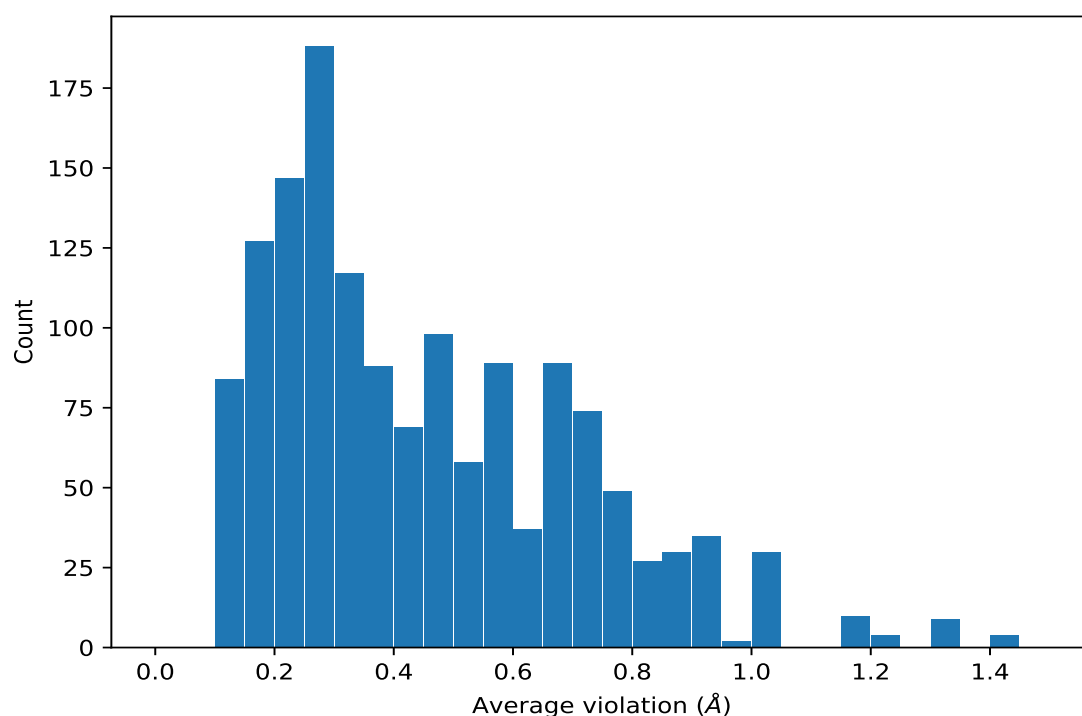
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD23	20	1.41	0.08	1.42
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD22	20	1.41	0.08	1.42
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD21	20	1.41	0.08	1.42
(1,3641)	1:73:A:ALA:H	1:74:A:LEU:HD23	20	1.41	0.08	1.42
(1,721)	1:44:A:LEU:HD21	1:47:A:TYR:H	20	1.32	0.08	1.32
(1,721)	1:45:A:LEU:HD23	1:47:A:TYR:H	20	1.32	0.08	1.32
(1,721)	1:45:A:LEU:HD21	1:47:A:TYR:H	20	1.32	0.08	1.32
(1,721)	1:45:A:LEU:HD22	1:47:A:TYR:H	20	1.32	0.08	1.32
(1,721)	1:48:A:LEU:HD11	1:47:A:TYR:H	20	1.32	0.08	1.32
(1,337)	1:110:A:ALA:HB3	1:102:A:ALA:H	20	1.32	0.12	1.33
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	20	1.32	0.12	1.33
(1,337)	1:103:A:ALA:HB3	1:102:A:ALA:H	20	1.32	0.12	1.33
(1,337)	1:103:A:ALA:HB1	1:102:A:ALA:H	20	1.32	0.12	1.33
(1,1295)	1:40:A:VAL:HG11	1:43:A:ARG:H	20	1.2	0.06	1.21
(1,1295)	1:80:A:ALA:HB3	1:43:A:ARG:H	20	1.2	0.06	1.21
(1,1295)	1:80:A:ALA:HB2	1:43:A:ARG:H	20	1.2	0.06	1.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1295)	1:40:A:VAL:HG13	1:43:A:ARG:H	20	1.2	0.06	1.21
(1,1295)	1:40:A:VAL:HG12	1:43:A:ARG:H	20	1.2	0.06	1.21
(1,1295)	1:80:A:ALA:HB1	1:43:A:ARG:H	20	1.2	0.06	1.21
(1,2898)	1:77:A:PHE:HE2	1:81:A:LEU:HD23	20	1.19	0.03	1.2
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD21	20	1.19	0.03	1.2
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD22	20	1.19	0.03	1.2
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD23	20	1.19	0.03	1.2
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD23	20	1.02	0.07	1.04
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD21	20	1.02	0.07	1.04
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD22	20	1.02	0.07	1.04
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD11	20	1.01	0.14	1.07
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD12	20	1.01	0.14	1.07
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD13	20	1.01	0.14	1.07
(1,3238)	1:89:A:LEU:HD23	1:90:A:MET:HE3	20	1.01	0.19	1.04
(1,3238)	1:89:A:LEU:HD23	1:90:A:MET:HE2	20	1.01	0.19	1.04
(1,3238)	1:89:A:LEU:HD21	1:90:A:MET:HE3	20	1.01	0.19	1.04
(1,3238)	1:40:A:VAL:HG23	1:90:A:MET:HE2	20	1.01	0.19	1.04
(1,3238)	1:40:A:VAL:HG22	1:90:A:MET:HE2	20	1.01	0.19	1.04
(1,3238)	1:40:A:VAL:HG21	1:90:A:MET:HE2	20	1.01	0.19	1.04
(1,3238)	1:40:A:VAL:HG22	1:90:A:MET:HE1	20	1.01	0.19	1.04
(1,3238)	1:89:A:LEU:HD22	1:90:A:MET:HE1	20	1.01	0.19	1.04
(1,3238)	1:40:A:VAL:HG21	1:90:A:MET:HE3	20	1.01	0.19	1.04
(1,3238)	1:89:A:LEU:HD22	1:90:A:MET:HE3	20	1.01	0.19	1.04
(1,3238)	1:40:A:VAL:HG23	1:90:A:MET:HE1	20	1.01	0.19	1.04
(1,3238)	1:89:A:LEU:HD21	1:90:A:MET:HE1	20	1.01	0.19	1.04
(1,3238)	1:40:A:VAL:HG22	1:90:A:MET:HE3	20	1.01	0.19	1.04
(1,1213)	1:34:A:ILE:HG21	1:41:A:GLN:H	20	1.01	0.2	1.08
(1,1213)	1:34:A:ILE:HG22	1:41:A:GLN:H	20	1.01	0.2	1.08
(1,1213)	1:34:A:ILE:HG23	1:41:A:GLN:H	20	1.01	0.2	1.08
(1,1213)	1:35:A:LEU:HD11	1:41:A:GLN:H	20	1.01	0.2	1.08
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	20	0.97	0.28	1.12
(1,2693)	1:36:A:ALA:H	1:33:A:PRO:HG2	20	0.97	0.28	1.12
(1,3568)	1:99:A:ALA:HB3	1:102:A:ALA:HB1	20	0.95	0.17	0.96
(1,3568)	1:114:A:ALA:HB2	1:102:A:ALA:HB1	20	0.95	0.17	0.96
(1,3568)	1:114:A:ALA:HB2	1:102:A:ALA:HB2	20	0.95	0.17	0.96
(1,3568)	1:99:A:ALA:HB2	1:102:A:ALA:HB3	20	0.95	0.17	0.96
(1,3568)	1:74:A:LEU:HG	1:31:A:MET:HE3	20	0.95	0.17	0.96
(1,3568)	1:99:A:ALA:HB3	1:102:A:ALA:HB3	20	0.95	0.17	0.96
(1,3568)	1:114:A:ALA:HB3	1:102:A:ALA:HB2	20	0.95	0.17	0.96
(1,3568)	1:114:A:ALA:HB3	1:102:A:ALA:HB1	20	0.95	0.17	0.96
(1,3568)	1:114:A:ALA:HB3	1:102:A:ALA:HB3	20	0.95	0.17	0.96
(1,3568)	1:114:A:ALA:HB1	1:102:A:ALA:HB1	20	0.95	0.17	0.96

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3568)	1:99:A:ALA:HB1	1:102:A:ALA:HB3	20	0.95	0.17	0.96
(1,3568)	1:114:A:ALA:HB2	1:102:A:ALA:HB3	20	0.95	0.17	0.96
(1,3568)	1:74:A:LEU:HG	1:31:A:MET:HE1	20	0.95	0.17	0.96
(1,3568)	1:114:A:ALA:HB1	1:102:A:ALA:HB2	20	0.95	0.17	0.96
(1,2915)	1:54:A:LEU:HA	1:54:A:LEU:HD13	20	0.9	0.12	0.94
(1,2915)	1:54:A:LEU:HA	1:54:A:LEU:HD11	20	0.9	0.12	0.94
(1,2915)	1:54:A:LEU:HA	1:54:A:LEU:HD12	20	0.9	0.12	0.94
(1,2915)	1:21:A:ASP:HA	1:22:A:LEU:HD12	20	0.9	0.12	0.94
(1,2915)	1:21:A:ASP:HA	1:22:A:LEU:HD13	20	0.9	0.12	0.94
(1,2915)	1:21:A:ASP:HA	1:22:A:LEU:HD11	20	0.9	0.12	0.94
(1,1135)	1:74:A:LEU:HD13	1:79:A:ALA:H	20	0.89	0.13	0.92
(1,1135)	1:44:A:LEU:HD12	1:79:A:ALA:H	20	0.89	0.13	0.92
(1,1135)	1:44:A:LEU:HD11	1:79:A:ALA:H	20	0.89	0.13	0.92
(1,1135)	1:44:A:LEU:HD13	1:79:A:ALA:H	20	0.89	0.13	0.92
(1,1135)	1:74:A:LEU:HD12	1:79:A:ALA:H	20	0.89	0.13	0.92
(1,3627)	1:33:A:PRO:HG2	1:93:A:PHE:HB2	20	0.89	0.21	0.88
(1,3627)	1:41:A:GLN:HB2	1:39:A:ASP:HB2	20	0.89	0.21	0.88
(1,3627)	1:90:A:MET:HE1	1:93:A:PHE:HB2	20	0.89	0.21	0.88
(1,3627)	1:90:A:MET:HE2	1:93:A:PHE:HB2	20	0.89	0.21	0.88
(1,505)	1:25:A:VAL:HG21	1:117:A:ASN:H	20	0.88	0.24	0.88
(1,505)	1:25:A:VAL:HG22	1:117:A:ASN:H	20	0.88	0.24	0.88
(1,505)	1:30:A:ILE:HD13	1:117:A:ASN:H	20	0.88	0.24	0.88
(1,505)	1:25:A:VAL:HG23	1:117:A:ASN:H	20	0.88	0.24	0.88
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD23	20	0.87	0.03	0.88
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD21	20	0.87	0.03	0.88
(1,3027)	1:103:A:ALA:HB3	1:81:A:LEU:HD22	20	0.87	0.03	0.88
(1,3027)	1:103:A:ALA:HB1	1:81:A:LEU:HD22	20	0.87	0.03	0.88
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD22	20	0.87	0.03	0.88
(1,3027)	1:103:A:ALA:HB2	1:81:A:LEU:HD23	20	0.87	0.03	0.88
(1,1014)	1:86:A:LEU:HD13	1:40:A:VAL:H	20	0.86	0.08	0.87
(1,1014)	1:86:A:LEU:HD12	1:40:A:VAL:H	20	0.86	0.08	0.87
(1,1014)	1:86:A:LEU:HD11	1:40:A:VAL:H	20	0.86	0.08	0.87
(1,1734)	1:44:A:LEU:HD11	1:76:A:MET:HA	20	0.84	0.15	0.86
(1,1734)	1:44:A:LEU:HD13	1:76:A:MET:HA	20	0.84	0.15	0.86
(1,1734)	1:44:A:LEU:HD12	1:76:A:MET:HA	20	0.84	0.15	0.86
(1,1170)	1:74:A:LEU:HG	1:23:A:ALA:H	20	0.82	0.13	0.8
(1,1170)	1:114:A:ALA:HB2	1:112:A:ALA:H	20	0.82	0.13	0.8
(1,1170)	1:114:A:ALA:HB1	1:112:A:ALA:H	20	0.82	0.13	0.8
(1,1170)	1:114:A:ALA:HB3	1:112:A:ALA:H	20	0.82	0.13	0.8
(1,1027)	1:100:A:VAL:HG23	1:92:A:GLN:H	20	0.82	0.13	0.86
(1,1027)	1:100:A:VAL:HG22	1:92:A:GLN:H	20	0.82	0.13	0.86
(1,1027)	1:100:A:VAL:HG21	1:92:A:GLN:H	20	0.82	0.13	0.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG22	20	0.82	0.21	0.82
(1,3080)	1:116:A:GLN:HA	1:25:A:VAL:HG21	20	0.82	0.21	0.82
(1,3080)	1:116:A:GLN:HA	1:25:A:VAL:HG22	20	0.82	0.21	0.82
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG21	20	0.82	0.21	0.82
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG23	20	0.82	0.21	0.82
(1,3080)	1:116:A:GLN:HA	1:25:A:VAL:HG23	20	0.82	0.21	0.82
(1,932)	1:103:A:ALA:HB1	1:106:A:GLY:H	20	0.82	0.09	0.8
(1,932)	1:103:A:ALA:HB3	1:106:A:GLY:H	20	0.82	0.09	0.8
(1,932)	1:103:A:ALA:HB2	1:106:A:GLY:H	20	0.82	0.09	0.8
(1,232)	1:73:A:ALA:HB2	1:76:A:MET:H	20	0.82	0.08	0.84
(1,232)	1:74:A:LEU:HB3	1:76:A:MET:H	20	0.82	0.08	0.84
(1,232)	1:73:A:ALA:HB3	1:76:A:MET:H	20	0.82	0.08	0.84
(1,232)	1:73:A:ALA:HB1	1:76:A:MET:H	20	0.82	0.08	0.84
(1,179)	1:38:A:ALA:HB1	1:40:A:VAL:H	20	0.79	0.06	0.81
(1,179)	1:38:A:ALA:HB3	1:40:A:VAL:H	20	0.79	0.06	0.81
(1,179)	1:38:A:ALA:HB2	1:40:A:VAL:H	20	0.79	0.06	0.81
(1,1345)	1:35:A:LEU:HD12	1:31:A:MET:H	20	0.78	0.13	0.74
(1,1345)	1:35:A:LEU:HD11	1:31:A:MET:H	20	0.78	0.13	0.74
(1,1345)	1:35:A:LEU:HD13	1:31:A:MET:H	20	0.78	0.13	0.74
(1,1345)	1:35:A:LEU:HD21	1:31:A:MET:H	20	0.78	0.13	0.74
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB1	20	0.78	0.09	0.79
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB3	20	0.78	0.09	0.79
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB2	20	0.78	0.09	0.79
(1,885)	1:80:A:ALA:HB2	1:83:A:SER:H	20	0.77	0.08	0.76
(1,885)	1:80:A:ALA:HB3	1:83:A:SER:H	20	0.77	0.08	0.76
(1,885)	1:80:A:ALA:HB1	1:83:A:SER:H	20	0.77	0.08	0.76
(1,3733)	1:90:A:MET:HE1	1:93:A:PHE:HZ	20	0.77	0.2	0.84
(1,3733)	1:90:A:MET:HE3	1:93:A:PHE:HZ	20	0.77	0.2	0.84
(1,3733)	1:90:A:MET:HE2	1:93:A:PHE:HZ	20	0.77	0.2	0.84
(1,3734)	1:90:A:MET:HE1	1:93:A:PHE:HZ	20	0.77	0.2	0.84
(1,3734)	1:90:A:MET:HE3	1:93:A:PHE:HZ	20	0.77	0.2	0.84
(1,3734)	1:90:A:MET:HE2	1:93:A:PHE:HZ	20	0.77	0.2	0.84
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE1	20	0.76	0.19	0.83
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE3	20	0.76	0.19	0.83
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE2	20	0.76	0.19	0.83
(1,3142)	1:111:A:PHE:HD1	1:90:A:MET:HE2	20	0.76	0.19	0.83
(1,3142)	1:93:A:PHE:HD2	1:90:A:MET:HE2	20	0.76	0.19	0.83
(1,2699)	1:93:A:PHE:HD2	1:34:A:ILE:HG13	20	0.74	0.24	0.73
(1,2699)	1:93:A:PHE:HD1	1:34:A:ILE:HG13	20	0.74	0.24	0.73
(1,1095)	1:23:A:ALA:HB2	1:22:A:LEU:H	20	0.73	0.11	0.76
(1,1095)	1:23:A:ALA:HB3	1:22:A:LEU:H	20	0.73	0.11	0.76
(1,1095)	1:23:A:ALA:HB1	1:22:A:LEU:H	20	0.73	0.11	0.76

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,82)	1:61:A:ILE:HD13	1:32:A:ALA:H	20	0.73	0.12	0.72
(1,82)	1:61:A:ILE:HD12	1:32:A:ALA:H	20	0.73	0.12	0.72
(1,82)	1:34:A:ILE:HD11	1:32:A:ALA:H	20	0.73	0.12	0.72
(1,82)	1:61:A:ILE:HD11	1:32:A:ALA:H	20	0.73	0.12	0.72
(1,82)	1:34:A:ILE:HD12	1:32:A:ALA:H	20	0.73	0.12	0.72
(1,82)	1:34:A:ILE:HD13	1:32:A:ALA:H	20	0.73	0.12	0.72
(1,3253)	1:32:A:ALA:H	1:61:A:ILE:HD13	20	0.73	0.12	0.72
(1,3253)	1:32:A:ALA:H	1:61:A:ILE:HD12	20	0.73	0.12	0.72
(1,3253)	1:32:A:ALA:H	1:34:A:ILE:HD11	20	0.73	0.12	0.72
(1,3253)	1:32:A:ALA:H	1:61:A:ILE:HD11	20	0.73	0.12	0.72
(1,3253)	1:32:A:ALA:H	1:34:A:ILE:HD12	20	0.73	0.12	0.72
(1,3253)	1:32:A:ALA:H	1:34:A:ILE:HD13	20	0.73	0.12	0.72
(1,307)	1:25:A:VAL:HG22	1:114:A:ALA:H	20	0.72	0.16	0.68
(1,307)	1:25:A:VAL:HG23	1:114:A:ALA:H	20	0.72	0.16	0.68
(1,307)	1:26:A:LEU:HD21	1:114:A:ALA:H	20	0.72	0.16	0.68
(1,307)	1:26:A:LEU:HD22	1:114:A:ALA:H	20	0.72	0.16	0.68
(1,307)	1:26:A:LEU:HD23	1:114:A:ALA:H	20	0.72	0.16	0.68
(1,307)	1:25:A:VAL:HG21	1:114:A:ALA:H	20	0.72	0.16	0.68
(1,3673)	1:114:A:ALA:H	1:111:A:PHE:HD2	20	0.72	0.11	0.74
(1,3673)	1:114:A:ALA:H	1:111:A:PHE:HD1	20	0.72	0.11	0.74
(1,3673)	1:107:A:ASP:H	1:111:A:PHE:HD1	20	0.72	0.11	0.74
(1,3561)	1:90:A:MET:HB3	1:34:A:ILE:HG22	20	0.72	0.22	0.65
(1,3561)	1:90:A:MET:HB3	1:34:A:ILE:HG21	20	0.72	0.22	0.65
(1,3561)	1:31:A:MET:HG3	1:34:A:ILE:HG21	20	0.72	0.22	0.65
(1,3561)	1:90:A:MET:HB3	1:34:A:ILE:HG23	20	0.72	0.22	0.65
(1,3561)	1:31:A:MET:HG3	1:34:A:ILE:HG23	20	0.72	0.22	0.65
(1,3561)	1:31:A:MET:HG2	1:34:A:ILE:HG21	20	0.72	0.22	0.65
(1,3561)	1:31:A:MET:HG2	1:34:A:ILE:HG23	20	0.72	0.22	0.65
(1,3561)	1:31:A:MET:HG3	1:34:A:ILE:HG22	20	0.72	0.22	0.65
(1,2872)	1:43:A:ARG:H	1:86:A:LEU:HD11	20	0.72	0.12	0.72
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD13	20	0.72	0.12	0.72
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD12	20	0.72	0.12	0.72
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD11	20	0.72	0.12	0.72
(1,365)	1:101:A:GLU:HG3	1:104:A:ASN:H	20	0.72	0.15	0.74
(1,365)	1:101:A:GLU:HG2	1:104:A:ASN:H	20	0.72	0.15	0.74
(1,365)	1:101:A:GLU:HG3	1:103:A:ALA:H	20	0.72	0.15	0.74
(1,376)	1:73:A:ALA:HB2	1:77:A:PHE:H	20	0.71	0.1	0.7
(1,376)	1:73:A:ALA:HB3	1:77:A:PHE:H	20	0.71	0.1	0.7
(1,376)	1:73:A:ALA:HB1	1:77:A:PHE:H	20	0.71	0.1	0.7
(1,3498)	1:102:A:ALA:HB1	1:81:A:LEU:HD11	20	0.71	0.16	0.72
(1,3498)	1:102:A:ALA:HB1	1:81:A:LEU:HD12	20	0.71	0.16	0.72
(1,3498)	1:102:A:ALA:HB2	1:81:A:LEU:HD13	20	0.71	0.16	0.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3498)	1:102:A:ALA:HB3	1:81:A:LEU:HD12	20	0.71	0.16	0.72
(1,3498)	1:31:A:MET:HE2	1:81:A:LEU:HD12	20	0.71	0.16	0.72
(1,3498)	1:31:A:MET:HE1	1:81:A:LEU:HD13	20	0.71	0.16	0.72
(1,3498)	1:102:A:ALA:HB2	1:81:A:LEU:HD12	20	0.71	0.16	0.72
(1,3498)	1:102:A:ALA:HB3	1:81:A:LEU:HD11	20	0.71	0.16	0.72
(1,3498)	1:31:A:MET:HE1	1:81:A:LEU:HD12	20	0.71	0.16	0.72
(1,3498)	1:31:A:MET:HE3	1:81:A:LEU:HD11	20	0.71	0.16	0.72
(1,3498)	1:31:A:MET:HE3	1:81:A:LEU:HD13	20	0.71	0.16	0.72
(1,3498)	1:31:A:MET:HE2	1:81:A:LEU:HD13	20	0.71	0.16	0.72
(1,3498)	1:102:A:ALA:HB1	1:81:A:LEU:HD13	20	0.71	0.16	0.72
(1,114)	1:81:A:LEU:HB2	1:79:A:ALA:H	20	0.7	0.08	0.71
(1,114)	1:82:A:ALA:HB1	1:79:A:ALA:H	20	0.7	0.08	0.71
(1,114)	1:82:A:ALA:HB2	1:79:A:ALA:H	20	0.7	0.08	0.71
(1,114)	1:82:A:ALA:HB3	1:79:A:ALA:H	20	0.7	0.08	0.71
(1,2513)	1:92:A:GLN:HE22	1:88:A:PRO:HB2	20	0.7	0.11	0.72
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	20	0.7	0.11	0.72
(1,338)	1:61:A:ILE:HG23	1:65:A:LEU:H	20	0.68	0.15	0.7
(1,338)	1:61:A:ILE:HG21	1:65:A:LEU:H	20	0.68	0.15	0.7
(1,338)	1:65:A:LEU:HD11	1:65:A:LEU:H	20	0.68	0.15	0.7
(1,338)	1:65:A:LEU:HD13	1:65:A:LEU:H	20	0.68	0.15	0.7
(1,338)	1:65:A:LEU:HD12	1:65:A:LEU:H	20	0.68	0.15	0.7
(1,338)	1:61:A:ILE:HG22	1:65:A:LEU:H	20	0.68	0.15	0.7
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	20	0.68	0.15	0.72
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG11	20	0.67	0.11	0.72
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG13	20	0.67	0.11	0.72
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG12	20	0.67	0.11	0.72
(1,3059)	1:111:A:PHE:HD2	1:108:A:VAL:HG12	20	0.67	0.11	0.72
(1,3059)	1:111:A:PHE:HD2	1:108:A:VAL:HG11	20	0.67	0.11	0.72
(1,3239)	1:34:A:ILE:HD12	1:90:A:MET:HE1	20	0.67	0.19	0.72
(1,3239)	1:86:A:LEU:HD13	1:90:A:MET:HE2	20	0.67	0.19	0.72
(1,3239)	1:86:A:LEU:HD12	1:90:A:MET:HE1	20	0.67	0.19	0.72
(1,3239)	1:34:A:ILE:HD13	1:90:A:MET:HE2	20	0.67	0.19	0.72
(1,3239)	1:86:A:LEU:HD12	1:90:A:MET:HE2	20	0.67	0.19	0.72
(1,3239)	1:86:A:LEU:HD13	1:90:A:MET:HE1	20	0.67	0.19	0.72
(1,3239)	1:86:A:LEU:HD13	1:90:A:MET:HE3	20	0.67	0.19	0.72
(1,3239)	1:34:A:ILE:HD12	1:90:A:MET:HE2	20	0.67	0.19	0.72
(1,3239)	1:86:A:LEU:HD12	1:90:A:MET:HE3	20	0.67	0.19	0.72
(1,3239)	1:86:A:LEU:HD11	1:90:A:MET:HE3	20	0.67	0.19	0.72
(1,3239)	1:34:A:ILE:HD11	1:90:A:MET:HE2	20	0.67	0.19	0.72
(1,3239)	1:34:A:ILE:HD11	1:90:A:MET:HE1	20	0.67	0.19	0.72
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	20	0.67	0.18	0.66
(1,234)	1:44:A:LEU:HD22	1:76:A:MET:H	20	0.67	0.06	0.66

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,234)	1:44:A:LEU:HD23	1:76:A:MET:H	20	0.67	0.06	0.66
(1,234)	1:44:A:LEU:HD21	1:76:A:MET:H	20	0.67	0.06	0.66
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD22	20	0.67	0.13	0.7
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD23	20	0.67	0.13	0.7
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD21	20	0.67	0.13	0.7
(1,2868)	1:43:A:ARG:H	1:86:A:LEU:HD21	20	0.67	0.13	0.7
(1,3441)	1:99:A:ALA:HB2	1:96:A:PRO:HB3	20	0.66	0.11	0.68
(1,3441)	1:114:A:ALA:HB1	1:96:A:PRO:HB3	20	0.66	0.11	0.68
(1,3441)	1:99:A:ALA:HB1	1:96:A:PRO:HB3	20	0.66	0.11	0.68
(1,3441)	1:99:A:ALA:HB3	1:96:A:PRO:HB3	20	0.66	0.11	0.68
(1,3441)	1:114:A:ALA:HB2	1:96:A:PRO:HB3	20	0.66	0.11	0.68
(1,3441)	1:114:A:ALA:HB3	1:96:A:PRO:HB3	20	0.66	0.11	0.68
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	20	0.66	0.07	0.64
(1,1719)	1:100:A:VAL:HG11	1:96:A:PRO:HA	20	0.66	0.11	0.68
(1,1719)	1:100:A:VAL:HG13	1:96:A:PRO:HA	20	0.66	0.11	0.68
(1,1719)	1:100:A:VAL:HG12	1:96:A:PRO:HA	20	0.66	0.11	0.68
(1,2075)	1:61:A:ILE:HG21	1:33:A:PRO:HD2	20	0.65	0.16	0.66
(1,2075)	1:61:A:ILE:HG23	1:33:A:PRO:HD2	20	0.65	0.16	0.66
(1,2075)	1:61:A:ILE:HG22	1:33:A:PRO:HD2	20	0.65	0.16	0.66
(1,3015)	1:97:A:ALA:HB3	1:100:A:VAL:HG11	20	0.65	0.08	0.66
(1,3015)	1:97:A:ALA:HB1	1:100:A:VAL:HG13	20	0.65	0.08	0.66
(1,3015)	1:97:A:ALA:HB1	1:100:A:VAL:HG12	20	0.65	0.08	0.66
(1,3015)	1:97:A:ALA:HB1	1:100:A:VAL:HG11	20	0.65	0.08	0.66
(1,3015)	1:97:A:ALA:HB2	1:100:A:VAL:HG13	20	0.65	0.08	0.66
(1,3015)	1:97:A:ALA:HB2	1:100:A:VAL:HG12	20	0.65	0.08	0.66
(1,3015)	1:97:A:ALA:HB3	1:100:A:VAL:HG12	20	0.65	0.08	0.66
(1,3015)	1:97:A:ALA:HB2	1:100:A:VAL:HG11	20	0.65	0.08	0.66
(1,578)	1:23:A:ALA:HB1	1:25:A:VAL:H	20	0.65	0.08	0.66
(1,578)	1:112:A:ALA:HB1	1:25:A:VAL:H	20	0.65	0.08	0.66
(1,578)	1:23:A:ALA:HB2	1:25:A:VAL:H	20	0.65	0.08	0.66
(1,578)	1:23:A:ALA:HB3	1:25:A:VAL:H	20	0.65	0.08	0.66
(1,578)	1:112:A:ALA:HB2	1:25:A:VAL:H	20	0.65	0.08	0.66
(1,906)	1:36:A:ALA:HB1	1:41:A:GLN:HE22	20	0.65	0.18	0.71
(1,906)	1:58:A:ALA:HB3	1:62:A:GLN:HE22	20	0.65	0.18	0.71
(1,906)	1:58:A:ALA:HB1	1:62:A:GLN:HE22	20	0.65	0.18	0.71
(1,906)	1:36:A:ALA:HB2	1:41:A:GLN:HE22	20	0.65	0.18	0.71
(1,906)	1:36:A:ALA:HB3	1:41:A:GLN:HE22	20	0.65	0.18	0.71
(1,906)	1:58:A:ALA:HB2	1:62:A:GLN:HE22	20	0.65	0.18	0.71
(1,2293)	1:34:A:ILE:HB	1:37:A:ASN:HB3	20	0.63	0.12	0.64
(1,2293)	1:38:A:ALA:HB3	1:37:A:ASN:HB3	20	0.63	0.12	0.64
(1,2293)	1:38:A:ALA:HB1	1:37:A:ASN:HB3	20	0.63	0.12	0.64
(1,2293)	1:38:A:ALA:HB2	1:37:A:ASN:HB3	20	0.63	0.12	0.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3380)	1:40:A:VAL:HG11	1:43:A:ARG:HD3	20	0.63	0.25	0.58
(1,3380)	1:40:A:VAL:HG12	1:43:A:ARG:HD3	20	0.63	0.25	0.58
(1,3380)	1:80:A:ALA:HB2	1:43:A:ARG:HD2	20	0.63	0.25	0.58
(1,3380)	1:80:A:ALA:HB1	1:43:A:ARG:HD2	20	0.63	0.25	0.58
(1,3380)	1:40:A:VAL:HG13	1:43:A:ARG:HD3	20	0.63	0.25	0.58
(1,3377)	1:45:A:LEU:HD23	1:46:A:PRO:HD2	20	0.62	0.07	0.66
(1,3377)	1:45:A:LEU:HD21	1:46:A:PRO:HD2	20	0.62	0.07	0.66
(1,3377)	1:45:A:LEU:HD22	1:46:A:PRO:HD2	20	0.62	0.07	0.66
(1,1975)	1:27:A:THR:HG21	1:26:A:LEU:HA	20	0.62	0.11	0.62
(1,1975)	1:27:A:THR:HG23	1:26:A:LEU:HA	20	0.62	0.11	0.62
(1,1975)	1:27:A:THR:HG22	1:26:A:LEU:HA	20	0.62	0.11	0.62
(1,375)	1:99:A:ALA:HB3	1:103:A:ALA:H	20	0.62	0.09	0.62
(1,375)	1:99:A:ALA:HB2	1:103:A:ALA:H	20	0.62	0.09	0.62
(1,375)	1:99:A:ALA:HB1	1:103:A:ALA:H	20	0.62	0.09	0.62
(1,849)	1:36:A:ALA:HB1	1:41:A:GLN:HE21	20	0.61	0.14	0.61
(1,849)	1:36:A:ALA:HB3	1:41:A:GLN:HE21	20	0.61	0.14	0.61
(1,849)	1:36:A:ALA:HB2	1:41:A:GLN:HE21	20	0.61	0.14	0.61
(1,849)	1:35:A:LEU:HB2	1:41:A:GLN:HE21	20	0.61	0.14	0.61
(1,305)	1:25:A:VAL:HG21	1:116:A:GLN:H	20	0.6	0.22	0.7
(1,305)	1:25:A:VAL:HG22	1:116:A:GLN:H	20	0.6	0.22	0.7
(1,305)	1:26:A:LEU:HD21	1:116:A:GLN:H	20	0.6	0.22	0.7
(1,305)	1:26:A:LEU:HD22	1:116:A:GLN:H	20	0.6	0.22	0.7
(1,305)	1:25:A:VAL:HG23	1:116:A:GLN:H	20	0.6	0.22	0.7
(1,305)	1:26:A:LEU:HD23	1:116:A:GLN:H	20	0.6	0.22	0.7
(1,1344)	1:30:A:ILE:HD12	1:31:A:MET:H	20	0.6	0.09	0.62
(1,1344)	1:30:A:ILE:HD11	1:31:A:MET:H	20	0.6	0.09	0.62
(1,1344)	1:26:A:LEU:HD21	1:31:A:MET:H	20	0.6	0.09	0.62
(1,1344)	1:30:A:ILE:HD13	1:31:A:MET:H	20	0.6	0.09	0.62
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB3	20	0.59	0.1	0.61
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB2	20	0.59	0.1	0.61
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB1	20	0.59	0.1	0.61
(1,3126)	1:111:A:PHE:H	1:114:A:ALA:HB3	20	0.59	0.1	0.61
(1,3126)	1:111:A:PHE:H	1:114:A:ALA:HB1	20	0.59	0.1	0.61
(1,3551)	1:56:A:GLN:HA	1:36:A:ALA:HB1	20	0.59	0.23	0.64
(1,3551)	1:56:A:GLN:HA	1:36:A:ALA:HB3	20	0.59	0.23	0.64
(1,3551)	1:57:A:THR:HB	1:36:A:ALA:HB1	20	0.59	0.23	0.64
(1,3551)	1:56:A:GLN:HA	1:36:A:ALA:HB2	20	0.59	0.23	0.64
(1,3551)	1:57:A:THR:HB	1:36:A:ALA:HB2	20	0.59	0.23	0.64
(1,3551)	1:57:A:THR:HB	1:36:A:ALA:HB3	20	0.59	0.23	0.64
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD12	20	0.58	0.12	0.6
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD11	20	0.58	0.12	0.6
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD13	20	0.58	0.12	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3054)	1:77:A:PHE:H	1:35:A:LEU:HD12	20	0.58	0.12	0.6
(1,1018)	1:77:A:PHE:HD2	1:81:A:LEU:H	20	0.57	0.11	0.56
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	20	0.57	0.11	0.56
(1,2296)	1:102:A:ALA:HB3	1:111:A:PHE:HB3	20	0.57	0.05	0.58
(1,2296)	1:102:A:ALA:HB1	1:111:A:PHE:HB3	20	0.57	0.05	0.58
(1,2296)	1:102:A:ALA:HB2	1:111:A:PHE:HB3	20	0.57	0.05	0.58
(1,2618)	1:36:A:ALA:HB2	1:33:A:PRO:HB2	20	0.57	0.09	0.57
(1,2618)	1:36:A:ALA:HB1	1:33:A:PRO:HB2	20	0.57	0.09	0.57
(1,2618)	1:36:A:ALA:HB3	1:33:A:PRO:HB2	20	0.57	0.09	0.57
(1,1193)	1:108:A:VAL:HG12	1:107:A:ASP:H	20	0.56	0.1	0.57
(1,1193)	1:108:A:VAL:HG11	1:107:A:ASP:H	20	0.56	0.1	0.57
(1,1193)	1:108:A:VAL:HG13	1:107:A:ASP:H	20	0.56	0.1	0.57
(1,921)	1:72:A:GLN:HB3	1:75:A:GLY:H	20	0.56	0.08	0.56
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	20	0.56	0.08	0.56
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	20	0.56	0.17	0.54
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD13	20	0.56	0.08	0.55
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD12	20	0.56	0.08	0.55
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD11	20	0.56	0.08	0.55
(1,36)	1:109:A:GLU:HA	1:108:A:VAL:H	20	0.55	0.06	0.56
(1,36)	1:106:A:GLY:HA2	1:108:A:VAL:H	20	0.55	0.06	0.56
(1,2801)	1:81:A:LEU:H	1:86:A:LEU:HD11	20	0.55	0.14	0.54
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD12	20	0.55	0.14	0.54
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD11	20	0.55	0.14	0.54
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD13	20	0.55	0.14	0.54
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB1	20	0.54	0.14	0.5
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB2	20	0.54	0.14	0.5
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB3	20	0.54	0.14	0.5
(1,3194)	1:44:A:LEU:HA	1:79:A:ALA:HB1	20	0.54	0.14	0.5
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD11	20	0.52	0.19	0.6
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD12	20	0.52	0.19	0.6
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD13	20	0.52	0.19	0.6
(1,1232)	1:57:A:THR:HG23	1:59:A:ASP:H	20	0.52	0.16	0.55
(1,1232)	1:57:A:THR:HG22	1:59:A:ASP:H	20	0.52	0.16	0.55
(1,1232)	1:57:A:THR:HG21	1:59:A:ASP:H	20	0.52	0.16	0.55
(1,2617)	1:95:A:LEU:HD21	1:90:A:MET:HB2	20	0.51	0.13	0.5
(1,2617)	1:95:A:LEU:HD22	1:90:A:MET:HB2	20	0.51	0.13	0.5
(1,2617)	1:95:A:LEU:HD23	1:90:A:MET:HB2	20	0.51	0.13	0.5
(1,2617)	1:99:A:ALA:HB3	1:100:A:VAL:HB	20	0.51	0.13	0.5
(1,2832)	1:103:A:ALA:H	1:81:A:LEU:HD11	20	0.51	0.1	0.51
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD12	20	0.51	0.1	0.51
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD13	20	0.51	0.1	0.51
(1,2832)	1:108:A:VAL:H	1:81:A:LEU:HD13	20	0.51	0.1	0.51

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2832)	1:108:A:VAL:H	1:81:A:LEU:HD12	20	0.51	0.1	0.51
(1,2832)	1:103:A:ALA:H	1:81:A:LEU:HD12	20	0.51	0.1	0.51
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD11	20	0.51	0.1	0.51
(1,2832)	1:103:A:ALA:H	1:81:A:LEU:HD13	20	0.51	0.1	0.51
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	20	0.5	0.11	0.5
(1,651)	1:34:A:ILE:HD13	1:34:A:ILE:H	20	0.49	0.03	0.49
(1,651)	1:34:A:ILE:HD11	1:34:A:ILE:H	20	0.49	0.03	0.49
(1,651)	1:34:A:ILE:HD12	1:34:A:ILE:H	20	0.49	0.03	0.49
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD13	20	0.49	0.03	0.49
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD11	20	0.49	0.03	0.49
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD12	20	0.49	0.03	0.49
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD12	20	0.49	0.2	0.49
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD11	20	0.49	0.2	0.49
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD13	20	0.49	0.2	0.49
(1,2859)	1:70:A:PHE:HE2	1:74:A:LEU:HD13	20	0.49	0.2	0.49
(1,231)	1:97:A:ALA:HB1	1:99:A:ALA:H	20	0.48	0.08	0.46
(1,231)	1:97:A:ALA:HB2	1:99:A:ALA:H	20	0.48	0.08	0.46
(1,231)	1:97:A:ALA:HB3	1:99:A:ALA:H	20	0.48	0.08	0.46
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	20	0.48	0.1	0.48
(1,1165)	1:70:A:PHE:HD2	1:23:A:ALA:H	20	0.48	0.1	0.48
(1,563)	1:40:A:VAL:HG23	1:42:A:GLU:H	20	0.48	0.1	0.49
(1,563)	1:54:A:LEU:HD12	1:42:A:GLU:H	20	0.48	0.1	0.49
(1,563)	1:40:A:VAL:HG22	1:42:A:GLU:H	20	0.48	0.1	0.49
(1,563)	1:40:A:VAL:HG21	1:42:A:GLU:H	20	0.48	0.1	0.49
(1,563)	1:54:A:LEU:HD11	1:42:A:GLU:H	20	0.48	0.1	0.49
(1,563)	1:54:A:LEU:HD13	1:42:A:GLU:H	20	0.48	0.1	0.49
(1,1275)	1:92:A:GLN:HB2	1:91:A:CYS:H	20	0.47	0.2	0.58
(1,1275)	1:88:A:PRO:HB2	1:91:A:CYS:H	20	0.47	0.2	0.58
(1,1275)	1:89:A:LEU:HB3	1:91:A:CYS:H	20	0.47	0.2	0.58
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB3	20	0.47	0.07	0.48
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB1	20	0.47	0.07	0.48
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB2	20	0.47	0.07	0.48
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	20	0.47	0.16	0.46
(1,1138)	1:87:A:GLY:HA2	1:81:A:LEU:H	20	0.47	0.16	0.46
(1,115)	1:80:A:ALA:HB3	1:79:A:ALA:H	20	0.47	0.07	0.46
(1,115)	1:80:A:ALA:HB1	1:79:A:ALA:H	20	0.47	0.07	0.46
(1,115)	1:108:A:VAL:HG11	1:79:A:ALA:H	20	0.47	0.07	0.46
(1,115)	1:80:A:ALA:HB2	1:79:A:ALA:H	20	0.47	0.07	0.46
(1,922)	1:82:A:ALA:HB3	1:84:A:GLY:H	20	0.46	0.08	0.44
(1,922)	1:82:A:ALA:HB1	1:84:A:GLY:H	20	0.46	0.08	0.44
(1,922)	1:82:A:ALA:HB2	1:84:A:GLY:H	20	0.46	0.08	0.44
(1,922)	1:86:A:LEU:HB2	1:84:A:GLY:H	20	0.46	0.08	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1042)	1:30:A:ILE:HD12	1:29:A:GLU:H	20	0.46	0.09	0.44
(1,1042)	1:30:A:ILE:HD11	1:29:A:GLU:H	20	0.46	0.09	0.44
(1,1042)	1:61:A:ILE:HG22	1:29:A:GLU:H	20	0.46	0.09	0.44
(1,1042)	1:30:A:ILE:HD13	1:29:A:GLU:H	20	0.46	0.09	0.44
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	20	0.45	0.17	0.42
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	20	0.45	0.12	0.44
(1,1225)	1:72:A:GLN:HG2	1:74:A:LEU:H	20	0.45	0.12	0.44
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	20	0.44	0.1	0.44
(1,1183)	1:99:A:ALA:HB1	1:101:A:GLU:H	20	0.44	0.04	0.42
(1,1183)	1:99:A:ALA:HB3	1:101:A:GLU:H	20	0.44	0.04	0.42
(1,1183)	1:99:A:ALA:HB2	1:101:A:GLU:H	20	0.44	0.04	0.42
(1,522)	1:114:A:ALA:HB3	1:113:A:LYS:H	20	0.43	0.12	0.41
(1,522)	1:114:A:ALA:HB2	1:113:A:LYS:H	20	0.43	0.12	0.41
(1,522)	1:114:A:ALA:HB1	1:113:A:LYS:H	20	0.43	0.12	0.41
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD22	20	0.42	0.12	0.44
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD23	20	0.42	0.12	0.44
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD21	20	0.42	0.12	0.44
(1,1563)	1:112:A:ALA:HB1	1:108:A:VAL:HA	20	0.41	0.12	0.38
(1,1563)	1:112:A:ALA:HB3	1:108:A:VAL:HA	20	0.41	0.12	0.38
(1,1563)	1:112:A:ALA:HB2	1:108:A:VAL:HA	20	0.41	0.12	0.38
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	20	0.4	0.09	0.4
(1,518)	1:43:A:ARG:HB3	1:44:A:LEU:H	20	0.4	0.09	0.4
(1,1534)	1:88:A:PRO:HG3	1:88:A:PRO:HA	20	0.39	0.01	0.39
(1,1534)	1:88:A:PRO:HG2	1:88:A:PRO:HA	20	0.39	0.01	0.39
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG3	20	0.39	0.01	0.39
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG2	20	0.39	0.01	0.39
(1,517)	1:42:A:GLU:HB2	1:44:A:LEU:H	20	0.38	0.09	0.39
(1,517)	1:42:A:GLU:HB3	1:44:A:LEU:H	20	0.38	0.09	0.39
(1,452)	1:44:A:LEU:HD12	1:45:A:LEU:H	20	0.38	0.14	0.36
(1,452)	1:44:A:LEU:HD11	1:45:A:LEU:H	20	0.38	0.14	0.36
(1,452)	1:44:A:LEU:HD13	1:45:A:LEU:H	20	0.38	0.14	0.36
(1,1299)	1:40:A:VAL:HG22	1:34:A:ILE:H	20	0.37	0.1	0.38
(1,1299)	1:40:A:VAL:HG23	1:34:A:ILE:H	20	0.37	0.1	0.38
(1,1299)	1:61:A:ILE:HG21	1:34:A:ILE:H	20	0.37	0.1	0.38
(1,1299)	1:61:A:ILE:HG23	1:34:A:ILE:H	20	0.37	0.1	0.38
(1,1299)	1:40:A:VAL:HG21	1:34:A:ILE:H	20	0.37	0.1	0.38
(1,1299)	1:61:A:ILE:HG22	1:34:A:ILE:H	20	0.37	0.1	0.38
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD22	20	0.37	0.02	0.38
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD23	20	0.37	0.02	0.38
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD21	20	0.37	0.02	0.38
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	20	0.36	0.06	0.38
(1,1287)	1:33:A:PRO:HG2	1:36:A:ALA:H	20	0.36	0.07	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1287)	1:61:A:ILE:HB	1:36:A:ALA:H	20	0.36	0.07	0.36
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	20	0.35	0.09	0.34
(1,786)	1:30:A:ILE:HG21	1:31:A:MET:H	20	0.35	0.07	0.36
(1,786)	1:30:A:ILE:HG22	1:31:A:MET:H	20	0.35	0.07	0.36
(1,786)	1:30:A:ILE:HG23	1:31:A:MET:H	20	0.35	0.07	0.36
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB2	20	0.35	0.06	0.35
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB3	20	0.35	0.06	0.35
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB1	20	0.35	0.06	0.35
(1,3530)	1:41:A:GLN:HE21	1:36:A:ALA:HB1	20	0.35	0.06	0.35
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	20	0.34	0.08	0.36
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB3	20	0.34	0.05	0.32
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB1	20	0.34	0.05	0.32
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB2	20	0.34	0.05	0.32
(1,635)	1:40:A:VAL:HG22	1:36:A:ALA:H	20	0.34	0.11	0.34
(1,635)	1:40:A:VAL:HG23	1:36:A:ALA:H	20	0.34	0.11	0.34
(1,635)	1:40:A:VAL:HG21	1:36:A:ALA:H	20	0.34	0.11	0.34
(1,635)	1:61:A:ILE:HG21	1:36:A:ALA:H	20	0.34	0.11	0.34
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	20	0.32	0.02	0.32
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	20	0.32	0.02	0.32
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	20	0.32	0.1	0.3
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	20	0.32	0.08	0.32
(1,494)	1:72:A:GLN:HB3	1:74:A:LEU:H	20	0.32	0.08	0.32
(1,2923)	1:43:A:ARG:HA	1:86:A:LEU:HD11	20	0.31	0.08	0.3
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD11	20	0.31	0.08	0.3
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD13	20	0.31	0.08	0.3
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD12	20	0.31	0.08	0.3
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	20	0.3	0.04	0.3
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD23	20	0.3	0.03	0.3
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD22	20	0.3	0.03	0.3
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD21	20	0.3	0.03	0.3
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	20	0.25	0.09	0.24
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	20	0.24	0.04	0.22
(1,248)	1:108:A:VAL:HA	1:112:A:ALA:H	20	0.24	0.04	0.22
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	20	0.23	0.05	0.23
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG11	20	0.22	0.02	0.23
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG13	20	0.22	0.02	0.23
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG12	20	0.22	0.02	0.23
(1,723)	1:86:A:LEU:HD12	1:86:A:LEU:H	20	0.22	0.05	0.23
(1,723)	1:86:A:LEU:HD11	1:86:A:LEU:H	20	0.22	0.05	0.23
(1,723)	1:86:A:LEU:HD13	1:86:A:LEU:H	20	0.22	0.05	0.23
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD12	20	0.22	0.05	0.23
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD11	20	0.22	0.05	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD13	20	0.22	0.05	0.23
(1,161)	1:39:A:ASP:HB2	1:40:A:VAL:H	20	0.22	0.01	0.22
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	20	0.22	0.01	0.22
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	20	0.21	0.06	0.2
(1,1005)	1:70:A:PHE:HD2	1:70:A:PHE:H	20	0.21	0.04	0.21
(1,1005)	1:70:A:PHE:HD1	1:70:A:PHE:H	20	0.21	0.04	0.21
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD13	20	0.2	0.02	0.2
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD12	20	0.2	0.02	0.2
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD11	20	0.2	0.02	0.2
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	20	0.19	0.03	0.19
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	20	0.17	0.04	0.17
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD13	20	0.17	0.03	0.16
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD11	20	0.17	0.03	0.16
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD12	20	0.17	0.03	0.16
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	20	0.16	0.02	0.16
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	20	0.15	0.02	0.15
(1,1154)	1:108:A:VAL:HG22	1:20:A:VAL:H	19	1.21	0.09	1.23
(1,1154)	1:108:A:VAL:HG21	1:111:A:PHE:H	19	1.21	0.09	1.23
(1,1154)	1:108:A:VAL:HG23	1:111:A:PHE:H	19	1.21	0.09	1.23
(1,1154)	1:108:A:VAL:HG22	1:111:A:PHE:H	19	1.21	0.09	1.23
(1,795)	1:65:A:LEU:HD23	1:64:A:THR:H	19	0.9	0.13	0.91
(1,795)	1:65:A:LEU:HD22	1:64:A:THR:H	19	0.9	0.13	0.91
(1,795)	1:65:A:LEU:HD21	1:64:A:THR:H	19	0.9	0.13	0.91
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	19	0.84	0.31	0.93
(1,2746)	1:43:A:ARG:HD2	1:88:A:PRO:HG2	19	0.84	0.31	0.93
(1,3504)	1:31:A:MET:HE2	1:86:A:LEU:HD23	19	0.76	0.36	0.68
(1,3504)	1:31:A:MET:HE1	1:86:A:LEU:HD21	19	0.76	0.36	0.68
(1,3504)	1:43:A:ARG:HG3	1:86:A:LEU:HD23	19	0.76	0.36	0.68
(1,3504)	1:43:A:ARG:HG3	1:86:A:LEU:HD21	19	0.76	0.36	0.68
(1,3504)	1:31:A:MET:HE3	1:86:A:LEU:HD23	19	0.76	0.36	0.68
(1,3504)	1:31:A:MET:HE1	1:86:A:LEU:HD22	19	0.76	0.36	0.68
(1,3504)	1:31:A:MET:HE2	1:86:A:LEU:HD21	19	0.76	0.36	0.68
(1,3504)	1:31:A:MET:HE1	1:86:A:LEU:HD23	19	0.76	0.36	0.68
(1,3504)	1:31:A:MET:HE3	1:86:A:LEU:HD21	19	0.76	0.36	0.68
(1,3504)	1:31:A:MET:HE3	1:86:A:LEU:HD22	19	0.76	0.36	0.68
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD11	19	0.75	0.1	0.76
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD13	19	0.75	0.1	0.76
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD12	19	0.75	0.1	0.76
(1,3484)	1:85:A:GLN:HB3	1:86:A:LEU:HD11	19	0.75	0.1	0.76
(1,523)	1:44:A:LEU:HD21	1:44:A:LEU:H	19	0.74	0.1	0.75
(1,523)	1:44:A:LEU:HD23	1:44:A:LEU:H	19	0.74	0.1	0.75
(1,523)	1:54:A:LEU:HD11	1:44:A:LEU:H	19	0.74	0.1	0.75

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,523)	1:44:A:LEU:HD22	1:44:A:LEU:H	19	0.74	0.1	0.75
(1,523)	1:54:A:LEU:HD12	1:44:A:LEU:H	19	0.74	0.1	0.75
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD22	19	0.72	0.18	0.78
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD21	19	0.72	0.18	0.78
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD23	19	0.72	0.18	0.78
(1,298)	1:119:A:ALA:HB3	1:116:A:GLN:H	19	0.69	0.14	0.69
(1,298)	1:112:A:ALA:HB3	1:116:A:GLN:H	19	0.69	0.14	0.69
(1,298)	1:119:A:ALA:HB1	1:116:A:GLN:H	19	0.69	0.14	0.69
(1,298)	1:112:A:ALA:HB2	1:116:A:GLN:H	19	0.69	0.14	0.69
(1,298)	1:119:A:ALA:HB2	1:116:A:GLN:H	19	0.69	0.14	0.69
(1,298)	1:112:A:ALA:HB1	1:116:A:GLN:H	19	0.69	0.14	0.69
(1,425)	1:57:A:THR:HG21	1:60:A:GLU:H	19	0.65	0.22	0.62
(1,425)	1:57:A:THR:HG22	1:60:A:GLU:H	19	0.65	0.22	0.62
(1,425)	1:57:A:THR:HG23	1:60:A:GLU:H	19	0.65	0.22	0.62
(1,3645)	1:55:A:PRO:HD2	1:35:A:LEU:HD12	19	0.64	0.2	0.65
(1,3645)	1:40:A:VAL:HA	1:35:A:LEU:HD12	19	0.64	0.2	0.65
(1,3645)	1:40:A:VAL:HA	1:35:A:LEU:HD13	19	0.64	0.2	0.65
(1,3645)	1:55:A:PRO:HD2	1:35:A:LEU:HD11	19	0.64	0.2	0.65
(1,3645)	1:55:A:PRO:HD2	1:35:A:LEU:HD13	19	0.64	0.2	0.65
(1,3645)	1:40:A:VAL:HA	1:35:A:LEU:HD11	19	0.64	0.2	0.65
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	19	0.59	0.09	0.59
(1,1146)	1:85:A:GLN:HB3	1:81:A:LEU:H	19	0.59	0.09	0.59
(1,3106)	1:40:A:VAL:HG22	1:35:A:LEU:HD13	19	0.55	0.16	0.55
(1,3106)	1:40:A:VAL:HG22	1:35:A:LEU:HD12	19	0.55	0.16	0.55
(1,3106)	1:40:A:VAL:HG23	1:35:A:LEU:HD13	19	0.55	0.16	0.55
(1,3106)	1:40:A:VAL:HG21	1:35:A:LEU:HD13	19	0.55	0.16	0.55
(1,3106)	1:40:A:VAL:HG23	1:35:A:LEU:HD12	19	0.55	0.16	0.55
(1,3106)	1:40:A:VAL:HG21	1:35:A:LEU:HD11	19	0.55	0.16	0.55
(1,3106)	1:40:A:VAL:HG22	1:35:A:LEU:HD11	19	0.55	0.16	0.55
(1,3106)	1:40:A:VAL:HG23	1:35:A:LEU:HD11	19	0.55	0.16	0.55
(1,236)	1:74:A:LEU:HD13	1:76:A:MET:H	19	0.55	0.09	0.55
(1,236)	1:74:A:LEU:HD12	1:76:A:MET:H	19	0.55	0.09	0.55
(1,236)	1:74:A:LEU:HD11	1:76:A:MET:H	19	0.55	0.09	0.55
(1,3497)	1:85:A:GLN:HB3	1:86:A:LEU:HD22	19	0.49	0.15	0.53
(1,3497)	1:85:A:GLN:HB3	1:86:A:LEU:HD23	19	0.49	0.15	0.53
(1,3497)	1:76:A:MET:HB2	1:86:A:LEU:HD23	19	0.49	0.15	0.53
(1,3497)	1:85:A:GLN:HB3	1:86:A:LEU:HD21	19	0.49	0.15	0.53
(1,3497)	1:76:A:MET:HB2	1:86:A:LEU:HD22	19	0.49	0.15	0.53
(1,3497)	1:76:A:MET:HB2	1:86:A:LEU:HD21	19	0.49	0.15	0.53
(1,2920)	1:43:A:ARG:HA	1:86:A:LEU:HD22	19	0.46	0.15	0.47
(1,2920)	1:43:A:ARG:HA	1:86:A:LEU:HD23	19	0.46	0.15	0.47
(1,2920)	1:43:A:ARG:HA	1:86:A:LEU:HD21	19	0.46	0.15	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2920)	1:87:A:GLY:HA3	1:86:A:LEU:HD21	19	0.46	0.15	0.47
(1,2920)	1:87:A:GLY:HA3	1:86:A:LEU:HD23	19	0.46	0.15	0.47
(1,2920)	1:87:A:GLY:HA3	1:86:A:LEU:HD22	19	0.46	0.15	0.47
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	19	0.41	0.12	0.43
(1,1335)	1:95:A:LEU:HD22	1:90:A:MET:H	19	0.41	0.12	0.43
(1,2147)	1:32:A:ALA:H	1:65:A:LEU:HB2	19	0.4	0.08	0.4
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	19	0.4	0.08	0.4
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	19	0.39	0.13	0.39
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD11	19	0.39	0.15	0.44
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD12	19	0.39	0.15	0.44
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD13	19	0.39	0.15	0.44
(1,449)	1:45:A:LEU:HD23	1:45:A:LEU:H	19	0.37	0.14	0.4
(1,449)	1:45:A:LEU:HD21	1:45:A:LEU:H	19	0.37	0.14	0.4
(1,449)	1:45:A:LEU:HD22	1:45:A:LEU:H	19	0.37	0.14	0.4
(1,449)	1:54:A:LEU:HD12	1:45:A:LEU:H	19	0.37	0.14	0.4
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD23	19	0.37	0.14	0.4
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD21	19	0.37	0.14	0.4
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD22	19	0.37	0.14	0.4
(1,2861)	1:45:A:LEU:H	1:54:A:LEU:HD12	19	0.37	0.14	0.4
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	19	0.34	0.1	0.32
(1,3332)	1:72:A:GLN:HB3	1:70:A:PHE:HA	19	0.34	0.1	0.32
(1,1562)	1:102:A:ALA:HB3	1:108:A:VAL:HA	19	0.33	0.11	0.37
(1,1562)	1:102:A:ALA:HB1	1:108:A:VAL:HA	19	0.33	0.11	0.37
(1,1562)	1:102:A:ALA:HB2	1:108:A:VAL:HA	19	0.33	0.11	0.37
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE2	19	0.29	0.11	0.27
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE3	19	0.29	0.11	0.27
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE1	19	0.29	0.11	0.27
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	19	0.29	0.12	0.27
(1,506)	1:74:A:LEU:HD23	1:74:A:LEU:H	19	0.29	0.04	0.3
(1,506)	1:35:A:LEU:HD21	1:74:A:LEU:H	19	0.29	0.04	0.3
(1,506)	1:35:A:LEU:HD22	1:74:A:LEU:H	19	0.29	0.04	0.3
(1,506)	1:74:A:LEU:HD22	1:74:A:LEU:H	19	0.29	0.04	0.3
(1,506)	1:74:A:LEU:HD21	1:74:A:LEU:H	19	0.29	0.04	0.3
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	19	0.28	0.11	0.25
(1,1320)	1:61:A:ILE:HD13	1:35:A:LEU:H	19	0.28	0.14	0.28
(1,1320)	1:61:A:ILE:HD12	1:35:A:LEU:H	19	0.28	0.14	0.28
(1,1320)	1:61:A:ILE:HD11	1:35:A:LEU:H	19	0.28	0.14	0.28
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD13	19	0.27	0.12	0.28
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD12	19	0.27	0.12	0.28
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD11	19	0.27	0.12	0.28
(1,3255)	1:41:A:GLN:HE21	1:61:A:ILE:HD13	19	0.27	0.12	0.28
(1,3255)	1:41:A:GLN:HE21	1:61:A:ILE:HD11	19	0.27	0.12	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3255)	1:41:A:GLN:HE21	1:61:A:ILE:HD12	19	0.27	0.12	0.28
(1,1222)	1:62:A:GLN:HG2	1:59:A:ASP:H	19	0.26	0.09	0.27
(1,1222)	1:60:A:GLU:HB2	1:59:A:ASP:H	19	0.26	0.09	0.27
(1,2638)	1:89:A:LEU:HD21	1:88:A:PRO:HB2	19	0.21	0.04	0.2
(1,2638)	1:89:A:LEU:HD12	1:88:A:PRO:HB2	19	0.21	0.04	0.2
(1,2638)	1:89:A:LEU:HD13	1:88:A:PRO:HB2	19	0.21	0.04	0.2
(1,2638)	1:89:A:LEU:HD23	1:88:A:PRO:HB2	19	0.21	0.04	0.2
(1,2638)	1:89:A:LEU:HD11	1:88:A:PRO:HB2	19	0.21	0.04	0.2
(1,2638)	1:89:A:LEU:HD22	1:88:A:PRO:HB2	19	0.21	0.04	0.2
(1,424)	1:110:A:ALA:HB3	1:107:A:ASP:H	19	0.21	0.07	0.19
(1,424)	1:110:A:ALA:HB2	1:107:A:ASP:H	19	0.21	0.07	0.19
(1,424)	1:110:A:ALA:HB1	1:107:A:ASP:H	19	0.21	0.07	0.19
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	19	0.2	0.06	0.2
(1,929)	1:105:A:LYS:HE3	1:106:A:GLY:H	19	0.2	0.06	0.2
(1,929)	1:105:A:LYS:HE2	1:106:A:GLY:H	19	0.2	0.06	0.2
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB3	19	0.19	0.07	0.17
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB2	19	0.19	0.07	0.17
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB1	19	0.19	0.07	0.17
(1,3158)	1:114:A:ALA:H	1:110:A:ALA:HB3	19	0.19	0.07	0.17
(1,1683)	1:29:A:GLU:HG3	1:29:A:GLU:HA	19	0.19	0.04	0.19
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	19	0.19	0.04	0.19
(1,1572)	1:48:A:LEU:HD13	1:53:A:SER:HB2	18	0.91	0.33	1.0
(1,1572)	1:48:A:LEU:HD11	1:53:A:SER:HB2	18	0.91	0.33	1.0
(1,1572)	1:48:A:LEU:HD12	1:53:A:SER:HB2	18	0.91	0.33	1.0
(1,1572)	1:65:A:LEU:HD23	1:53:A:SER:HB2	18	0.91	0.33	1.0
(1,1572)	1:65:A:LEU:HD22	1:53:A:SER:HB2	18	0.91	0.33	1.0
(1,1572)	1:48:A:LEU:HD21	1:53:A:SER:HB2	18	0.91	0.33	1.0
(1,1572)	1:48:A:LEU:HD23	1:53:A:SER:HB2	18	0.91	0.33	1.0
(1,1572)	1:48:A:LEU:HD22	1:53:A:SER:HB2	18	0.91	0.33	1.0
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG21	18	0.77	0.14	0.78
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG22	18	0.77	0.14	0.78
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG23	18	0.77	0.14	0.78
(1,1883)	1:35:A:LEU:HD21	1:74:A:LEU:HA	18	0.48	0.23	0.51
(1,1883)	1:35:A:LEU:HD22	1:74:A:LEU:HA	18	0.48	0.23	0.51
(1,1883)	1:74:A:LEU:HD21	1:74:A:LEU:HA	18	0.48	0.23	0.51
(1,1883)	1:74:A:LEU:HD23	1:74:A:LEU:HA	18	0.48	0.23	0.51
(1,1883)	1:35:A:LEU:HD23	1:74:A:LEU:HA	18	0.48	0.23	0.51
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	18	0.4	0.15	0.41
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD13	18	0.38	0.14	0.38
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD11	18	0.38	0.14	0.38
(1,3259)	1:77:A:PHE:HE1	1:34:A:ILE:HD12	18	0.38	0.14	0.38
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD12	18	0.38	0.14	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	18	0.37	0.13	0.39
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG13	18	0.37	0.17	0.36
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG12	18	0.37	0.17	0.36
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG11	18	0.37	0.17	0.36
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD22	18	0.35	0.13	0.36
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD23	18	0.35	0.13	0.36
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD21	18	0.35	0.13	0.36
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	18	0.33	0.11	0.37
(1,303)	1:73:A:ALA:HB3	1:72:A:GLN:H	18	0.32	0.1	0.31
(1,303)	1:73:A:ALA:HB1	1:72:A:GLN:H	18	0.32	0.1	0.31
(1,303)	1:73:A:ALA:HB2	1:72:A:GLN:H	18	0.32	0.1	0.31
(1,499)	1:115:A:MET:HB2	1:117:A:ASN:H	18	0.31	0.13	0.31
(1,499)	1:115:A:MET:HB3	1:117:A:ASN:H	18	0.31	0.13	0.31
(1,499)	1:120:A:LYS:HB2	1:117:A:ASN:H	18	0.31	0.13	0.31
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	18	0.31	0.15	0.26
(1,870)	1:25:A:VAL:HG11	1:24:A:SER:H	18	0.3	0.11	0.3
(1,870)	1:25:A:VAL:HG12	1:24:A:SER:H	18	0.3	0.11	0.3
(1,870)	1:25:A:VAL:HG13	1:24:A:SER:H	18	0.3	0.11	0.3
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	18	0.3	0.08	0.3
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	18	0.25	0.09	0.24
(1,740)	1:111:A:PHE:HA	1:115:A:MET:H	18	0.25	0.09	0.24
(1,468)	1:57:A:THR:HG22	1:56:A:GLN:H	18	0.23	0.08	0.24
(1,468)	1:57:A:THR:HG23	1:56:A:GLN:H	18	0.23	0.08	0.24
(1,468)	1:57:A:THR:HG21	1:56:A:GLN:H	18	0.23	0.08	0.24
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	18	0.23	0.02	0.23
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE3	18	0.22	0.07	0.22
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE1	18	0.22	0.07	0.22
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE2	18	0.22	0.07	0.22
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	18	0.2	0.04	0.21
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB1	18	0.19	0.04	0.2
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB3	18	0.19	0.04	0.2
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB2	18	0.19	0.04	0.2
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	18	0.18	0.02	0.19
(1,2582)	1:28:A:PRO:HD2	1:28:A:PRO:HB2	18	0.16	0.02	0.16
(1,2582)	1:28:A:PRO:HA	1:28:A:PRO:HB2	18	0.16	0.02	0.16
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB3	17	0.45	0.12	0.45
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB2	17	0.45	0.12	0.45
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB1	17	0.45	0.12	0.45
(1,1429)	1:116:A:GLN:HB3	1:119:A:ALA:H	17	0.45	0.2	0.46
(1,1429)	1:116:A:GLN:HB2	1:119:A:ALA:H	17	0.45	0.2	0.46
(1,562)	1:95:A:LEU:HD21	1:93:A:PHE:H	17	0.42	0.16	0.43
(1,562)	1:95:A:LEU:HD22	1:93:A:PHE:H	17	0.42	0.16	0.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,562)	1:95:A:LEU:HD23	1:93:A:PHE:H	17	0.42	0.16	0.43
(1,3556)	1:43:A:ARG:HD3	1:80:A:ALA:HB2	17	0.36	0.11	0.37
(1,3556)	1:43:A:ARG:HD3	1:80:A:ALA:HB3	17	0.36	0.11	0.37
(1,3556)	1:77:A:PHE:HB3	1:80:A:ALA:HB3	17	0.36	0.11	0.37
(1,3556)	1:77:A:PHE:HB3	1:80:A:ALA:HB2	17	0.36	0.11	0.37
(1,3556)	1:77:A:PHE:HB3	1:80:A:ALA:HB1	17	0.36	0.11	0.37
(1,3556)	1:43:A:ARG:HD3	1:80:A:ALA:HB1	17	0.36	0.11	0.37
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	17	0.25	0.09	0.25
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD2	17	0.24	0.09	0.23
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD3	17	0.24	0.09	0.23
(1,1548)	1:61:A:ILE:HB	1:61:A:ILE:HA	17	0.22	0.04	0.24
(1,1548)	1:65:A:LEU:HG	1:61:A:ILE:HA	17	0.22	0.04	0.24
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	17	0.21	0.07	0.19
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD22	17	0.19	0.06	0.17
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD21	17	0.19	0.06	0.17
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD23	17	0.19	0.06	0.17
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	17	0.17	0.04	0.16
(1,2769)	1:99:A:ALA:HB2	1:115:A:MET:HB2	16	1.01	0.58	1.33
(1,2769)	1:30:A:ILE:HG13	1:29:A:GLU:HB3	16	1.01	0.58	1.33
(1,2769)	1:99:A:ALA:HB1	1:115:A:MET:HB2	16	1.01	0.58	1.33
(1,2769)	1:114:A:ALA:HB3	1:115:A:MET:HB2	16	1.01	0.58	1.33
(1,2769)	1:95:A:LEU:HD22	1:115:A:MET:HB3	16	1.01	0.58	1.33
(1,2769)	1:114:A:ALA:HB1	1:115:A:MET:HB2	16	1.01	0.58	1.33
(1,2769)	1:99:A:ALA:HB3	1:115:A:MET:HB2	16	1.01	0.58	1.33
(1,1558)	1:30:A:ILE:HG13	1:28:A:PRO:HA	16	0.61	0.16	0.6
(1,1558)	1:64:A:THR:HG23	1:53:A:SER:HB3	16	0.61	0.16	0.6
(1,1558)	1:64:A:THR:HG21	1:53:A:SER:HB3	16	0.61	0.16	0.6
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD23	16	0.52	0.2	0.46
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD11	16	0.52	0.2	0.46
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD12	16	0.52	0.2	0.46
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD13	16	0.52	0.2	0.46
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD21	16	0.52	0.2	0.46
(1,2921)	1:32:A:ALA:HA	1:35:A:LEU:HD21	16	0.49	0.16	0.5
(1,2921)	1:73:A:ALA:HA	1:35:A:LEU:HD22	16	0.49	0.16	0.5
(1,2921)	1:32:A:ALA:HA	1:35:A:LEU:HD23	16	0.49	0.16	0.5
(1,2921)	1:73:A:ALA:HA	1:35:A:LEU:HD23	16	0.49	0.16	0.5
(1,2921)	1:73:A:ALA:HA	1:35:A:LEU:HD21	16	0.49	0.16	0.5
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE3	16	0.39	0.23	0.3
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE2	16	0.39	0.23	0.3
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE1	16	0.39	0.23	0.3
(1,2630)	1:34:A:ILE:HD12	1:90:A:MET:HG3	16	0.35	0.15	0.32
(1,2630)	1:34:A:ILE:HD13	1:90:A:MET:HG3	16	0.35	0.15	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2630)	1:34:A:ILE:HD11	1:90:A:MET:HG3	16	0.35	0.15	0.32
(1,3231)	1:107:A:ASP:HB2	1:110:A:ALA:HB2	16	0.32	0.08	0.34
(1,3231)	1:107:A:ASP:HB2	1:110:A:ALA:HB3	16	0.32	0.08	0.34
(1,3231)	1:107:A:ASP:HB2	1:110:A:ALA:HB1	16	0.32	0.08	0.34
(1,3231)	1:109:A:GLU:HG3	1:110:A:ALA:HB2	16	0.32	0.08	0.34
(1,3231)	1:109:A:GLU:HG3	1:110:A:ALA:HB1	16	0.32	0.08	0.34
(1,3231)	1:109:A:GLU:HG3	1:110:A:ALA:HB3	16	0.32	0.08	0.34
(1,896)	1:72:A:GLN:HG2	1:72:A:GLN:HE22	16	0.3	0.02	0.3
(1,896)	1:72:A:GLN:HG3	1:72:A:GLN:HE22	16	0.3	0.02	0.3
(1,896)	1:69:A:GLN:HB3	1:72:A:GLN:HE22	16	0.3	0.02	0.3
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	16	0.21	0.05	0.19
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	16	0.2	0.05	0.2
(1,1206)	1:34:A:ILE:HB	1:37:A:ASN:H	16	0.17	0.05	0.16
(1,1206)	1:35:A:LEU:HG	1:37:A:ASN:H	16	0.17	0.05	0.16
(1,109)	1:48:A:LEU:HD12	1:48:A:LEU:H	16	0.16	0.04	0.16
(1,109)	1:48:A:LEU:HD13	1:48:A:LEU:H	16	0.16	0.04	0.16
(1,109)	1:48:A:LEU:HD11	1:48:A:LEU:H	16	0.16	0.04	0.16
(1,109)	1:48:A:LEU:HD23	1:48:A:LEU:H	16	0.16	0.04	0.16
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	16	0.13	0.02	0.14
(1,2857)	1:44:A:LEU:H	1:44:A:LEU:HD21	15	0.69	0.22	0.75
(1,2857)	1:44:A:LEU:H	1:44:A:LEU:HD23	15	0.69	0.22	0.75
(1,2857)	1:44:A:LEU:H	1:44:A:LEU:HD22	15	0.69	0.22	0.75
(1,2857)	1:52:A:GLU:H	1:48:A:LEU:HD22	15	0.69	0.22	0.75
(1,2857)	1:52:A:GLU:H	1:48:A:LEU:HD21	15	0.69	0.22	0.75
(1,3272)	1:96:A:PRO:HD3	1:115:A:MET:HE3	15	0.6	0.31	0.57
(1,3272)	1:96:A:PRO:HD3	1:115:A:MET:HE2	15	0.6	0.31	0.57
(1,3272)	1:30:A:ILE:HA	1:115:A:MET:HE3	15	0.6	0.31	0.57
(1,3272)	1:96:A:PRO:HD3	1:115:A:MET:HE1	15	0.6	0.31	0.57
(1,1116)	1:96:A:PRO:HA	1:119:A:ALA:H	15	0.56	0.23	0.7
(1,1116)	1:95:A:LEU:HA	1:119:A:ALA:H	15	0.56	0.23	0.7
(1,3634)	1:65:A:LEU:HD12	1:70:A:PHE:HB3	15	0.5	0.17	0.56
(1,3634)	1:22:A:LEU:HD12	1:70:A:PHE:HB3	15	0.5	0.17	0.56
(1,3634)	1:65:A:LEU:HD11	1:70:A:PHE:HB3	15	0.5	0.17	0.56
(1,3634)	1:65:A:LEU:HD13	1:70:A:PHE:HB3	15	0.5	0.17	0.56
(1,3642)	1:74:A:LEU:HD21	1:70:A:PHE:HA	15	0.48	0.17	0.44
(1,3642)	1:35:A:LEU:HD21	1:70:A:PHE:HA	15	0.48	0.17	0.44
(1,3642)	1:74:A:LEU:HD23	1:70:A:PHE:HA	15	0.48	0.17	0.44
(1,3642)	1:74:A:LEU:HD22	1:70:A:PHE:HA	15	0.48	0.17	0.44
(1,3642)	1:35:A:LEU:HD23	1:70:A:PHE:HA	15	0.48	0.17	0.44
(1,3642)	1:35:A:LEU:HD22	1:70:A:PHE:HA	15	0.48	0.17	0.44
(1,1145)	1:85:A:GLN:HB2	1:81:A:LEU:H	15	0.45	0.17	0.47
(1,1145)	1:43:A:ARG:HB3	1:81:A:LEU:H	15	0.45	0.17	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3565)	1:90:A:MET:HE1	1:31:A:MET:HE2	15	0.44	0.31	0.4
(1,3565)	1:90:A:MET:HE3	1:31:A:MET:HE1	15	0.44	0.31	0.4
(1,3565)	1:101:A:GLU:HB2	1:102:A:ALA:HB1	15	0.44	0.31	0.4
(1,3565)	1:90:A:MET:HE3	1:31:A:MET:HE2	15	0.44	0.31	0.4
(1,3565)	1:90:A:MET:HE1	1:31:A:MET:HE1	15	0.44	0.31	0.4
(1,3565)	1:90:A:MET:HE2	1:31:A:MET:HE3	15	0.44	0.31	0.4
(1,3565)	1:90:A:MET:HE2	1:31:A:MET:HE1	15	0.44	0.31	0.4
(1,3565)	1:90:A:MET:HE2	1:31:A:MET:HE2	15	0.44	0.31	0.4
(1,3565)	1:90:A:MET:HE1	1:31:A:MET:HE3	15	0.44	0.31	0.4
(1,3565)	1:90:A:MET:HE3	1:31:A:MET:HE3	15	0.44	0.31	0.4
(1,60)	1:54:A:LEU:HD11	1:54:A:LEU:H	15	0.41	0.13	0.36
(1,60)	1:54:A:LEU:HD12	1:54:A:LEU:H	15	0.41	0.13	0.36
(1,60)	1:48:A:LEU:HD11	1:54:A:LEU:H	15	0.41	0.13	0.36
(1,60)	1:54:A:LEU:HD13	1:54:A:LEU:H	15	0.41	0.13	0.36
(1,60)	1:48:A:LEU:HD12	1:54:A:LEU:H	15	0.41	0.13	0.36
(1,60)	1:48:A:LEU:HD13	1:54:A:LEU:H	15	0.41	0.13	0.36
(1,2081)	1:95:A:LEU:HD13	1:96:A:PRO:HD2	15	0.4	0.14	0.38
(1,2081)	1:65:A:LEU:HD11	1:55:A:PRO:HD2	15	0.4	0.14	0.38
(1,2081)	1:65:A:LEU:HD13	1:55:A:PRO:HD2	15	0.4	0.14	0.38
(1,2081)	1:95:A:LEU:HD11	1:96:A:PRO:HD2	15	0.4	0.14	0.38
(1,2081)	1:95:A:LEU:HD12	1:96:A:PRO:HD2	15	0.4	0.14	0.38
(1,2081)	1:65:A:LEU:HD12	1:55:A:PRO:HD2	15	0.4	0.14	0.38
(1,2081)	1:54:A:LEU:HD21	1:55:A:PRO:HD2	15	0.4	0.14	0.38
(1,3766)	1:45:A:LEU:H	1:47:A:TYR:HE2	15	0.37	0.15	0.4
(1,3766)	1:83:A:SER:H	1:47:A:TYR:HE2	15	0.37	0.15	0.4
(1,3766)	1:83:A:SER:H	1:47:A:TYR:HE1	15	0.37	0.15	0.4
(1,3402)	1:22:A:LEU:HD12	1:21:A:ASP:HB2	15	0.37	0.11	0.37
(1,3402)	1:25:A:VAL:HG11	1:21:A:ASP:HB2	15	0.37	0.11	0.37
(1,3402)	1:22:A:LEU:HD11	1:21:A:ASP:HB2	15	0.37	0.11	0.37
(1,3402)	1:25:A:VAL:HG12	1:21:A:ASP:HB2	15	0.37	0.11	0.37
(1,3402)	1:22:A:LEU:HD13	1:21:A:ASP:HB2	15	0.37	0.11	0.37
(1,3402)	1:25:A:VAL:HG13	1:21:A:ASP:HB2	15	0.37	0.11	0.37
(1,2066)	1:119:A:ALA:HB1	1:96:A:PRO:HD2	15	0.34	0.12	0.36
(1,2066)	1:54:A:LEU:HB3	1:55:A:PRO:HD2	15	0.34	0.12	0.36
(1,2066)	1:95:A:LEU:HB2	1:96:A:PRO:HD2	15	0.34	0.12	0.36
(1,2530)	1:56:A:GLN:HA	1:56:A:GLN:HG2	15	0.32	0.04	0.33
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD13	15	0.29	0.1	0.29
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD11	15	0.29	0.1	0.29
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD12	15	0.29	0.1	0.29
(1,3337)	1:14:A:PRO:HD3	1:14:A:PRO:HA	15	0.28	0.09	0.26
(1,3337)	1:11:A:PRO:HD3	1:11:A:PRO:HA	15	0.28	0.09	0.26
(1,3337)	1:11:A:PRO:HD2	1:11:A:PRO:HA	15	0.28	0.09	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3337)	1:121:A:PRO:HD2	1:121:A:PRO:HA	15	0.28	0.09	0.26
(1,3337)	1:14:A:PRO:HD2	1:14:A:PRO:HA	15	0.28	0.09	0.26
(1,3434)	1:114:A:ALA:HA	1:113:A:LYS:HB3	15	0.27	0.11	0.22
(1,3434)	1:116:A:GLN:HA	1:120:A:LYS:HB2	15	0.27	0.11	0.22
(1,297)	1:113:A:LYS:HG3	1:114:A:ALA:H	15	0.26	0.07	0.26
(1,297)	1:112:A:ALA:HB3	1:114:A:ALA:H	15	0.26	0.07	0.26
(1,1273)	1:80:A:ALA:HB3	1:85:A:GLN:H	15	0.25	0.12	0.21
(1,1273)	1:80:A:ALA:HB2	1:85:A:GLN:H	15	0.25	0.12	0.21
(1,1273)	1:80:A:ALA:HB1	1:85:A:GLN:H	15	0.25	0.12	0.21
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG13	15	0.24	0.1	0.21
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG12	15	0.24	0.1	0.21
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG11	15	0.24	0.1	0.21
(1,2109)	1:49:A:PRO:HD3	1:48:A:LEU:HB3	15	0.23	0.05	0.23
(1,2109)	1:49:A:PRO:HD2	1:48:A:LEU:HB3	15	0.23	0.05	0.23
(1,2552)	1:27:A:THR:HA	1:28:A:PRO:HB3	15	0.12	0.02	0.12
(1,2552)	1:27:A:THR:HB	1:28:A:PRO:HB3	15	0.12	0.02	0.12
(1,3558)	1:118:A:ASN:HB3	1:114:A:ALA:HB1	14	0.86	0.49	0.82
(1,3558)	1:118:A:ASN:HB3	1:114:A:ALA:HB3	14	0.86	0.49	0.82
(1,3558)	1:117:A:ASN:HB2	1:114:A:ALA:HB2	14	0.86	0.49	0.82
(1,3558)	1:117:A:ASN:HB2	1:114:A:ALA:HB1	14	0.86	0.49	0.82
(1,3558)	1:118:A:ASN:HB3	1:114:A:ALA:HB2	14	0.86	0.49	0.82
(1,3558)	1:118:A:ASN:HB3	1:99:A:ALA:HB2	14	0.86	0.49	0.82
(1,3558)	1:117:A:ASN:HB2	1:114:A:ALA:HB3	14	0.86	0.49	0.82
(1,3558)	1:90:A:MET:HG2	1:99:A:ALA:HB2	14	0.86	0.49	0.82
(1,1063)	1:95:A:LEU:HD22	1:94:A:GLY:H	14	0.38	0.13	0.38
(1,1063)	1:95:A:LEU:HD21	1:94:A:GLY:H	14	0.38	0.13	0.38
(1,1063)	1:95:A:LEU:HD23	1:94:A:GLY:H	14	0.38	0.13	0.38
(1,2694)	1:99:A:ALA:H	1:96:A:PRO:HG3	14	0.35	0.18	0.36
(1,2694)	1:72:A:GLN:HE21	1:49:A:PRO:HG3	14	0.35	0.18	0.36
(1,3455)	1:104:A:ASN:H	1:105:A:LYS:HG3	14	0.33	0.1	0.33
(1,1707)	1:30:A:ILE:HG13	1:30:A:ILE:HA	14	0.28	0.06	0.28
(1,1707)	1:114:A:ALA:HB2	1:111:A:PHE:HA	14	0.28	0.06	0.28
(1,1707)	1:114:A:ALA:HB3	1:111:A:PHE:HA	14	0.28	0.06	0.28
(1,1307)	1:51:A:GLY:HA3	1:53:A:SER:H	14	0.26	0.07	0.24
(1,1255)	1:26:A:LEU:HG	1:25:A:VAL:H	14	0.22	0.07	0.22
(1,3698)	1:90:A:MET:HE2	1:111:A:PHE:HD1	14	0.21	0.07	0.22
(1,3698)	1:90:A:MET:HE3	1:111:A:PHE:HD1	14	0.21	0.07	0.22
(1,3698)	1:108:A:VAL:HB	1:111:A:PHE:HD2	14	0.21	0.07	0.22
(1,3698)	1:90:A:MET:HE1	1:111:A:PHE:HD1	14	0.21	0.07	0.22
(1,3698)	1:90:A:MET:HE1	1:93:A:PHE:HD2	14	0.21	0.07	0.22
(1,3698)	1:90:A:MET:HE3	1:93:A:PHE:HD2	14	0.21	0.07	0.22
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD22	14	0.19	0.06	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD23	14	0.19	0.06	0.17
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD21	14	0.19	0.06	0.17
(1,1181)	1:111:A:PHE:HA	1:102:A:ALA:H	14	0.17	0.03	0.17
(1,334)	1:81:A:LEU:HB2	1:80:A:ALA:H	14	0.17	0.04	0.17
(1,633)	1:34:A:ILE:HB	1:36:A:ALA:H	14	0.14	0.03	0.14
(1,2912)	1:43:A:ARG:HA	1:44:A:LEU:HD21	13	0.79	0.27	0.72
(1,2912)	1:85:A:GLN:HA	1:89:A:LEU:HD23	13	0.79	0.27	0.72
(1,2912)	1:50:A:SER:HA	1:48:A:LEU:HD22	13	0.79	0.27	0.72
(1,2912)	1:43:A:ARG:HA	1:89:A:LEU:HD22	13	0.79	0.27	0.72
(1,2912)	1:50:A:SER:HA	1:48:A:LEU:HD21	13	0.79	0.27	0.72
(1,2912)	1:85:A:GLN:HA	1:89:A:LEU:HD22	13	0.79	0.27	0.72
(1,2912)	1:43:A:ARG:HA	1:89:A:LEU:HD23	13	0.79	0.27	0.72
(1,2912)	1:50:A:SER:HA	1:48:A:LEU:HD23	13	0.79	0.27	0.72
(1,1859)	1:64:A:THR:HG21	1:60:A:GLU:HA	13	0.47	0.22	0.5
(1,1859)	1:64:A:THR:HG22	1:60:A:GLU:HA	13	0.47	0.22	0.5
(1,1859)	1:64:A:THR:HG23	1:60:A:GLU:HA	13	0.47	0.22	0.5
(1,2456)	1:63:A:ASN:H	1:55:A:PRO:HB3	13	0.37	0.17	0.36
(1,2456)	1:120:A:LYS:H	1:121:A:PRO:HB3	13	0.37	0.17	0.36
(1,1703)	1:114:A:ALA:HB1	1:98:A:GLU:HA	13	0.35	0.28	0.29
(1,1703)	1:114:A:ALA:HB3	1:98:A:GLU:HA	13	0.35	0.28	0.29
(1,1703)	1:114:A:ALA:HB2	1:98:A:GLU:HA	13	0.35	0.28	0.29
(1,3258)	1:111:A:PHE:HE2	1:34:A:ILE:HD13	13	0.31	0.09	0.33
(1,3258)	1:37:A:ASN:H	1:61:A:ILE:HD11	13	0.31	0.09	0.33
(1,3258)	1:111:A:PHE:HE2	1:34:A:ILE:HD11	13	0.31	0.09	0.33
(1,3258)	1:37:A:ASN:H	1:61:A:ILE:HD12	13	0.31	0.09	0.33
(1,3258)	1:111:A:PHE:HE2	1:34:A:ILE:HD12	13	0.31	0.09	0.33
(1,2958)	1:103:A:ALA:HA	1:81:A:LEU:HD12	13	0.31	0.1	0.32
(1,2958)	1:103:A:ALA:HA	1:81:A:LEU:HD13	13	0.31	0.1	0.32
(1,2958)	1:103:A:ALA:HA	1:81:A:LEU:HD11	13	0.31	0.1	0.32
(1,2958)	1:78:A:SER:HB3	1:81:A:LEU:HD13	13	0.31	0.1	0.32
(1,2958)	1:78:A:SER:HB3	1:81:A:LEU:HD11	13	0.31	0.1	0.32
(1,2482)	1:93:A:PHE:HZ	1:40:A:VAL:HB	13	0.29	0.14	0.22
(1,264)	1:110:A:ALA:HB3	1:109:A:GLU:H	13	0.23	0.06	0.22
(1,264)	1:110:A:ALA:HB2	1:109:A:GLU:H	13	0.23	0.06	0.22
(1,264)	1:110:A:ALA:HB1	1:109:A:GLU:H	13	0.23	0.06	0.22
(1,1274)	1:95:A:LEU:HD22	1:91:A:CYS:H	13	0.2	0.06	0.19
(1,1274)	1:95:A:LEU:HD21	1:91:A:CYS:H	13	0.2	0.06	0.19
(1,1274)	1:95:A:LEU:HD23	1:91:A:CYS:H	13	0.2	0.06	0.19
(1,3009)	1:26:A:LEU:HB3	1:74:A:LEU:HD11	13	0.19	0.04	0.2
(1,3009)	1:74:A:LEU:HB3	1:74:A:LEU:HD11	13	0.19	0.04	0.2
(1,3009)	1:74:A:LEU:HB3	1:74:A:LEU:HD12	13	0.19	0.04	0.2
(1,3009)	1:74:A:LEU:HB3	1:74:A:LEU:HD13	13	0.19	0.04	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3009)	1:26:A:LEU:HB3	1:74:A:LEU:HD13	13	0.19	0.04	0.2
(1,1097)	1:74:A:LEU:HG	1:22:A:LEU:H	13	0.17	0.05	0.16
(1,614)	1:95:A:LEU:HB2	1:91:A:CYS:H	12	0.49	0.06	0.47
(1,614)	1:89:A:LEU:HB2	1:91:A:CYS:H	12	0.49	0.06	0.47
(1,3712)	1:65:A:LEU:HD12	1:70:A:PHE:HD1	12	0.42	0.2	0.34
(1,3712)	1:65:A:LEU:HD13	1:70:A:PHE:HD1	12	0.42	0.2	0.34
(1,3712)	1:26:A:LEU:HD22	1:111:A:PHE:HE2	12	0.42	0.2	0.34
(1,3712)	1:65:A:LEU:HD11	1:70:A:PHE:HD1	12	0.42	0.2	0.34
(1,3712)	1:61:A:ILE:HG22	1:70:A:PHE:HE1	12	0.42	0.2	0.34
(1,3712)	1:26:A:LEU:HD21	1:111:A:PHE:HE2	12	0.42	0.2	0.34
(1,3117)	1:116:A:GLN:H	1:115:A:MET:HE2	12	0.41	0.35	0.23
(1,3117)	1:116:A:GLN:H	1:115:A:MET:HE3	12	0.41	0.35	0.23
(1,3117)	1:119:A:ALA:H	1:115:A:MET:HE1	12	0.41	0.35	0.23
(1,3117)	1:116:A:GLN:H	1:115:A:MET:HE1	12	0.41	0.35	0.23
(1,3117)	1:119:A:ALA:H	1:115:A:MET:HE2	12	0.41	0.35	0.23
(1,2994)	1:31:A:MET:HG3	1:35:A:LEU:HD23	12	0.32	0.21	0.26
(1,2994)	1:41:A:GLN:HG2	1:35:A:LEU:HD23	12	0.32	0.21	0.26
(1,2994)	1:31:A:MET:HG3	1:35:A:LEU:HD21	12	0.32	0.21	0.26
(1,2994)	1:31:A:MET:HG3	1:35:A:LEU:HD22	12	0.32	0.21	0.26
(1,3737)	1:92:A:GLN:HB3	1:93:A:PHE:HZ	12	0.31	0.1	0.32
(1,3737)	1:89:A:LEU:HG	1:93:A:PHE:HZ	12	0.31	0.1	0.32
(1,3527)	1:82:A:ALA:HB1	1:108:A:VAL:HG23	12	0.3	0.06	0.28
(1,3527)	1:112:A:ALA:HB3	1:108:A:VAL:HG21	12	0.3	0.06	0.28
(1,3527)	1:82:A:ALA:HB2	1:108:A:VAL:HG21	12	0.3	0.06	0.28
(1,3527)	1:82:A:ALA:HB2	1:108:A:VAL:HG22	12	0.3	0.06	0.28
(1,3527)	1:82:A:ALA:HB3	1:108:A:VAL:HG22	12	0.3	0.06	0.28
(1,3527)	1:82:A:ALA:HB2	1:108:A:VAL:HG23	12	0.3	0.06	0.28
(1,2417)	1:114:A:ALA:HB1	1:98:A:GLU:HG3	12	0.28	0.13	0.28
(1,2417)	1:114:A:ALA:HB2	1:98:A:GLU:HG3	12	0.28	0.13	0.28
(1,2417)	1:114:A:ALA:HB3	1:98:A:GLU:HG3	12	0.28	0.13	0.28
(1,2417)	1:114:A:ALA:HB1	1:98:A:GLU:HG2	12	0.28	0.13	0.28
(1,2417)	1:114:A:ALA:HB2	1:98:A:GLU:HG2	12	0.28	0.13	0.28
(1,2417)	1:114:A:ALA:HB3	1:98:A:GLU:HG2	12	0.28	0.13	0.28
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB1	12	0.28	0.13	0.28
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB2	12	0.28	0.13	0.28
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB3	12	0.28	0.13	0.28
(1,3229)	1:98:A:GLU:HG2	1:114:A:ALA:HB1	12	0.28	0.13	0.28
(1,3229)	1:98:A:GLU:HG2	1:114:A:ALA:HB2	12	0.28	0.13	0.28
(1,3229)	1:98:A:GLU:HG2	1:114:A:ALA:HB3	12	0.28	0.13	0.28
(1,105)	1:76:A:MET:HB3	1:48:A:LEU:H	12	0.26	0.12	0.26
(1,1849)	1:115:A:MET:HB2	1:112:A:ALA:HA	12	0.26	0.11	0.22
(1,1849)	1:115:A:MET:HB3	1:112:A:ALA:HA	12	0.26	0.11	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1849)	1:26:A:LEU:HG	1:112:A:ALA:HA	12	0.26	0.11	0.22
(1,3407)	1:32:A:ALA:H	1:29:A:GLU:HG3	12	0.24	0.12	0.22
(1,291)	1:116:A:GLN:HB3	1:116:A:GLN:H	12	0.14	0.03	0.12
(1,2551)	1:55:A:PRO:HA	1:55:A:PRO:HB2	12	0.13	0.01	0.13
(1,2551)	1:49:A:PRO:HA	1:49:A:PRO:HB2	12	0.13	0.01	0.13
(1,868)	1:65:A:LEU:HD22	1:69:A:GLN:HE21	11	0.56	0.31	0.54
(1,868)	1:65:A:LEU:HD23	1:69:A:GLN:HE21	11	0.56	0.31	0.54
(1,868)	1:65:A:LEU:HD23	1:72:A:GLN:HE21	11	0.56	0.31	0.54
(1,868)	1:65:A:LEU:HD21	1:72:A:GLN:HE21	11	0.56	0.31	0.54
(1,868)	1:65:A:LEU:HD21	1:69:A:GLN:HE21	11	0.56	0.31	0.54
(1,3267)	1:31:A:MET:HG2	1:34:A:ILE:HD13	11	0.52	0.16	0.48
(1,3267)	1:31:A:MET:HG2	1:34:A:ILE:HD11	11	0.52	0.16	0.48
(1,3267)	1:31:A:MET:HG3	1:34:A:ILE:HD11	11	0.52	0.16	0.48
(1,3267)	1:31:A:MET:HG2	1:34:A:ILE:HD12	11	0.52	0.16	0.48
(1,3584)	1:48:A:LEU:HD13	1:49:A:PRO:HA	11	0.5	0.29	0.42
(1,3584)	1:10:A:VAL:HG12	1:11:A:PRO:HA	11	0.5	0.29	0.42
(1,3584)	1:48:A:LEU:HD11	1:49:A:PRO:HA	11	0.5	0.29	0.42
(1,3584)	1:10:A:VAL:HG11	1:11:A:PRO:HA	11	0.5	0.29	0.42
(1,3584)	1:48:A:LEU:HD12	1:49:A:PRO:HA	11	0.5	0.29	0.42
(1,3584)	1:10:A:VAL:HG13	1:11:A:PRO:HA	11	0.5	0.29	0.42
(1,1296)	1:26:A:LEU:HD22	1:115:A:MET:H	11	0.34	0.14	0.37
(1,1296)	1:26:A:LEU:HD21	1:115:A:MET:H	11	0.34	0.14	0.37
(1,1296)	1:26:A:LEU:HD23	1:115:A:MET:H	11	0.34	0.14	0.37
(1,1187)	1:116:A:GLN:HB2	1:118:A:ASN:H	11	0.33	0.12	0.34
(1,2770)	1:99:A:ALA:HB1	1:96:A:PRO:HG3	11	0.32	0.12	0.36
(1,2770)	1:99:A:ALA:HB3	1:96:A:PRO:HG3	11	0.32	0.12	0.36
(1,2770)	1:99:A:ALA:HB2	1:96:A:PRO:HG3	11	0.32	0.12	0.36
(1,192)	1:108:A:VAL:HG13	1:82:A:ALA:H	11	0.3	0.1	0.3
(1,192)	1:108:A:VAL:HG12	1:82:A:ALA:H	11	0.3	0.1	0.3
(1,192)	1:108:A:VAL:HG11	1:82:A:ALA:H	11	0.3	0.1	0.3
(1,3228)	1:61:A:ILE:HB	1:32:A:ALA:HB1	11	0.29	0.13	0.3
(1,3228)	1:61:A:ILE:HB	1:32:A:ALA:HB2	11	0.29	0.13	0.3
(1,3228)	1:61:A:ILE:HB	1:32:A:ALA:HB3	11	0.29	0.13	0.3
(1,618)	1:37:A:ASN:HA	1:37:A:ASN:HD22	11	0.28	0.04	0.3
(1,3547)	1:54:A:LEU:HG	1:76:A:MET:HE1	11	0.27	0.1	0.29
(1,3547)	1:54:A:LEU:HG	1:76:A:MET:HE3	11	0.27	0.1	0.29
(1,3547)	1:48:A:LEU:HG	1:76:A:MET:HE3	11	0.27	0.1	0.29
(1,2631)	1:100:A:VAL:HG21	1:90:A:MET:HB3	11	0.25	0.08	0.24
(1,2631)	1:100:A:VAL:HG23	1:90:A:MET:HB3	11	0.25	0.08	0.24
(1,2631)	1:100:A:VAL:HG22	1:90:A:MET:HB3	11	0.25	0.08	0.24
(1,3375)	1:58:A:ALA:HB3	1:33:A:PRO:HD2	11	0.25	0.1	0.25
(1,3375)	1:58:A:ALA:HB1	1:33:A:PRO:HD2	11	0.25	0.1	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3375)	1:58:A:ALA:HB2	1:33:A:PRO:HD2	11	0.25	0.1	0.25
(1,3375)	1:35:A:LEU:HB2	1:33:A:PRO:HD2	11	0.25	0.1	0.25
(1,1282)	1:91:A:CYS:HB3	1:89:A:LEU:H	11	0.23	0.14	0.15
(1,1282)	1:91:A:CYS:HB2	1:89:A:LEU:H	11	0.23	0.14	0.15
(1,1144)	1:90:A:MET:HE3	1:81:A:LEU:H	11	0.23	0.16	0.17
(1,1144)	1:44:A:LEU:HG	1:81:A:LEU:H	11	0.23	0.16	0.17
(1,1202)	1:40:A:VAL:HA	1:45:A:LEU:H	11	0.22	0.07	0.21
(1,399)	1:118:A:ASN:HB3	1:118:A:ASN:H	11	0.21	0.06	0.2
(1,399)	1:117:A:ASN:HB3	1:118:A:ASN:H	11	0.21	0.06	0.2
(1,2585)	1:77:A:PHE:HB3	1:76:A:MET:HG3	11	0.2	0.05	0.19
(1,3783)	1:26:A:LEU:HD12	1:77:A:PHE:HZ	11	0.2	0.09	0.18
(1,3783)	1:26:A:LEU:HD11	1:77:A:PHE:HZ	11	0.2	0.09	0.18
(1,3783)	1:26:A:LEU:HD13	1:77:A:PHE:HZ	11	0.2	0.09	0.18
(1,866)	1:22:A:LEU:HG	1:24:A:SER:H	11	0.19	0.08	0.17
(1,1552)	1:89:A:LEU:HB2	1:88:A:PRO:HA	11	0.19	0.03	0.17
(1,1552)	1:103:A:ALA:HB3	1:88:A:PRO:HA	11	0.19	0.03	0.17
(1,1552)	1:103:A:ALA:HB1	1:88:A:PRO:HA	11	0.19	0.03	0.17
(1,3196)	1:31:A:MET:HA	1:30:A:ILE:HG21	11	0.19	0.04	0.18
(1,3196)	1:31:A:MET:HA	1:30:A:ILE:HG23	11	0.19	0.04	0.18
(1,3196)	1:31:A:MET:HA	1:30:A:ILE:HG22	11	0.19	0.04	0.18
(1,459)	1:37:A:ASN:HB3	1:41:A:GLN:H	11	0.17	0.06	0.15
(1,547)	1:40:A:VAL:HB	1:42:A:GLU:H	11	0.16	0.06	0.13
(1,547)	1:39:A:ASP:HB2	1:42:A:GLU:H	11	0.16	0.06	0.13
(2,13)	1:43:A:ARG:H	1:39:A:ASP:O	11	0.13	0.02	0.13
(1,637)	1:44:A:LEU:HD21	1:43:A:ARG:H	10	0.73	0.24	0.86
(1,637)	1:40:A:VAL:HG23	1:43:A:ARG:H	10	0.73	0.24	0.86
(1,637)	1:89:A:LEU:HD22	1:43:A:ARG:H	10	0.73	0.24	0.86
(1,637)	1:89:A:LEU:HD21	1:43:A:ARG:H	10	0.73	0.24	0.86
(1,637)	1:40:A:VAL:HG21	1:43:A:ARG:H	10	0.73	0.24	0.86
(1,637)	1:40:A:VAL:HG22	1:43:A:ARG:H	10	0.73	0.24	0.86
(1,637)	1:89:A:LEU:HD12	1:43:A:ARG:H	10	0.73	0.24	0.86
(1,3383)	1:42:A:GLU:HG3	1:43:A:ARG:HD2	10	0.6	0.35	0.6
(1,3646)	1:62:A:GLN:HB2	1:59:A:ASP:HB3	10	0.43	0.22	0.42
(1,3646)	1:62:A:GLN:HB2	1:59:A:ASP:HB2	10	0.43	0.22	0.42
(1,3646)	1:136:A:GLU:HB2	1:137:A:ASP:HB3	10	0.43	0.22	0.42
(1,3646)	1:138:A:MET:HB2	1:137:A:ASP:HB3	10	0.43	0.22	0.42
(1,1737)	1:54:A:LEU:HD22	1:41:A:GLN:HA	10	0.3	0.17	0.25
(1,1737)	1:44:A:LEU:HD21	1:41:A:GLN:HA	10	0.3	0.17	0.25
(1,1737)	1:44:A:LEU:HD22	1:41:A:GLN:HA	10	0.3	0.17	0.25
(1,1737)	1:54:A:LEU:HD21	1:41:A:GLN:HA	10	0.3	0.17	0.25
(1,1737)	1:54:A:LEU:HD13	1:41:A:GLN:HA	10	0.3	0.17	0.25
(1,1737)	1:44:A:LEU:HD23	1:41:A:GLN:HA	10	0.3	0.17	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1737)	1:54:A:LEU:HD11	1:41:A:GLN:HA	10	0.3	0.17	0.25
(1,1915)	1:70:A:PHE:HE2	1:26:A:LEU:HA	10	0.25	0.09	0.23
(1,755)	1:116:A:GLN:HB3	1:115:A:MET:H	10	0.22	0.09	0.21
(1,972)	1:96:A:PRO:HD2	1:97:A:ALA:H	10	0.16	0.03	0.16
(1,844)	1:36:A:ALA:HA	1:41:A:GLN:HE21	10	0.16	0.04	0.15
(1,996)	1:70:A:PHE:HB2	1:73:A:ALA:H	10	0.14	0.03	0.13
(1,2347)	1:73:A:ALA:H	1:70:A:PHE:HB2	10	0.14	0.04	0.13
(1,2347)	1:72:A:GLN:H	1:70:A:PHE:HB2	10	0.14	0.04	0.13
(1,1102)	1:60:A:GLU:HG2	1:58:A:ALA:H	9	0.69	0.26	0.74
(1,1102)	1:56:A:GLN:HB3	1:58:A:ALA:H	9	0.69	0.26	0.74
(1,827)	1:4:A:ILE:HD13	1:2:A:ASN:HD21	9	0.63	0.14	0.64
(1,827)	1:4:A:ILE:HD12	1:2:A:ASN:HD21	9	0.63	0.14	0.64
(1,827)	1:4:A:ILE:HD11	1:2:A:ASN:HD21	9	0.63	0.14	0.64
(1,1007)	1:30:A:ILE:HD11	1:119:A:ALA:H	9	0.62	0.42	0.54
(1,1007)	1:30:A:ILE:HD13	1:119:A:ALA:H	9	0.62	0.42	0.54
(1,1007)	1:30:A:ILE:HD12	1:119:A:ALA:H	9	0.62	0.42	0.54
(1,683)	1:40:A:VAL:HG11	1:37:A:ASN:HD21	9	0.58	0.27	0.62
(1,683)	1:40:A:VAL:HG13	1:37:A:ASN:HD21	9	0.58	0.27	0.62
(1,683)	1:40:A:VAL:HG12	1:37:A:ASN:HD21	9	0.58	0.27	0.62
(1,683)	1:128:A:THR:HG21	1:128:A:THR:H	9	0.58	0.27	0.62
(1,683)	1:128:A:THR:HG22	1:128:A:THR:H	9	0.58	0.27	0.62
(1,1158)	1:119:A:ALA:HB3	1:120:A:LYS:H	9	0.5	0.23	0.51
(1,1158)	1:119:A:ALA:HB2	1:120:A:LYS:H	9	0.5	0.23	0.51
(1,1158)	1:119:A:ALA:HB1	1:120:A:LYS:H	9	0.5	0.23	0.51
(1,3464)	1:31:A:MET:HG2	1:26:A:LEU:HD11	9	0.36	0.12	0.35
(1,3464)	1:31:A:MET:HG3	1:26:A:LEU:HD11	9	0.36	0.12	0.35
(1,3464)	1:31:A:MET:HG2	1:26:A:LEU:HD12	9	0.36	0.12	0.35
(1,3464)	1:31:A:MET:HG2	1:26:A:LEU:HD13	9	0.36	0.12	0.35
(1,3464)	1:31:A:MET:HG3	1:26:A:LEU:HD12	9	0.36	0.12	0.35
(1,316)	1:47:A:TYR:HE2	1:80:A:ALA:H	9	0.32	0.14	0.34
(1,221)	1:96:A:PRO:HD2	1:99:A:ALA:H	9	0.32	0.13	0.34
(1,2252)	1:41:A:GLN:HA	1:54:A:LEU:HB3	9	0.29	0.15	0.25
(1,2252)	1:53:A:SER:HB3	1:54:A:LEU:HB2	9	0.29	0.15	0.25
(1,3473)	1:55:A:PRO:HD2	1:65:A:LEU:HD22	9	0.28	0.13	0.32
(1,3473)	1:55:A:PRO:HD2	1:65:A:LEU:HD21	9	0.28	0.13	0.32
(1,3473)	1:55:A:PRO:HD2	1:65:A:LEU:HD23	9	0.28	0.13	0.32
(1,3271)	1:55:A:PRO:HB2	1:61:A:ILE:HD12	9	0.25	0.07	0.25
(1,3271)	1:31:A:MET:HE2	1:34:A:ILE:HD11	9	0.25	0.07	0.25
(1,3271)	1:31:A:MET:HE1	1:34:A:ILE:HD12	9	0.25	0.07	0.25
(1,3271)	1:31:A:MET:HE3	1:34:A:ILE:HD11	9	0.25	0.07	0.25
(1,3271)	1:55:A:PRO:HB2	1:61:A:ILE:HD13	9	0.25	0.07	0.25
(1,3271)	1:31:A:MET:HE3	1:34:A:ILE:HD12	9	0.25	0.07	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3271)	1:31:A:MET:HE2	1:34:A:ILE:HD12	9	0.25	0.07	0.25
(1,3271)	1:31:A:MET:HE3	1:34:A:ILE:HD13	9	0.25	0.07	0.25
(1,3758)	1:26:A:LEU:HD13	1:77:A:PHE:HD1	9	0.25	0.12	0.2
(1,3758)	1:26:A:LEU:HD11	1:77:A:PHE:HD1	9	0.25	0.12	0.2
(1,3758)	1:26:A:LEU:HD12	1:77:A:PHE:HD1	9	0.25	0.12	0.2
(1,504)	1:65:A:LEU:HD12	1:74:A:LEU:H	9	0.25	0.11	0.23
(1,504)	1:65:A:LEU:HD13	1:74:A:LEU:H	9	0.25	0.11	0.23
(1,504)	1:22:A:LEU:HD12	1:74:A:LEU:H	9	0.25	0.11	0.23
(1,504)	1:22:A:LEU:HD13	1:74:A:LEU:H	9	0.25	0.11	0.23
(1,504)	1:65:A:LEU:HD11	1:74:A:LEU:H	9	0.25	0.11	0.23
(1,3094)	1:56:A:GLN:HB3	1:57:A:THR:HG22	9	0.23	0.11	0.18
(1,3094)	1:56:A:GLN:HB3	1:57:A:THR:HG23	9	0.23	0.11	0.18
(1,3094)	1:56:A:GLN:HB3	1:57:A:THR:HG21	9	0.23	0.11	0.18
(1,3493)	1:76:A:MET:HG2	1:74:A:LEU:HD13	9	0.23	0.06	0.22
(1,3493)	1:76:A:MET:HG2	1:74:A:LEU:HD12	9	0.23	0.06	0.22
(1,3493)	1:76:A:MET:HG2	1:74:A:LEU:HD11	9	0.23	0.06	0.22
(1,3536)	1:44:A:LEU:H	1:80:A:ALA:HB2	9	0.21	0.09	0.14
(1,3536)	1:44:A:LEU:H	1:80:A:ALA:HB3	9	0.21	0.09	0.14
(1,3536)	1:44:A:LEU:H	1:80:A:ALA:HB1	9	0.21	0.09	0.14
(1,3536)	1:85:A:GLN:H	1:80:A:ALA:HB1	9	0.21	0.09	0.14
(1,3536)	1:85:A:GLN:H	1:80:A:ALA:HB2	9	0.21	0.09	0.14
(1,3457)	1:105:A:LYS:H	1:81:A:LEU:HD22	9	0.18	0.05	0.15
(1,3457)	1:105:A:LYS:H	1:81:A:LEU:HD23	9	0.18	0.05	0.15
(1,3457)	1:105:A:LYS:H	1:81:A:LEU:HD21	9	0.18	0.05	0.15
(1,129)	1:122:A:GLU:HB3	1:122:A:GLU:H	9	0.17	0.06	0.15
(1,129)	1:121:A:PRO:HB2	1:122:A:GLU:H	9	0.17	0.06	0.15
(1,3188)	1:57:A:THR:HA	1:58:A:ALA:HB2	9	0.16	0.06	0.14
(1,3188)	1:57:A:THR:HA	1:58:A:ALA:HB1	9	0.16	0.06	0.14
(1,3188)	1:57:A:THR:HA	1:58:A:ALA:HB3	9	0.16	0.06	0.14
(1,571)	1:25:A:VAL:HA	1:25:A:VAL:H	9	0.12	0.01	0.11
(1,3519)	1:109:A:GLU:HG3	1:20:A:VAL:HG12	8	0.54	0.23	0.55
(1,3519)	1:109:A:GLU:HG3	1:20:A:VAL:HG13	8	0.54	0.23	0.55
(1,3519)	1:109:A:GLU:HG3	1:20:A:VAL:HG11	8	0.54	0.23	0.55
(1,3519)	1:19:A:GLN:HG2	1:20:A:VAL:HG12	8	0.54	0.23	0.55
(1,1276)	1:95:A:LEU:HB3	1:91:A:CYS:H	8	0.47	0.06	0.48
(1,1276)	1:92:A:GLN:HB3	1:91:A:CYS:H	8	0.47	0.06	0.48
(1,3192)	1:33:A:PRO:HA	1:58:A:ALA:HB2	8	0.33	0.14	0.3
(1,3192)	1:33:A:PRO:HA	1:58:A:ALA:HB3	8	0.33	0.14	0.3
(1,3192)	1:33:A:PRO:HA	1:58:A:ALA:HB1	8	0.33	0.14	0.3
(1,2297)	1:99:A:ALA:HB2	1:111:A:PHE:HB3	8	0.28	0.12	0.29
(1,2297)	1:114:A:ALA:HB2	1:111:A:PHE:HB3	8	0.28	0.12	0.29
(1,2297)	1:99:A:ALA:HB1	1:111:A:PHE:HB3	8	0.28	0.12	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2297)	1:114:A:ALA:HB3	1:111:A:PHE:HB3	8	0.28	0.12	0.29
(1,2297)	1:99:A:ALA:HB3	1:111:A:PHE:HB3	8	0.28	0.12	0.29
(1,2265)	1:37:A:ASN:HB3	1:89:A:LEU:HB3	8	0.26	0.08	0.28
(1,2265)	1:43:A:ARG:HD3	1:89:A:LEU:HB3	8	0.26	0.08	0.28
(1,3177)	1:27:A:THR:H	1:30:A:ILE:HG21	8	0.25	0.1	0.23
(1,3177)	1:27:A:THR:H	1:30:A:ILE:HG23	8	0.25	0.1	0.23
(1,3177)	1:27:A:THR:H	1:30:A:ILE:HG22	8	0.25	0.1	0.23
(1,1565)	1:64:A:THR:HG23	1:61:A:ILE:HA	8	0.22	0.13	0.18
(1,1565)	1:64:A:THR:HG22	1:61:A:ILE:HA	8	0.22	0.13	0.18
(1,1565)	1:64:A:THR:HG21	1:61:A:ILE:HA	8	0.22	0.13	0.18
(1,1997)	1:108:A:VAL:HG11	1:82:A:ALA:HA	8	0.2	0.06	0.22
(1,1997)	1:108:A:VAL:HG12	1:82:A:ALA:HA	8	0.2	0.06	0.22
(1,1997)	1:108:A:VAL:HG13	1:82:A:ALA:HA	8	0.2	0.06	0.22
(1,699)	1:64:A:THR:HB	1:63:A:ASN:H	8	0.18	0.04	0.2
(1,699)	1:59:A:ASP:HA	1:63:A:ASN:H	8	0.18	0.04	0.2
(1,1654)	1:100:A:VAL:HA	1:91:A:CYS:HA	8	0.13	0.01	0.12
(1,1079)	1:107:A:ASP:HB2	1:106:A:GLY:H	8	0.12	0.02	0.12
(1,916)	1:84:A:GLY:HA3	1:84:A:GLY:H	8	0.12	0.01	0.11
(1,3533)	1:111:A:PHE:HD2	1:115:A:MET:HE2	7	0.45	0.09	0.46
(1,3533)	1:111:A:PHE:HD2	1:115:A:MET:HE1	7	0.45	0.09	0.46
(1,3533)	1:111:A:PHE:HD2	1:115:A:MET:HE3	7	0.45	0.09	0.46
(1,3533)	1:93:A:PHE:HD2	1:115:A:MET:HE3	7	0.45	0.09	0.46
(1,3533)	1:93:A:PHE:HD2	1:115:A:MET:HE2	7	0.45	0.09	0.46
(1,760)	1:96:A:PRO:HB2	1:118:A:ASN:HD22	7	0.35	0.13	0.34
(1,1168)	1:132:A:LYS:HB3	1:134:A:GLU:H	7	0.34	0.17	0.33
(1,1168)	1:131:A:LYS:HB3	1:134:A:GLU:H	7	0.34	0.17	0.33
(1,3314)	1:93:A:PHE:HB2	1:34:A:ILE:HA	7	0.33	0.17	0.25
(1,3314)	1:40:A:VAL:HB	1:34:A:ILE:HA	7	0.33	0.17	0.25
(1,3782)	1:103:A:ALA:HA	1:111:A:PHE:HZ	7	0.29	0.14	0.27
(1,3541)	1:103:A:ALA:HB2	1:90:A:MET:HE3	7	0.28	0.09	0.32
(1,3541)	1:103:A:ALA:HB3	1:90:A:MET:HE3	7	0.28	0.09	0.32
(1,3541)	1:89:A:LEU:HB2	1:90:A:MET:HE1	7	0.28	0.09	0.32
(1,3541)	1:103:A:ALA:HB2	1:90:A:MET:HE2	7	0.28	0.09	0.32
(1,3541)	1:89:A:LEU:HB2	1:90:A:MET:HE2	7	0.28	0.09	0.32
(1,2189)	1:93:A:PHE:HZ	1:89:A:LEU:HB2	7	0.26	0.11	0.24
(1,2189)	1:92:A:GLN:HE22	1:89:A:LEU:HB2	7	0.26	0.11	0.24
(1,2768)	1:64:A:THR:HG22	1:60:A:GLU:HB2	7	0.26	0.12	0.24
(1,2768)	1:64:A:THR:HG21	1:60:A:GLU:HB2	7	0.26	0.12	0.24
(1,2768)	1:64:A:THR:HG23	1:60:A:GLU:HB2	7	0.26	0.12	0.24
(1,2768)	1:57:A:THR:HG22	1:60:A:GLU:HB2	7	0.26	0.12	0.24
(1,2542)	1:107:A:ASP:HA	1:108:A:VAL:HB	7	0.24	0.03	0.22
(1,2542)	1:9:A:ASN:HA	1:10:A:VAL:HB	7	0.24	0.03	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1569)	1:35:A:LEU:HD23	1:28:A:PRO:HA	7	0.23	0.08	0.21
(1,1569)	1:35:A:LEU:HD21	1:28:A:PRO:HA	7	0.23	0.08	0.21
(1,1569)	1:74:A:LEU:HD12	1:28:A:PRO:HA	7	0.23	0.08	0.21
(1,2842)	1:105:A:LYS:H	1:105:A:LYS:HG3	7	0.2	0.06	0.22
(1,3704)	1:102:A:ALA:HB1	1:111:A:PHE:HD1	7	0.2	0.05	0.2
(1,3704)	1:102:A:ALA:HB3	1:111:A:PHE:HD1	7	0.2	0.05	0.2
(1,3704)	1:102:A:ALA:HB2	1:111:A:PHE:HD1	7	0.2	0.05	0.2
(1,3707)	1:95:A:LEU:HD11	1:93:A:PHE:HD2	7	0.2	0.05	0.2
(1,3707)	1:95:A:LEU:HD12	1:93:A:PHE:HD2	7	0.2	0.05	0.2
(1,3707)	1:26:A:LEU:HD21	1:111:A:PHE:HD2	7	0.2	0.05	0.2
(1,3707)	1:95:A:LEU:HD13	1:93:A:PHE:HD2	7	0.2	0.05	0.2
(1,965)	1:36:A:ALA:H	1:38:A:ALA:H	7	0.18	0.05	0.18
(1,965)	1:93:A:PHE:HE1	1:38:A:ALA:H	7	0.18	0.05	0.18
(1,3554)	1:83:A:SER:HB2	1:80:A:ALA:HB3	7	0.18	0.08	0.16
(1,3554)	1:43:A:ARG:HA	1:80:A:ALA:HB3	7	0.18	0.08	0.16
(1,3554)	1:43:A:ARG:HA	1:80:A:ALA:HB1	7	0.18	0.08	0.16
(1,3554)	1:43:A:ARG:HA	1:80:A:ALA:HB2	7	0.18	0.08	0.16
(1,3446)	1:93:A:PHE:H	1:91:A:CYS:HB2	7	0.15	0.03	0.16
(1,3446)	1:89:A:LEU:H	1:91:A:CYS:HB2	7	0.15	0.03	0.16
(1,2900)	1:27:A:THR:HB	1:28:A:PRO:HG2	7	0.13	0.02	0.13
(1,2900)	1:27:A:THR:HA	1:28:A:PRO:HG2	7	0.13	0.02	0.13
(1,2063)	1:32:A:ALA:HB1	1:33:A:PRO:HD2	7	0.13	0.02	0.13
(1,2063)	1:32:A:ALA:HB2	1:33:A:PRO:HD2	7	0.13	0.02	0.13
(1,2063)	1:32:A:ALA:HB3	1:33:A:PRO:HD2	7	0.13	0.02	0.13
(1,2277)	1:60:A:GLU:HB2	1:63:A:ASN:HB3	6	0.82	0.27	0.94
(1,2277)	1:60:A:GLU:HG3	1:63:A:ASN:HB3	6	0.82	0.27	0.94
(1,1310)	1:40:A:VAL:HG21	1:37:A:ASN:HD21	6	0.55	0.34	0.52
(1,1310)	1:89:A:LEU:HD22	1:86:A:LEU:H	6	0.55	0.34	0.52
(1,1310)	1:89:A:LEU:HD23	1:86:A:LEU:H	6	0.55	0.34	0.52
(1,1310)	1:40:A:VAL:HG22	1:37:A:ASN:HD21	6	0.55	0.34	0.52
(1,1310)	1:89:A:LEU:HD21	1:86:A:LEU:H	6	0.55	0.34	0.52
(1,1365)	1:88:A:PRO:HG3	1:104:A:ASN:HD22	6	0.51	0.26	0.48
(1,1365)	1:101:A:GLU:HB2	1:104:A:ASN:HD22	6	0.51	0.26	0.48
(1,3615)	1:29:A:GLU:HG3	1:30:A:ILE:HD12	6	0.5	0.17	0.56
(1,3615)	1:29:A:GLU:HG3	1:30:A:ILE:HD13	6	0.5	0.17	0.56
(1,3615)	1:31:A:MET:HG2	1:30:A:ILE:HD12	6	0.5	0.17	0.56
(1,2030)	1:41:A:GLN:HE22	1:55:A:PRO:HD2	6	0.43	0.11	0.44
(1,2030)	1:62:A:GLN:HE22	1:28:A:PRO:HD3	6	0.43	0.11	0.44
(1,3388)	1:20:A:VAL:HA	1:21:A:ASP:HB2	6	0.4	0.18	0.44
(1,2369)	1:43:A:ARG:H	1:42:A:GLU:HG2	6	0.39	0.1	0.42
(1,2369)	1:43:A:ARG:HE	1:42:A:GLU:HG3	6	0.39	0.1	0.42
(1,2369)	1:43:A:ARG:H	1:42:A:GLU:HG3	6	0.39	0.1	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,905)	1:58:A:ALA:HB3	1:62:A:GLN:HE22	6	0.38	0.15	0.44
(1,905)	1:58:A:ALA:HB2	1:62:A:GLN:HE22	6	0.38	0.15	0.44
(1,775)	1:62:A:GLN:HB2	1:63:A:ASN:HD22	6	0.36	0.09	0.37
(1,2067)	1:99:A:ALA:HB1	1:96:A:PRO:HD2	6	0.35	0.08	0.33
(1,2067)	1:99:A:ALA:HB3	1:96:A:PRO:HD2	6	0.35	0.08	0.33
(1,2067)	1:27:A:THR:HG21	1:28:A:PRO:HD3	6	0.35	0.08	0.33
(1,2644)	1:89:A:LEU:HD21	1:92:A:GLN:HG3	6	0.35	0.09	0.38
(1,2644)	1:89:A:LEU:HD22	1:92:A:GLN:HG3	6	0.35	0.09	0.38
(1,2644)	1:89:A:LEU:HD23	1:92:A:GLN:HG3	6	0.35	0.09	0.38
(1,3379)	1:86:A:LEU:HA	1:43:A:ARG:HD3	6	0.3	0.11	0.27
(1,3663)	1:46:A:PRO:HB3	1:47:A:TYR:HD2	6	0.27	0.17	0.23
(1,3663)	1:44:A:LEU:HG	1:47:A:TYR:HD2	6	0.27	0.17	0.23
(1,1251)	1:92:A:GLN:HE22	1:92:A:GLN:H	6	0.22	0.06	0.21
(1,2785)	1:74:A:LEU:HD11	1:31:A:MET:HB2	6	0.21	0.09	0.18
(1,2785)	1:74:A:LEU:HD13	1:31:A:MET:HB2	6	0.21	0.09	0.18
(1,2785)	1:74:A:LEU:HD12	1:31:A:MET:HB2	6	0.21	0.09	0.18
(1,263)	1:102:A:ALA:HB3	1:109:A:GLU:H	6	0.21	0.05	0.22
(1,263)	1:102:A:ALA:HB1	1:109:A:GLU:H	6	0.21	0.05	0.22
(1,263)	1:102:A:ALA:HB2	1:109:A:GLU:H	6	0.21	0.05	0.22
(1,1129)	1:44:A:LEU:HA	1:79:A:ALA:H	6	0.21	0.04	0.21
(1,3591)	1:44:A:LEU:HA	1:76:A:MET:HE1	6	0.19	0.07	0.18
(1,3591)	1:44:A:LEU:HA	1:76:A:MET:HE2	6	0.19	0.07	0.18
(1,3591)	1:44:A:LEU:HA	1:76:A:MET:HE3	6	0.19	0.07	0.18
(1,3286)	1:89:A:LEU:HG	1:40:A:VAL:HA	6	0.19	0.06	0.17
(1,47)	1:20:A:VAL:HG11	1:21:A:ASP:H	6	0.19	0.05	0.2
(1,47)	1:20:A:VAL:HG12	1:21:A:ASP:H	6	0.19	0.05	0.2
(1,47)	1:20:A:VAL:HG13	1:21:A:ASP:H	6	0.19	0.05	0.2
(1,3735)	1:34:A:ILE:HB	1:93:A:PHE:HZ	6	0.16	0.05	0.18
(1,3735)	1:89:A:LEU:HB2	1:93:A:PHE:HZ	6	0.16	0.05	0.18
(1,3682)	1:91:A:CYS:HA	1:93:A:PHE:HD2	6	0.16	0.05	0.16
(1,3682)	1:89:A:LEU:HA	1:93:A:PHE:HD2	6	0.16	0.05	0.16
(1,2622)	1:64:A:THR:HG22	1:55:A:PRO:HB2	5	0.59	0.3	0.64
(1,2622)	1:95:A:LEU:HD23	1:115:A:MET:HG3	5	0.59	0.3	0.64
(1,2622)	1:30:A:ILE:HG13	1:115:A:MET:HG3	5	0.59	0.3	0.64
(1,2622)	1:99:A:ALA:HB3	1:115:A:MET:HG3	5	0.59	0.3	0.64
(1,2622)	1:95:A:LEU:HD22	1:115:A:MET:HG3	5	0.59	0.3	0.64
(1,803)	1:46:A:PRO:HG2	1:85:A:GLN:HE21	5	0.47	0.25	0.43
(1,1306)	1:49:A:PRO:HD2	1:53:A:SER:H	5	0.38	0.16	0.33
(1,1067)	1:124:A:LYS:HB3	1:126:A:GLY:H	5	0.3	0.06	0.33
(1,1067)	1:124:A:LYS:HB2	1:126:A:GLY:H	5	0.3	0.06	0.33
(1,3187)	1:115:A:MET:HA	1:99:A:ALA:HB1	5	0.28	0.17	0.18
(1,3187)	1:115:A:MET:HA	1:99:A:ALA:HB3	5	0.28	0.17	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3187)	1:115:A:MET:HA	1:99:A:ALA:HB2	5	0.28	0.17	0.18
(1,3449)	1:94:A:GLY:HA2	1:91:A:CYS:HB2	5	0.26	0.13	0.21
(1,3449)	1:97:A:ALA:HA	1:91:A:CYS:HB2	5	0.26	0.13	0.21
(1,1122)	1:114:A:ALA:HB1	1:119:A:ALA:H	5	0.23	0.07	0.21
(1,1122)	1:99:A:ALA:HB2	1:119:A:ALA:H	5	0.23	0.07	0.21
(1,1122)	1:114:A:ALA:HB3	1:119:A:ALA:H	5	0.23	0.07	0.21
(1,1122)	1:99:A:ALA:HB1	1:119:A:ALA:H	5	0.23	0.07	0.21
(1,2930)	1:103:A:ALA:HA	1:105:A:LYS:HG2	5	0.22	0.07	0.24
(1,3167)	1:70:A:PHE:HD1	1:61:A:ILE:HG23	5	0.19	0.09	0.14
(1,3167)	1:70:A:PHE:HD1	1:61:A:ILE:HG21	5	0.19	0.09	0.14
(1,3167)	1:70:A:PHE:HD1	1:61:A:ILE:HG22	5	0.19	0.09	0.14
(1,3167)	1:70:A:PHE:HE1	1:61:A:ILE:HG22	5	0.19	0.09	0.14
(1,1078)	1:81:A:LEU:HG	1:106:A:GLY:H	5	0.17	0.07	0.14
(1,1556)	1:36:A:ALA:HB2	1:33:A:PRO:HA	5	0.17	0.05	0.15
(1,1556)	1:36:A:ALA:HB1	1:33:A:PRO:HA	5	0.17	0.05	0.15
(1,765)	1:114:A:ALA:HB3	1:115:A:MET:H	5	0.16	0.05	0.2
(1,765)	1:114:A:ALA:HB1	1:115:A:MET:H	5	0.16	0.05	0.2
(1,765)	1:114:A:ALA:HB2	1:115:A:MET:H	5	0.16	0.05	0.2
(1,3141)	1:89:A:LEU:H	1:90:A:MET:HE1	5	0.16	0.06	0.13
(1,3141)	1:89:A:LEU:H	1:90:A:MET:HE3	5	0.16	0.06	0.13
(1,3403)	1:79:A:ALA:HB2	1:47:A:TYR:HB2	5	0.16	0.06	0.13
(1,3403)	1:79:A:ALA:HB1	1:47:A:TYR:HB2	5	0.16	0.06	0.13
(1,3403)	1:79:A:ALA:HB3	1:47:A:TYR:HB2	5	0.16	0.06	0.13
(1,261)	1:22:A:LEU:HG	1:23:A:ALA:H	5	0.15	0.04	0.14
(1,1009)	1:116:A:GLN:HG3	1:119:A:ALA:H	5	0.14	0.04	0.12
(1,3775)	1:46:A:PRO:HG2	1:47:A:TYR:HE2	5	0.14	0.03	0.13
(1,145)	1:19:A:GLN:HA	1:19:A:GLN:H	5	0.11	0.0	0.11
(1,2640)	1:95:A:LEU:HD12	1:115:A:MET:HG3	4	0.9	0.19	0.82
(1,2640)	1:30:A:ILE:HD11	1:115:A:MET:HG3	4	0.9	0.19	0.82
(1,2640)	1:65:A:LEU:HD13	1:55:A:PRO:HB2	4	0.9	0.19	0.82
(1,2640)	1:30:A:ILE:HD12	1:115:A:MET:HG3	4	0.9	0.19	0.82
(1,2116)	1:86:A:LEU:HD12	1:43:A:ARG:HD3	4	0.46	0.22	0.45
(1,2116)	1:86:A:LEU:HD11	1:43:A:ARG:HD3	4	0.46	0.22	0.45
(1,2116)	1:86:A:LEU:HD13	1:43:A:ARG:HD2	4	0.46	0.22	0.45
(1,2875)	1:93:A:PHE:HZ	1:86:A:LEU:HD13	4	0.4	0.27	0.29
(1,2875)	1:47:A:TYR:HD2	1:44:A:LEU:HD13	4	0.4	0.27	0.29
(1,2875)	1:47:A:TYR:HD2	1:44:A:LEU:HD12	4	0.4	0.27	0.29
(1,1246)	1:44:A:LEU:HD13	1:42:A:GLU:H	4	0.36	0.3	0.24
(1,1246)	1:44:A:LEU:HD12	1:42:A:GLU:H	4	0.36	0.3	0.24
(1,2782)	1:26:A:LEU:HD22	1:115:A:MET:HB3	4	0.36	0.13	0.33
(1,2782)	1:26:A:LEU:HD23	1:115:A:MET:HB3	4	0.36	0.13	0.33
(1,341)	1:44:A:LEU:HD11	1:80:A:ALA:H	4	0.35	0.4	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,341)	1:86:A:LEU:HD11	1:80:A:ALA:H	4	0.35	0.4	0.12
(1,341)	1:44:A:LEU:HD12	1:80:A:ALA:H	4	0.35	0.4	0.12
(1,2972)	1:43:A:ARG:HD3	1:86:A:LEU:HD12	4	0.33	0.14	0.31
(1,2972)	1:43:A:ARG:HD3	1:86:A:LEU:HD11	4	0.33	0.14	0.31
(1,2972)	1:77:A:PHE:HB3	1:44:A:LEU:HD11	4	0.33	0.14	0.31
(1,1543)	1:31:A:MET:HB3	1:28:A:PRO:HA	4	0.32	0.16	0.28
(1,2575)	1:14:A:PRO:HD3	1:14:A:PRO:HB2	4	0.31	0.1	0.3
(1,2575)	1:14:A:PRO:HD2	1:14:A:PRO:HB2	4	0.31	0.1	0.3
(1,2575)	1:11:A:PRO:HD2	1:11:A:PRO:HB2	4	0.31	0.1	0.3
(1,2871)	1:80:A:ALA:H	1:44:A:LEU:HD11	4	0.26	0.25	0.12
(1,2871)	1:87:A:GLY:H	1:86:A:LEU:HD12	4	0.26	0.25	0.12
(1,2871)	1:80:A:ALA:H	1:44:A:LEU:HD12	4	0.26	0.25	0.12
(1,1676)	1:42:A:GLU:HG3	1:42:A:GLU:HA	4	0.26	0.08	0.26
(1,1676)	1:98:A:GLU:HG2	1:98:A:GLU:HA	4	0.26	0.08	0.26
(1,2620)	1:64:A:THR:HG21	1:60:A:GLU:HB2	4	0.26	0.14	0.22
(1,2620)	1:64:A:THR:HG22	1:60:A:GLU:HB2	4	0.26	0.14	0.22
(1,3470)	1:80:A:ALA:HA	1:44:A:LEU:HD21	4	0.25	0.08	0.25
(1,3470)	1:35:A:LEU:HA	1:44:A:LEU:HD22	4	0.25	0.08	0.25
(1,3470)	1:35:A:LEU:HA	1:44:A:LEU:HD23	4	0.25	0.08	0.25
(1,2669)	1:86:A:LEU:H	1:43:A:ARG:HG3	4	0.23	0.11	0.24
(1,2940)	1:55:A:PRO:HD3	1:54:A:LEU:HD21	4	0.22	0.06	0.21
(1,2940)	1:55:A:PRO:HD3	1:65:A:LEU:HD13	4	0.22	0.06	0.21
(1,2914)	1:45:A:LEU:HA	1:48:A:LEU:HD22	4	0.18	0.07	0.15
(1,2914)	1:45:A:LEU:HA	1:48:A:LEU:HD11	4	0.18	0.07	0.15
(1,1309)	1:54:A:LEU:HG	1:53:A:SER:H	4	0.18	0.06	0.16
(1,1309)	1:48:A:LEU:HG	1:53:A:SER:H	4	0.18	0.06	0.16
(1,2450)	1:86:A:LEU:H	1:85:A:GLN:HG3	4	0.18	0.06	0.15
(1,1462)	1:56:A:GLN:HB2	1:57:A:THR:HB	4	0.17	0.05	0.17
(1,1462)	1:60:A:GLU:HB3	1:57:A:THR:HB	4	0.17	0.05	0.17
(1,3416)	1:114:A:ALA:HA	1:117:A:ASN:HB3	4	0.16	0.05	0.15
(1,1525)	1:31:A:MET:HA	1:34:A:ILE:HA	4	0.16	0.06	0.16
(1,2934)	1:71:A:GLN:HA	1:74:A:LEU:HG	4	0.15	0.02	0.16
(1,2934)	1:93:A:PHE:HB3	1:95:A:LEU:HD21	4	0.15	0.02	0.16
(1,2934)	1:93:A:PHE:HB3	1:95:A:LEU:HD23	4	0.15	0.02	0.16
(1,411)	1:40:A:VAL:HG21	1:39:A:ASP:H	4	0.15	0.04	0.14
(1,411)	1:40:A:VAL:HG22	1:39:A:ASP:H	4	0.15	0.04	0.14
(1,2042)	1:104:A:ASN:HB3	1:87:A:GLY:HA2	4	0.15	0.03	0.15
(1,784)	1:32:A:ALA:HB1	1:31:A:MET:H	4	0.15	0.02	0.15
(1,784)	1:32:A:ALA:HB2	1:31:A:MET:H	4	0.15	0.02	0.15
(1,941)	1:27:A:THR:HG23	1:27:A:THR:H	4	0.14	0.01	0.14
(1,941)	1:27:A:THR:HG21	1:27:A:THR:H	4	0.14	0.01	0.14
(1,2997)	1:43:A:ARG:HB2	1:86:A:LEU:HD11	4	0.14	0.03	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2997)	1:43:A:ARG:HB2	1:86:A:LEU:HD13	4	0.14	0.03	0.13
(1,2506)	1:52:A:GLU:H	1:52:A:GLU:HB3	4	0.12	0.01	0.12
(1,2506)	1:60:A:GLU:H	1:60:A:GLU:HB2	4	0.12	0.01	0.12
(1,909)	1:54:A:LEU:HD13	1:41:A:GLN:HE22	3	0.65	0.14	0.59
(1,909)	1:61:A:ILE:HG23	1:62:A:GLN:HE22	3	0.65	0.14	0.59
(1,909)	1:61:A:ILE:HG21	1:62:A:GLN:HE22	3	0.65	0.14	0.59
(1,404)	1:96:A:PRO:HG2	1:118:A:ASN:H	3	0.53	0.26	0.6
(1,759)	1:60:A:GLU:HB3	1:63:A:ASN:HD21	3	0.5	0.15	0.56
(1,759)	1:62:A:GLN:HB2	1:63:A:ASN:HD21	3	0.5	0.15	0.56
(1,886)	1:61:A:ILE:HG22	1:62:A:GLN:HE21	3	0.48	0.04	0.47
(1,886)	1:61:A:ILE:HG21	1:62:A:GLN:HE21	3	0.48	0.04	0.47
(1,886)	1:89:A:LEU:HD13	1:92:A:GLN:HE21	3	0.48	0.04	0.47
(1,617)	1:92:A:GLN:HE22	1:37:A:ASN:HD22	3	0.38	0.12	0.44
(1,617)	1:93:A:PHE:HZ	1:37:A:ASN:HD22	3	0.38	0.12	0.44
(1,1457)	1:20:A:VAL:HG11	1:109:A:GLU:H	3	0.34	0.16	0.31
(1,1457)	1:20:A:VAL:HG12	1:109:A:GLU:H	3	0.34	0.16	0.31
(1,1457)	1:20:A:VAL:HG13	1:109:A:GLU:H	3	0.34	0.16	0.31
(1,1457)	1:20:A:VAL:HG21	1:109:A:GLU:H	3	0.34	0.16	0.31
(1,1457)	1:20:A:VAL:HG22	1:109:A:GLU:H	3	0.34	0.16	0.31
(1,1457)	1:20:A:VAL:HG23	1:109:A:GLU:H	3	0.34	0.16	0.31
(1,75)	1:132:A:LYS:HB2	1:132:A:LYS:H	3	0.3	0.15	0.21
(1,75)	1:131:A:LYS:HB3	1:132:A:LYS:H	3	0.3	0.15	0.21
(1,1175)	1:110:A:ALA:HB2	1:114:A:ALA:H	3	0.29	0.09	0.32
(1,1175)	1:113:A:LYS:HG2	1:114:A:ALA:H	3	0.29	0.09	0.32
(1,3756)	1:22:A:LEU:HB3	1:77:A:PHE:HD1	3	0.29	0.12	0.27
(1,767)	1:100:A:VAL:HG23	1:90:A:MET:H	3	0.29	0.16	0.24
(1,767)	1:100:A:VAL:HG22	1:90:A:MET:H	3	0.29	0.16	0.24
(1,684)	1:48:A:LEU:HD11	1:53:A:SER:H	3	0.25	0.16	0.18
(1,684)	1:65:A:LEU:HD22	1:53:A:SER:H	3	0.25	0.16	0.18
(1,684)	1:48:A:LEU:HD23	1:53:A:SER:H	3	0.25	0.16	0.18
(1,3273)	1:96:A:PRO:HD2	1:115:A:MET:HE2	3	0.25	0.06	0.28
(1,3273)	1:96:A:PRO:HD2	1:115:A:MET:HE3	3	0.25	0.06	0.28
(1,1571)	1:61:A:ILE:HG23	1:28:A:PRO:HA	3	0.23	0.11	0.17
(1,1571)	1:61:A:ILE:HG22	1:28:A:PRO:HA	3	0.23	0.11	0.17
(1,1398)	1:27:A:THR:HG22	1:24:A:SER:H	3	0.23	0.07	0.23
(1,1398)	1:27:A:THR:HG21	1:24:A:SER:H	3	0.23	0.07	0.23
(1,1398)	1:27:A:THR:HG23	1:24:A:SER:H	3	0.23	0.07	0.23
(1,377)	1:100:A:VAL:HG21	1:104:A:ASN:H	3	0.22	0.07	0.18
(1,377)	1:100:A:VAL:HG22	1:104:A:ASN:H	3	0.22	0.07	0.18
(1,2398)	1:98:A:GLU:HA	1:98:A:GLU:HG2	3	0.21	0.01	0.21
(1,2894)	1:77:A:PHE:HE1	1:35:A:LEU:HD21	3	0.2	0.05	0.22
(1,2894)	1:77:A:PHE:HE2	1:35:A:LEU:HD21	3	0.2	0.05	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3392)	1:87:A:GLY:HA2	1:86:A:LEU:HB2	3	0.2	0.04	0.18
(1,3392)	1:40:A:VAL:HA	1:86:A:LEU:HB2	3	0.2	0.04	0.18
(1,2496)	1:65:A:LEU:H	1:62:A:GLN:HG2	3	0.19	0.09	0.15
(1,2976)	1:111:A:PHE:HB3	1:81:A:LEU:HD23	3	0.19	0.08	0.14
(1,2976)	1:111:A:PHE:HB3	1:81:A:LEU:HD22	3	0.19	0.08	0.14
(1,2976)	1:111:A:PHE:HB3	1:81:A:LEU:HD21	3	0.19	0.08	0.14
(1,164)	1:133:A:ASP:HB3	1:133:A:ASP:H	3	0.18	0.08	0.15
(1,3052)	1:20:A:VAL:H	1:20:A:VAL:HG13	3	0.18	0.03	0.19
(1,3052)	1:20:A:VAL:H	1:20:A:VAL:HG11	3	0.18	0.03	0.19
(1,3052)	1:20:A:VAL:H	1:20:A:VAL:HG12	3	0.18	0.03	0.19
(1,3422)	1:28:A:PRO:HD3	1:29:A:GLU:HG2	3	0.16	0.03	0.16
(1,588)	1:114:A:ALA:HB2	1:98:A:GLU:H	3	0.15	0.03	0.14
(1,588)	1:99:A:ALA:HB2	1:98:A:GLU:H	3	0.15	0.03	0.14
(1,588)	1:114:A:ALA:HB3	1:98:A:GLU:H	3	0.15	0.03	0.14
(1,2324)	1:25:A:VAL:HG13	1:26:A:LEU:HB2	3	0.15	0.03	0.16
(1,2313)	1:81:A:LEU:HG	1:111:A:PHE:HB2	3	0.15	0.02	0.14
(1,3668)	1:46:A:PRO:HB2	1:47:A:TYR:HD2	3	0.15	0.03	0.13
(1,3792)	1:40:A:VAL:HG22	1:93:A:PHE:HE2	3	0.14	0.02	0.15
(1,3792)	1:89:A:LEU:HD22	1:93:A:PHE:HE2	3	0.14	0.02	0.15
(1,3792)	1:40:A:VAL:HG21	1:93:A:PHE:HE2	3	0.14	0.02	0.15
(1,2309)	1:22:A:LEU:HB2	1:26:A:LEU:HB3	3	0.14	0.04	0.12
(1,272)	1:115:A:MET:H	1:116:A:GLN:H	3	0.13	0.03	0.12
(1,173)	1:19:A:GLN:HB3	1:19:A:GLN:H	3	0.13	0.0	0.13
(1,3352)	1:111:A:PHE:HB2	1:112:A:ALA:HA	3	0.12	0.02	0.11
(1,1550)	1:33:A:PRO:HB3	1:34:A:ILE:HA	3	0.12	0.01	0.12
(1,1956)	1:96:A:PRO:HB3	1:95:A:LEU:HA	3	0.12	0.02	0.11
(1,1866)	1:28:A:PRO:HB3	1:62:A:GLN:HA	3	0.12	0.01	0.11
(1,3232)	1:31:A:MET:HG2	1:30:A:ILE:HG23	2	0.72	0.12	0.72
(1,3232)	1:31:A:MET:HG2	1:30:A:ILE:HG21	2	0.72	0.12	0.72
(1,1361)	1:88:A:PRO:HA	1:104:A:ASN:HD21	2	0.56	0.1	0.56
(1,2281)	1:61:A:ILE:HB	1:35:A:LEU:HB2	2	0.54	0.07	0.54
(1,172)	1:136:A:GLU:HB2	1:136:A:GLU:H	2	0.44	0.09	0.44
(1,172)	1:136:A:GLU:HB3	1:136:A:GLU:H	2	0.44	0.09	0.44
(1,770)	1:64:A:THR:HB	1:63:A:ASN:HD22	2	0.38	0.16	0.38
(1,770)	1:59:A:ASP:HA	1:63:A:ASN:HD22	2	0.38	0.16	0.38
(1,1759)	1:137:A:ASP:H	1:136:A:GLU:HA	2	0.38	0.03	0.38
(1,3242)	1:95:A:LEU:HD11	1:115:A:MET:HE3	2	0.37	0.09	0.37
(1,3242)	1:95:A:LEU:HD12	1:115:A:MET:HE3	2	0.37	0.09	0.37
(1,3394)	1:33:A:PRO:HG2	1:93:A:PHE:HB3	2	0.37	0.08	0.37
(1,1510)	1:80:A:ALA:H	1:78:A:SER:HB2	2	0.34	0.06	0.34
(1,1838)	1:18:A:GLN:HG2	1:18:A:GLN:HA	2	0.32	0.12	0.32
(1,3418)	1:98:A:GLU:HA	1:101:A:GLU:HG3	2	0.3	0.01	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3557)	1:40:A:VAL:HA	1:80:A:ALA:HB3	2	0.3	0.13	0.3
(1,3557)	1:47:A:TYR:HB3	1:80:A:ALA:HB1	2	0.3	0.13	0.3
(1,1153)	1:19:A:GLN:HB2	1:19:A:GLN:H	2	0.3	0.1	0.3
(1,997)	1:123:A:GLN:HG2	1:124:A:LYS:H	2	0.3	0.07	0.3
(1,997)	1:122:A:GLU:HG2	1:124:A:LYS:H	2	0.3	0.07	0.3
(1,95)	1:119:A:ALA:HB1	1:119:A:ALA:H	2	0.28	0.04	0.28
(1,95)	1:119:A:ALA:HB2	1:119:A:ALA:H	2	0.28	0.04	0.28
(1,1432)	1:119:A:ALA:HB2	1:117:A:ASN:H	2	0.27	0.04	0.27
(1,209)	1:131:A:LYS:HB2	1:131:A:LYS:H	2	0.25	0.02	0.25
(1,423)	1:105:A:LYS:HG2	1:107:A:ASP:H	2	0.22	0.06	0.22
(1,2911)	1:53:A:SER:HA	1:48:A:LEU:HD12	2	0.22	0.09	0.22
(1,402)	1:42:A:GLU:HB2	1:39:A:ASP:H	2	0.22	0.06	0.22
(1,2715)	1:123:A:GLN:HA	1:123:A:GLN:HB3	2	0.22	0.02	0.22
(1,299)	1:114:A:ALA:HB3	1:116:A:GLN:H	2	0.22	0.01	0.22
(1,299)	1:114:A:ALA:HB1	1:116:A:GLN:H	2	0.22	0.01	0.22
(1,3191)	1:107:A:ASP:HA	1:82:A:ALA:HB2	2	0.21	0.05	0.21
(1,3191)	1:107:A:ASP:HA	1:82:A:ALA:HB1	2	0.21	0.05	0.21
(1,1887)	1:25:A:VAL:HG22	1:112:A:ALA:HA	2	0.2	0.0	0.2
(1,1887)	1:26:A:LEU:HD22	1:112:A:ALA:HA	2	0.2	0.0	0.2
(1,1468)	1:44:A:LEU:H	1:40:A:VAL:HA	2	0.2	0.09	0.2
(1,1257)	1:27:A:THR:HG22	1:25:A:VAL:H	2	0.19	0.06	0.19
(1,165)	1:130:A:ASP:HB3	1:130:A:ASP:H	2	0.18	0.06	0.18
(1,2856)	1:92:A:GLN:HE22	1:89:A:LEU:HD21	2	0.18	0.06	0.18
(1,2856)	1:92:A:GLN:HE22	1:89:A:LEU:HD23	2	0.18	0.06	0.18
(1,3428)	1:35:A:LEU:H	1:40:A:VAL:HB	2	0.18	0.06	0.18
(1,2906)	1:114:A:ALA:HA	1:113:A:LYS:HG2	2	0.17	0.0	0.17
(1,3574)	1:57:A:THR:H	1:61:A:ILE:HD13	2	0.17	0.05	0.17
(1,3574)	1:57:A:THR:H	1:61:A:ILE:HD11	2	0.17	0.05	0.17
(1,97)	1:35:A:LEU:HD22	1:73:A:ALA:H	2	0.16	0.02	0.16
(1,1061)	1:73:A:ALA:HB2	1:72:A:GLN:HE21	2	0.16	0.02	0.16
(1,1061)	1:73:A:ALA:HB3	1:72:A:GLN:HE21	2	0.16	0.02	0.16
(1,1072)	1:80:A:ALA:HB3	1:84:A:GLY:H	2	0.16	0.02	0.16
(1,1072)	1:81:A:LEU:HG	1:84:A:GLY:H	2	0.16	0.02	0.16
(1,1131)	1:47:A:TYR:HB2	1:79:A:ALA:H	2	0.16	0.05	0.16
(1,2629)	1:100:A:VAL:HG23	1:90:A:MET:HG3	2	0.16	0.01	0.16
(1,2629)	1:100:A:VAL:HG22	1:90:A:MET:HG3	2	0.16	0.01	0.16
(1,3442)	1:99:A:ALA:HB2	1:96:A:PRO:HB2	2	0.15	0.03	0.15
(1,3517)	1:77:A:PHE:HA	1:35:A:LEU:HD13	2	0.14	0.03	0.14
(1,3517)	1:77:A:PHE:HA	1:35:A:LEU:HD11	2	0.14	0.03	0.14
(1,1760)	1:136:A:GLU:H	1:136:A:GLU:HA	2	0.14	0.01	0.14
(1,2238)	1:70:A:PHE:HA	1:74:A:LEU:HB2	2	0.14	0.0	0.14
(1,2954)	1:61:A:ILE:HA	1:35:A:LEU:HD21	2	0.14	0.01	0.14

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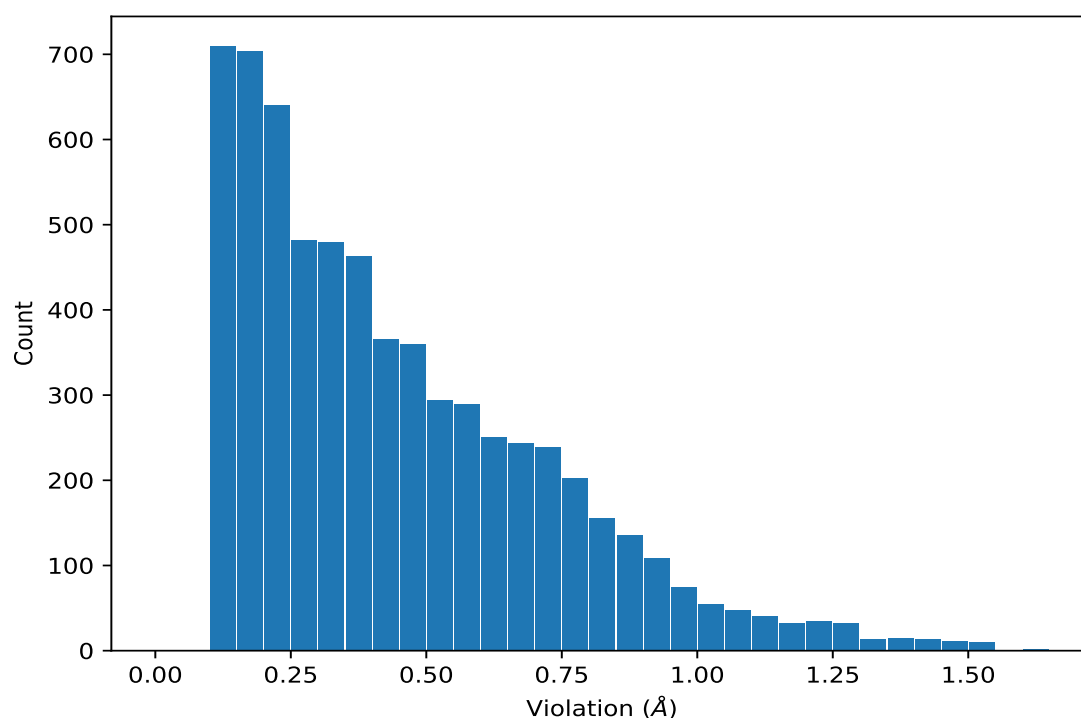
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2954)	1:28:A:PRO:HA	1:35:A:LEU:HD21	2	0.14	0.01	0.14
(1,884)	1:92:A:GLN:HG3	1:92:A:GLN:HE21	2	0.14	0.01	0.14
(1,884)	1:82:A:ALA:HB2	1:83:A:SER:H	2	0.14	0.01	0.14
(1,790)	1:7:A:THR:HA	1:7:A:THR:H	2	0.13	0.01	0.13
(1,1064)	1:92:A:GLN:HB3	1:94:A:GLY:H	2	0.13	0.0	0.13
(1,1541)	1:121:A:PRO:HB2	1:121:A:PRO:HA	2	0.13	0.02	0.13
(1,1541)	1:11:A:PRO:HB2	1:11:A:PRO:HA	2	0.13	0.02	0.13
(1,2543)	1:121:A:PRO:HA	1:121:A:PRO:HB2	2	0.13	0.02	0.13
(1,2543)	1:11:A:PRO:HA	1:11:A:PRO:HB2	2	0.13	0.02	0.13
(1,3769)	1:44:A:LEU:HA	1:47:A:TYR:HE2	2	0.13	0.01	0.13
(1,879)	1:62:A:GLN:HB3	1:62:A:GLN:HE21	2	0.12	0.01	0.12
(1,879)	1:92:A:GLN:HG2	1:92:A:GLN:HE21	2	0.12	0.01	0.12
(1,3592)	1:85:A:GLN:HB3	1:80:A:ALA:HB2	2	0.12	0.02	0.12
(1,3592)	1:85:A:GLN:HB3	1:80:A:ALA:HB1	2	0.12	0.02	0.12
(1,146)	1:136:A:GLU:HA	1:136:A:GLU:H	2	0.12	0.01	0.12
(1,2822)	1:91:A:CYS:H	1:100:A:VAL:HG12	2	0.12	0.01	0.12
(1,2822)	1:95:A:LEU:H	1:100:A:VAL:HG13	2	0.12	0.01	0.12
(1,3221)	1:93:A:PHE:HB3	1:34:A:ILE:HG23	2	0.12	0.02	0.12
(1,3145)	1:115:A:MET:H	1:115:A:MET:HE1	2	0.12	0.0	0.12
(1,3145)	1:115:A:MET:H	1:115:A:MET:HE2	2	0.12	0.0	0.12
(1,3145)	1:115:A:MET:H	1:115:A:MET:HE3	2	0.12	0.0	0.12

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)
(1,3558)	1:90:A:MET:HG2	1:99:A:ALA:HB2	19	1.62
(1,2769)	1:114:A:ALA:HB1	1:115:A:MET:HB2	12	1.61
(1,3558)	1:118:A:ASN:HB3	1:114:A:ALA:HB1	2	1.58
(1,2769)	1:99:A:ALA:HB1	1:115:A:MET:HB2	4	1.54
(1,2769)	1:114:A:ALA:HB1	1:115:A:MET:HB2	11	1.53
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD23	2	1.52
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD21	9	1.52
(1,2769)	1:114:A:ALA:HB3	1:115:A:MET:HB2	5	1.52
(1,3641)	1:73:A:ALA:H	1:74:A:LEU:HD23	18	1.51
(1,1007)	1:30:A:ILE:HD12	1:119:A:ALA:H	19	1.51
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD22	14	1.5
(1,2769)	1:30:A:ILE:HG13	1:29:A:GLU:HB3	2	1.5
(1,337)	1:103:A:ALA:HB1	1:102:A:ALA:H	20	1.5
(1,2769)	1:95:A:LEU:HD22	1:115:A:MET:HB3	8	1.49
(1,1572)	1:48:A:LEU:HD23	1:53:A:SER:HB2	20	1.49
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD22	8	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3504)	1:31:A:MET:HE1	1:86:A:LEU:HD22	9	1.47
(1,721)	1:45:A:LEU:HD23	1:47:A:TYR:H	19	1.47
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	4	1.47
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD22	15	1.46
(1,721)	1:45:A:LEU:HD21	1:47:A:TYR:H	9	1.46
(1,337)	1:110:A:ALA:HB3	1:102:A:ALA:H	1	1.46
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD22	5	1.45
(1,3504)	1:31:A:MET:HE2	1:86:A:LEU:HD23	1	1.45
(1,3558)	1:118:A:ASN:HB3	1:114:A:ALA:HB2	7	1.44
(1,2769)	1:99:A:ALA:HB2	1:115:A:MET:HB2	9	1.44
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD22	3	1.43
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD23	16	1.43
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD21	11	1.42
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD21	17	1.42
(1,721)	1:45:A:LEU:HD23	1:47:A:TYR:H	20	1.42
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	11	1.42
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	16	1.42
(1,337)	1:103:A:ALA:HB3	1:102:A:ALA:H	12	1.41
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD22	12	1.4
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD23	19	1.4
(1,721)	1:45:A:LEU:HD22	1:47:A:TYR:H	16	1.4
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD23	20	1.39
(1,721)	1:45:A:LEU:HD23	1:47:A:TYR:H	17	1.39
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	14	1.39
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD23	1	1.38
(1,3504)	1:31:A:MET:HE2	1:86:A:LEU:HD21	10	1.38
(1,721)	1:45:A:LEU:HD22	1:47:A:TYR:H	15	1.38
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD22	7	1.37
(1,721)	1:45:A:LEU:HD23	1:47:A:TYR:H	12	1.37
(1,337)	1:103:A:ALA:HB3	1:102:A:ALA:H	8	1.37
(1,2769)	1:114:A:ALA:HB1	1:115:A:MET:HB2	17	1.36
(1,721)	1:45:A:LEU:HD21	1:47:A:TYR:H	8	1.36
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	5	1.36
(1,1154)	1:108:A:VAL:HG22	1:111:A:PHE:H	8	1.35
(1,721)	1:45:A:LEU:HD22	1:47:A:TYR:H	10	1.35
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	18	1.35
(1,3238)	1:40:A:VAL:HG22	1:90:A:MET:HE2	5	1.34
(1,2912)	1:43:A:ARG:HA	1:89:A:LEU:HD23	18	1.34
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	16	1.33
(1,721)	1:45:A:LEU:HD22	1:47:A:TYR:H	4	1.33
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD22	10	1.32
(1,3238)	1:40:A:VAL:HG23	1:90:A:MET:HE2	16	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1295)	1:40:A:VAL:HG13	1:43:A:ARG:H	9	1.31
(1,3565)	1:101:A:GLU:HB2	1:102:A:ALA:HB1	4	1.3
(1,3558)	1:118:A:ASN:HB3	1:114:A:ALA:HB1	15	1.3
(1,721)	1:45:A:LEU:HD21	1:47:A:TYR:H	6	1.3
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	2	1.3
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	13	1.3
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	19	1.3
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD23	4	1.29
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD22	6	1.29
(1,2769)	1:114:A:ALA:HB3	1:115:A:MET:HB2	18	1.29
(1,2693)	1:36:A:ALA:H	1:33:A:PRO:HG2	6	1.29
(1,1345)	1:35:A:LEU:HD21	1:31:A:MET:H	10	1.29
(1,2769)	1:30:A:ILE:HG13	1:29:A:GLU:HB3	15	1.28
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	20	1.28
(1,1154)	1:108:A:VAL:HG22	1:111:A:PHE:H	20	1.28
(1,721)	1:45:A:LEU:HD21	1:47:A:TYR:H	3	1.28
(1,721)	1:48:A:LEU:HD11	1:47:A:TYR:H	11	1.28
(1,721)	1:45:A:LEU:HD22	1:47:A:TYR:H	18	1.28
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	9	1.28
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	10	1.28
(1,3238)	1:89:A:LEU:HD23	1:90:A:MET:HE2	12	1.27
(1,1295)	1:80:A:ALA:HB2	1:43:A:ARG:H	18	1.27
(1,1295)	1:40:A:VAL:HG11	1:43:A:ARG:H	20	1.27
(1,1154)	1:108:A:VAL:HG21	1:111:A:PHE:H	7	1.27
(1,721)	1:44:A:LEU:HD21	1:47:A:TYR:H	1	1.27
(1,3641)	1:72:A:GLN:H	1:74:A:LEU:HD22	13	1.26
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	5	1.26
(1,1572)	1:48:A:LEU:HD11	1:53:A:SER:HB2	2	1.26
(1,1295)	1:40:A:VAL:HG11	1:43:A:ARG:H	8	1.26
(1,1295)	1:80:A:ALA:HB2	1:43:A:ARG:H	12	1.26
(1,1295)	1:40:A:VAL:HG12	1:43:A:ARG:H	14	1.26
(1,1154)	1:108:A:VAL:HG22	1:111:A:PHE:H	9	1.26
(1,1154)	1:108:A:VAL:HG23	1:111:A:PHE:H	11	1.26
(1,1154)	1:108:A:VAL:HG21	1:111:A:PHE:H	14	1.26
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	17	1.26
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD22	5	1.25
(1,1154)	1:108:A:VAL:HG21	1:111:A:PHE:H	15	1.25
(1,1154)	1:108:A:VAL:HG23	1:111:A:PHE:H	16	1.25
(1,721)	1:45:A:LEU:HD23	1:47:A:TYR:H	5	1.25
(1,3568)	1:114:A:ALA:HB3	1:102:A:ALA:HB2	7	1.24
(1,1572)	1:48:A:LEU:HD11	1:53:A:SER:HB2	12	1.24
(1,1295)	1:40:A:VAL:HG11	1:43:A:ARG:H	7	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,721)	1:45:A:LEU:HD23	1:47:A:TYR:H	2	1.24
(1,505)	1:25:A:VAL:HG21	1:117:A:ASN:H	1	1.24
(1,3504)	1:31:A:MET:HE1	1:86:A:LEU:HD22	17	1.23
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD23	12	1.23
(1,2640)	1:95:A:LEU:HD12	1:115:A:MET:HG3	19	1.23
(1,1295)	1:80:A:ALA:HB3	1:43:A:ARG:H	2	1.23
(1,1154)	1:108:A:VAL:HG21	1:111:A:PHE:H	10	1.23
(1,1154)	1:108:A:VAL:HG23	1:111:A:PHE:H	19	1.23
(1,721)	1:48:A:LEU:HD11	1:47:A:TYR:H	14	1.23
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD22	13	1.22
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD23	16	1.22
(1,1295)	1:80:A:ALA:HB3	1:43:A:ARG:H	11	1.22
(1,721)	1:45:A:LEU:HD21	1:47:A:TYR:H	7	1.22
(1,3238)	1:40:A:VAL:HG23	1:90:A:MET:HE2	4	1.21
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD22	8	1.21
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD21	17	1.21
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD23	19	1.21
(1,1295)	1:40:A:VAL:HG11	1:43:A:ARG:H	4	1.21
(1,1295)	1:80:A:ALA:HB2	1:43:A:ARG:H	17	1.21
(1,1154)	1:108:A:VAL:HG22	1:111:A:PHE:H	4	1.21
(1,1154)	1:108:A:VAL:HG21	1:111:A:PHE:H	5	1.21
(1,505)	1:25:A:VAL:HG22	1:117:A:ASN:H	12	1.21
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	15	1.21
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD22	4	1.2
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD21	9	1.2
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD23	11	1.2
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD23	14	1.2
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD23	20	1.2
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	11	1.2
(1,1295)	1:40:A:VAL:HG11	1:43:A:ARG:H	1	1.2
(1,1295)	1:40:A:VAL:HG13	1:43:A:ARG:H	16	1.2
(1,505)	1:25:A:VAL:HG22	1:117:A:ASN:H	5	1.2
(1,3627)	1:41:A:GLN:HB2	1:39:A:ASP:HB2	11	1.19
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD11	6	1.19
(1,2898)	1:77:A:PHE:HE2	1:81:A:LEU:HD23	1	1.19
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD22	15	1.19
(1,1295)	1:80:A:ALA:HB1	1:43:A:ARG:H	19	1.19
(1,3561)	1:31:A:MET:HG2	1:34:A:ILE:HG23	17	1.18
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD21	2	1.18
(1,1295)	1:80:A:ALA:HB2	1:43:A:ARG:H	13	1.18
(1,3627)	1:33:A:PRO:HG2	1:93:A:PHE:HB2	12	1.17
(1,3568)	1:99:A:ALA:HB3	1:102:A:ALA:HB3	6	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3561)	1:90:A:MET:HB3	1:34:A:ILE:HG22	1	1.17
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD13	18	1.17
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD22	3	1.17
(1,2898)	1:77:A:PHE:HE2	1:81:A:LEU:HD23	7	1.17
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD21	18	1.17
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	2	1.17
(1,1572)	1:48:A:LEU:HD13	1:53:A:SER:HB2	13	1.17
(1,1154)	1:108:A:VAL:HG23	1:111:A:PHE:H	3	1.17
(1,1154)	1:108:A:VAL:HG22	1:20:A:VAL:H	18	1.17
(1,721)	1:45:A:LEU:HD21	1:47:A:TYR:H	13	1.17
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	3	1.17
(1,2912)	1:43:A:ARG:HA	1:89:A:LEU:HD22	4	1.16
(1,1154)	1:108:A:VAL:HG21	1:111:A:PHE:H	2	1.16
(1,1154)	1:108:A:VAL:HG21	1:111:A:PHE:H	6	1.16
(1,1154)	1:108:A:VAL:HG21	1:111:A:PHE:H	13	1.16
(1,3383)	1:42:A:GLU:HG3	1:43:A:ARG:HD2	18	1.15
(1,3272)	1:96:A:PRO:HD3	1:115:A:MET:HE3	13	1.15
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD13	12	1.15
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	3	1.15
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	9	1.15
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	10	1.15
(1,1213)	1:34:A:ILE:HG22	1:41:A:GLN:H	17	1.15
(1,3627)	1:33:A:PRO:HG2	1:93:A:PHE:HB2	8	1.14
(1,3558)	1:118:A:ASN:HB3	1:114:A:ALA:HB3	11	1.14
(1,3238)	1:40:A:VAL:HG21	1:90:A:MET:HE3	15	1.14
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD21	10	1.14
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	1	1.14
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	18	1.14
(1,1572)	1:48:A:LEU:HD23	1:53:A:SER:HB2	11	1.14
(1,1135)	1:74:A:LEU:HD12	1:79:A:ALA:H	18	1.14
(1,505)	1:25:A:VAL:HG23	1:117:A:ASN:H	15	1.14
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD11	3	1.13
(1,2912)	1:50:A:SER:HA	1:48:A:LEU:HD21	5	1.13
(1,1213)	1:34:A:ILE:HG23	1:41:A:GLN:H	19	1.13
(1,795)	1:65:A:LEU:HD21	1:64:A:THR:H	15	1.13
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD23	10	1.12
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD23	14	1.12
(1,2898)	1:77:A:PHE:HE1	1:81:A:LEU:HD22	6	1.12
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	19	1.12
(1,1572)	1:48:A:LEU:HD13	1:53:A:SER:HB2	1	1.12
(1,1572)	1:48:A:LEU:HD22	1:53:A:SER:HB2	17	1.12
(1,1213)	1:34:A:ILE:HG23	1:41:A:GLN:H	14	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1213)	1:34:A:ILE:HG22	1:41:A:GLN:H	16	1.12
(1,505)	1:25:A:VAL:HG22	1:117:A:ASN:H	4	1.12
(1,3568)	1:74:A:LEU:HG	1:31:A:MET:HE3	5	1.11
(1,3238)	1:89:A:LEU:HD23	1:90:A:MET:HE3	7	1.11
(1,2699)	1:93:A:PHE:HD1	1:34:A:ILE:HG13	20	1.11
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	12	1.11
(1,1295)	1:80:A:ALA:HB2	1:43:A:ARG:H	5	1.11
(1,1295)	1:80:A:ALA:HB3	1:43:A:ARG:H	10	1.11
(1,1154)	1:108:A:VAL:HG22	1:111:A:PHE:H	17	1.11
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	7	1.11
(1,3627)	1:90:A:MET:HE1	1:93:A:PHE:HB2	3	1.1
(1,3568)	1:99:A:ALA:HB3	1:102:A:ALA:HB3	9	1.1
(1,3238)	1:89:A:LEU:HD23	1:90:A:MET:HE3	14	1.1
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD11	1	1.1
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD12	17	1.1
(1,2699)	1:93:A:PHE:HD1	1:34:A:ILE:HG13	6	1.1
(1,1295)	1:80:A:ALA:HB2	1:43:A:ARG:H	3	1.1
(1,1295)	1:80:A:ALA:HB3	1:43:A:ARG:H	6	1.1
(1,1295)	1:80:A:ALA:HB1	1:43:A:ARG:H	15	1.1
(1,1213)	1:34:A:ILE:HG23	1:41:A:GLN:H	5	1.1
(1,3380)	1:80:A:ALA:HB1	1:43:A:ARG:HD2	4	1.09
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG22	5	1.09
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD23	15	1.09
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD12	15	1.09
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	10	1.09
(1,2277)	1:60:A:GLU:HB2	1:63:A:ASN:HB3	4	1.09
(1,1213)	1:34:A:ILE:HG23	1:41:A:GLN:H	3	1.09
(1,1213)	1:34:A:ILE:HG21	1:41:A:GLN:H	7	1.09
(1,1213)	1:34:A:ILE:HG22	1:41:A:GLN:H	8	1.09
(1,1213)	1:34:A:ILE:HG23	1:41:A:GLN:H	12	1.09
(1,1213)	1:34:A:ILE:HG21	1:41:A:GLN:H	18	1.09
(1,1170)	1:74:A:LEU:HG	1:23:A:ALA:H	6	1.09
(1,505)	1:25:A:VAL:HG21	1:117:A:ASN:H	3	1.09
(1,3568)	1:114:A:ALA:HB3	1:102:A:ALA:HB1	8	1.08
(1,3568)	1:99:A:ALA:HB3	1:102:A:ALA:HB1	18	1.08
(1,3117)	1:119:A:ALA:H	1:115:A:MET:HE1	3	1.08
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD23	8	1.08
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD11	2	1.08
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD11	16	1.08
(1,1572)	1:48:A:LEU:HD12	1:53:A:SER:HB2	9	1.08
(1,1135)	1:44:A:LEU:HD12	1:79:A:ALA:H	14	1.08
(1,307)	1:25:A:VAL:HG22	1:114:A:ALA:H	1	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3238)	1:40:A:VAL:HG23	1:90:A:MET:HE1	18	1.07
(1,3238)	1:89:A:LEU:HD21	1:90:A:MET:HE1	19	1.07
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG22	9	1.07
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD22	9	1.07
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD21	13	1.07
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD13	7	1.07
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD13	14	1.07
(1,1572)	1:48:A:LEU:HD11	1:53:A:SER:HB2	3	1.07
(1,3238)	1:40:A:VAL:HG22	1:90:A:MET:HE2	11	1.06
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD22	16	1.06
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD12	5	1.06
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	2	1.06
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	4	1.06
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	11	1.06
(1,2699)	1:93:A:PHE:HD1	1:34:A:ILE:HG13	19	1.06
(1,1213)	1:34:A:ILE:HG23	1:41:A:GLN:H	6	1.06
(1,1213)	1:34:A:ILE:HG22	1:41:A:GLN:H	15	1.06
(1,337)	1:95:A:LEU:HB2	1:100:A:VAL:H	6	1.06
(1,3568)	1:74:A:LEU:HG	1:31:A:MET:HE1	15	1.05
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD21	2	1.05
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD22	17	1.05
(1,2622)	1:95:A:LEU:HD23	1:115:A:MET:HG3	3	1.05
(1,1213)	1:34:A:ILE:HG21	1:41:A:GLN:H	20	1.05
(1,1007)	1:30:A:ILE:HD12	1:119:A:ALA:H	14	1.05
(1,365)	1:101:A:GLU:HG3	1:103:A:ALA:H	17	1.05
(1,3627)	1:41:A:GLN:HB2	1:39:A:ASP:HB2	20	1.04
(1,3558)	1:118:A:ASN:HB3	1:114:A:ALA:HB3	4	1.04
(1,3272)	1:30:A:ILE:HA	1:115:A:MET:HE3	8	1.04
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG23	13	1.04
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD22	20	1.04
(1,2872)	1:43:A:ARG:H	1:86:A:LEU:HD11	1	1.04
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	14	1.04
(1,2699)	1:93:A:PHE:HD2	1:34:A:ILE:HG13	12	1.04
(1,1213)	1:34:A:ILE:HG23	1:41:A:GLN:H	11	1.04
(1,341)	1:86:A:LEU:HD11	1:80:A:ALA:H	1	1.04
(1,3568)	1:99:A:ALA:HB2	1:102:A:ALA:HB3	4	1.03
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG22	16	1.03
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD22	5	1.03
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD22	11	1.03
(1,2915)	1:21:A:ASP:HA	1:22:A:LEU:HD13	8	1.03
(1,2915)	1:54:A:LEU:HA	1:54:A:LEU:HD11	9	1.03
(1,2277)	1:60:A:GLU:HB2	1:63:A:ASN:HB3	8	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,795)	1:65:A:LEU:HD23	1:64:A:THR:H	5	1.03
(1,795)	1:65:A:LEU:HD23	1:64:A:THR:H	16	1.03
(1,505)	1:25:A:VAL:HG21	1:117:A:ASN:H	2	1.03
(1,3117)	1:116:A:GLN:H	1:115:A:MET:HE1	20	1.02
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	8	1.02
(1,1703)	1:114:A:ALA:HB3	1:98:A:GLU:HA	12	1.02
(1,1365)	1:88:A:PRO:HG3	1:104:A:ASN:HD22	6	1.02
(1,868)	1:65:A:LEU:HD22	1:69:A:GLN:HE21	9	1.02
(1,795)	1:65:A:LEU:HD22	1:64:A:THR:H	4	1.02
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	14	1.01
(1,3380)	1:40:A:VAL:HG11	1:43:A:ARG:HD3	8	1.01
(1,3272)	1:96:A:PRO:HD3	1:115:A:MET:HE2	19	1.01
(1,3238)	1:40:A:VAL:HG23	1:90:A:MET:HE2	10	1.01
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG22	8	1.01
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD22	3	1.01
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD23	4	1.01
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	19	1.01
(1,1102)	1:56:A:GLN:HB3	1:58:A:ALA:H	17	1.01
(1,795)	1:65:A:LEU:HD23	1:64:A:THR:H	3	1.01
(1,795)	1:65:A:LEU:HD22	1:64:A:THR:H	19	1.01
(1,3734)	1:90:A:MET:HE2	1:93:A:PHE:HZ	5	1.0
(1,3734)	1:90:A:MET:HE2	1:93:A:PHE:HZ	19	1.0
(1,3733)	1:90:A:MET:HE2	1:93:A:PHE:HZ	5	1.0
(1,3733)	1:90:A:MET:HE2	1:93:A:PHE:HZ	19	1.0
(1,3627)	1:41:A:GLN:HB2	1:39:A:ASP:HB2	7	1.0
(1,3568)	1:74:A:LEU:HG	1:31:A:MET:HE3	13	1.0
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG21	1	1.0
(1,3498)	1:102:A:ALA:HB2	1:81:A:LEU:HD12	7	1.0
(1,2915)	1:54:A:LEU:HA	1:54:A:LEU:HD13	3	1.0
(1,1170)	1:74:A:LEU:HG	1:23:A:ALA:H	16	1.0
(1,1135)	1:44:A:LEU:HD11	1:79:A:ALA:H	3	1.0
(1,1027)	1:100:A:VAL:HG21	1:92:A:GLN:H	11	1.0
(1,932)	1:103:A:ALA:HB2	1:106:A:GLY:H	6	1.0
(1,932)	1:103:A:ALA:HB1	1:106:A:GLY:H	13	1.0
(1,795)	1:65:A:LEU:HD22	1:64:A:THR:H	9	1.0
(1,425)	1:57:A:THR:HG22	1:60:A:GLU:H	15	1.0
(1,307)	1:25:A:VAL:HG23	1:114:A:ALA:H	13	1.0
(1,3646)	1:62:A:GLN:HB2	1:59:A:ASP:HB3	20	0.99
(1,3627)	1:90:A:MET:HE1	1:93:A:PHE:HB2	17	0.99
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG23	12	0.99
(1,2915)	1:21:A:ASP:HA	1:22:A:LEU:HD13	14	0.99
(1,1734)	1:44:A:LEU:HD11	1:76:A:MET:HA	14	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1213)	1:34:A:ILE:HG21	1:41:A:GLN:H	4	0.99
(1,1170)	1:74:A:LEU:HG	1:23:A:ALA:H	12	0.99
(1,868)	1:65:A:LEU:HD23	1:69:A:GLN:HE21	11	0.99
(1,3253)	1:32:A:ALA:H	1:34:A:ILE:HD13	18	0.98
(1,3238)	1:40:A:VAL:HG21	1:90:A:MET:HE2	9	0.98
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD21	6	0.98
(1,1734)	1:44:A:LEU:HD11	1:76:A:MET:HA	16	0.98
(1,1135)	1:44:A:LEU:HD11	1:79:A:ALA:H	5	0.98
(1,1135)	1:44:A:LEU:HD12	1:79:A:ALA:H	16	0.98
(1,1014)	1:86:A:LEU:HD11	1:40:A:VAL:H	14	0.98
(1,82)	1:34:A:ILE:HD13	1:32:A:ALA:H	18	0.98
(1,3568)	1:99:A:ALA:HB3	1:102:A:ALA:HB1	1	0.97
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD21	18	0.97
(1,2915)	1:54:A:LEU:HA	1:54:A:LEU:HD13	4	0.97
(1,2915)	1:54:A:LEU:HA	1:54:A:LEU:HD12	12	0.97
(1,2915)	1:21:A:ASP:HA	1:22:A:LEU:HD13	16	0.97
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD12	4	0.97
(1,1213)	1:34:A:ILE:HG22	1:41:A:GLN:H	13	0.97
(1,1135)	1:44:A:LEU:HD11	1:79:A:ALA:H	12	0.97
(1,1135)	1:44:A:LEU:HD12	1:79:A:ALA:H	17	0.97
(1,1135)	1:44:A:LEU:HD12	1:79:A:ALA:H	20	0.97
(1,1102)	1:60:A:GLU:HG2	1:58:A:ALA:H	3	0.97
(1,1027)	1:100:A:VAL:HG21	1:92:A:GLN:H	20	0.97
(1,1014)	1:86:A:LEU:HD11	1:40:A:VAL:H	16	0.97
(1,795)	1:65:A:LEU:HD23	1:64:A:THR:H	7	0.97
(1,505)	1:25:A:VAL:HG21	1:117:A:ASN:H	16	0.97
(1,452)	1:44:A:LEU:HD12	1:45:A:LEU:H	1	0.97
(1,425)	1:57:A:THR:HG23	1:60:A:GLU:H	4	0.97
(1,3712)	1:61:A:ILE:HG22	1:70:A:PHE:HE1	8	0.96
(1,3627)	1:41:A:GLN:HB2	1:39:A:ASP:HB2	2	0.96
(1,3568)	1:114:A:ALA:HB2	1:102:A:ALA:HB1	2	0.96
(1,3568)	1:114:A:ALA:HB2	1:102:A:ALA:HB1	20	0.96
(1,3383)	1:42:A:GLU:HG3	1:43:A:ARG:HD2	10	0.96
(1,3380)	1:40:A:VAL:HG13	1:43:A:ARG:HD3	15	0.96
(1,3272)	1:96:A:PRO:HD3	1:115:A:MET:HE2	14	0.96
(1,3253)	1:32:A:ALA:H	1:34:A:ILE:HD11	3	0.96
(1,3238)	1:89:A:LEU:HD22	1:90:A:MET:HE3	17	0.96
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE3	15	0.96
(1,3080)	1:116:A:GLN:HA	1:25:A:VAL:HG21	2	0.96
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD23	1	0.96
(1,2915)	1:54:A:LEU:HA	1:54:A:LEU:HD11	2	0.96
(1,2277)	1:60:A:GLU:HB2	1:63:A:ASN:HB3	20	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1310)	1:40:A:VAL:HG21	1:37:A:ASN:HD21	3	0.96
(1,885)	1:80:A:ALA:HB3	1:83:A:SER:H	9	0.96
(1,365)	1:101:A:GLU:HG3	1:104:A:ASN:H	5	0.96
(1,82)	1:34:A:ILE:HD11	1:32:A:ALA:H	3	0.96
(1,3734)	1:90:A:MET:HE3	1:93:A:PHE:HZ	2	0.95
(1,3734)	1:90:A:MET:HE1	1:93:A:PHE:HZ	17	0.95
(1,3733)	1:90:A:MET:HE3	1:93:A:PHE:HZ	2	0.95
(1,3733)	1:90:A:MET:HE1	1:93:A:PHE:HZ	17	0.95
(1,3561)	1:90:A:MET:HB3	1:34:A:ILE:HG23	7	0.95
(1,3561)	1:31:A:MET:HG3	1:34:A:ILE:HG23	13	0.95
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG22	11	0.95
(1,2915)	1:54:A:LEU:HA	1:54:A:LEU:HD13	1	0.95
(1,2915)	1:54:A:LEU:HA	1:54:A:LEU:HD12	6	0.95
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD11	19	0.95
(1,2912)	1:50:A:SER:HA	1:48:A:LEU:HD21	8	0.95
(1,1734)	1:44:A:LEU:HD13	1:76:A:MET:HA	5	0.95
(1,1734)	1:44:A:LEU:HD13	1:76:A:MET:HA	8	0.95
(1,1734)	1:44:A:LEU:HD12	1:76:A:MET:HA	13	0.95
(1,1310)	1:40:A:VAL:HG22	1:37:A:ASN:HD21	18	0.95
(1,1213)	1:34:A:ILE:HG22	1:41:A:GLN:H	2	0.95
(1,1135)	1:44:A:LEU:HD12	1:79:A:ALA:H	4	0.95
(1,1135)	1:44:A:LEU:HD11	1:79:A:ALA:H	8	0.95
(1,1027)	1:100:A:VAL:HG23	1:92:A:GLN:H	4	0.95
(1,1014)	1:86:A:LEU:HD13	1:40:A:VAL:H	2	0.95
(1,1014)	1:86:A:LEU:HD12	1:40:A:VAL:H	20	0.95
(1,505)	1:25:A:VAL:HG21	1:117:A:ASN:H	8	0.95
(1,376)	1:73:A:ALA:HB2	1:77:A:PHE:H	20	0.95
(1,3734)	1:90:A:MET:HE1	1:93:A:PHE:HZ	14	0.94
(1,3734)	1:90:A:MET:HE2	1:93:A:PHE:HZ	16	0.94
(1,3733)	1:90:A:MET:HE1	1:93:A:PHE:HZ	14	0.94
(1,3733)	1:90:A:MET:HE2	1:93:A:PHE:HZ	16	0.94
(1,3568)	1:114:A:ALA:HB1	1:102:A:ALA:HB2	17	0.94
(1,3551)	1:56:A:GLN:HA	1:36:A:ALA:HB1	3	0.94
(1,3380)	1:40:A:VAL:HG13	1:43:A:ARG:HD3	17	0.94
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE2	19	0.94
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE3	12	0.94
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD22	12	0.94
(1,2915)	1:21:A:ASP:HA	1:22:A:LEU:HD13	18	0.94
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	7	0.94
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	8	0.94
(1,1572)	1:48:A:LEU:HD21	1:53:A:SER:HB2	10	0.94
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	14	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1170)	1:114:A:ALA:HB2	1:112:A:ALA:H	3	0.94
(1,1170)	1:74:A:LEU:HG	1:23:A:ALA:H	15	0.94
(1,1027)	1:100:A:VAL:HG23	1:92:A:GLN:H	17	0.94
(1,1027)	1:100:A:VAL:HG22	1:92:A:GLN:H	19	0.94
(1,885)	1:80:A:ALA:HB3	1:83:A:SER:H	10	0.94
(1,298)	1:119:A:ALA:HB1	1:116:A:GLN:H	11	0.94
(1,3645)	1:40:A:VAL:HA	1:35:A:LEU:HD11	13	0.93
(1,3584)	1:48:A:LEU:HD13	1:49:A:PRO:HA	2	0.93
(1,3498)	1:102:A:ALA:HB3	1:81:A:LEU:HD11	9	0.93
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD13	5	0.93
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE2	5	0.93
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD23	10	0.93
(1,2915)	1:54:A:LEU:HA	1:54:A:LEU:HD11	17	0.93
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD13	9	0.93
(1,2859)	1:70:A:PHE:HE2	1:74:A:LEU:HD13	8	0.93
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	18	0.93
(1,2699)	1:93:A:PHE:HD1	1:34:A:ILE:HG13	3	0.93
(1,2277)	1:60:A:GLU:HG3	1:63:A:ASN:HB3	15	0.93
(1,2075)	1:61:A:ILE:HG23	1:33:A:PRO:HD2	19	0.93
(1,1734)	1:44:A:LEU:HD13	1:76:A:MET:HA	3	0.93
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	17	0.93
(1,1213)	1:34:A:ILE:HG21	1:41:A:GLN:H	9	0.93
(1,1154)	1:108:A:VAL:HG22	1:20:A:VAL:H	1	0.93
(1,1014)	1:86:A:LEU:HD12	1:40:A:VAL:H	5	0.93
(1,683)	1:128:A:THR:HG22	1:128:A:THR:H	19	0.93
(1,505)	1:25:A:VAL:HG23	1:117:A:ASN:H	19	0.93
(1,298)	1:112:A:ALA:HB2	1:116:A:GLN:H	20	0.93
(1,232)	1:73:A:ALA:HB1	1:76:A:MET:H	8	0.93
(1,3627)	1:33:A:PRO:HG2	1:93:A:PHE:HB2	9	0.92
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	10	0.92
(1,3142)	1:111:A:PHE:HD1	1:90:A:MET:HE2	7	0.92
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE2	16	0.92
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG21	20	0.92
(1,2915)	1:54:A:LEU:HA	1:54:A:LEU:HD11	5	0.92
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD13	8	0.92
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	4	0.92
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	12	0.92
(1,1703)	1:114:A:ALA:HB1	1:98:A:GLU:HA	18	0.92
(1,1558)	1:30:A:ILE:HG13	1:28:A:PRO:HA	3	0.92
(1,1170)	1:74:A:LEU:HG	1:23:A:ALA:H	7	0.92
(1,1170)	1:74:A:LEU:HG	1:23:A:ALA:H	13	0.92
(1,932)	1:103:A:ALA:HB3	1:106:A:GLY:H	2	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,932)	1:103:A:ALA:HB2	1:106:A:GLY:H	18	0.92
(1,827)	1:4:A:ILE:HD12	1:2:A:ASN:HD21	6	0.92
(1,637)	1:40:A:VAL:HG21	1:43:A:ARG:H	7	0.92
(1,305)	1:25:A:VAL:HG23	1:116:A:GLN:H	19	0.92
(1,3734)	1:90:A:MET:HE1	1:93:A:PHE:HZ	18	0.91
(1,3733)	1:90:A:MET:HE1	1:93:A:PHE:HZ	18	0.91
(1,3645)	1:55:A:PRO:HD2	1:35:A:LEU:HD13	18	0.91
(1,3551)	1:56:A:GLN:HA	1:36:A:ALA:HB3	16	0.91
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG23	10	0.91
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG21	14	0.91
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD13	3	0.91
(1,3383)	1:42:A:GLU:HG3	1:43:A:ARG:HD2	16	0.91
(1,3239)	1:34:A:ILE:HD11	1:90:A:MET:HE2	16	0.91
(1,3238)	1:40:A:VAL:HG22	1:90:A:MET:HE3	20	0.91
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG22	19	0.91
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD22	20	0.91
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD11	13	0.91
(1,1734)	1:44:A:LEU:HD11	1:76:A:MET:HA	4	0.91
(1,1734)	1:44:A:LEU:HD11	1:76:A:MET:HA	20	0.91
(1,1572)	1:48:A:LEU:HD12	1:53:A:SER:HB2	18	0.91
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	7	0.91
(1,1027)	1:100:A:VAL:HG23	1:92:A:GLN:H	12	0.91
(1,1027)	1:100:A:VAL:HG23	1:92:A:GLN:H	15	0.91
(1,1014)	1:86:A:LEU:HD12	1:40:A:VAL:H	10	0.91
(1,795)	1:65:A:LEU:HD22	1:64:A:THR:H	2	0.91
(1,795)	1:65:A:LEU:HD21	1:64:A:THR:H	6	0.91
(1,683)	1:40:A:VAL:HG12	1:37:A:ASN:HD21	13	0.91
(1,637)	1:89:A:LEU:HD21	1:43:A:ARG:H	6	0.91
(1,637)	1:40:A:VAL:HG23	1:43:A:ARG:H	13	0.91
(1,307)	1:25:A:VAL:HG22	1:114:A:ALA:H	3	0.91
(1,307)	1:25:A:VAL:HG23	1:114:A:ALA:H	12	0.91
(1,232)	1:73:A:ALA:HB2	1:76:A:MET:H	19	0.91
(1,3584)	1:48:A:LEU:HD11	1:49:A:PRO:HA	4	0.9
(1,3238)	1:89:A:LEU:HD22	1:90:A:MET:HE1	13	0.9
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE1	17	0.9
(1,3106)	1:40:A:VAL:HG22	1:35:A:LEU:HD11	13	0.9
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD21	9	0.9
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD22	11	0.9
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD21	15	0.9
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD21	19	0.9
(1,2915)	1:21:A:ASP:HA	1:22:A:LEU:HD11	15	0.9
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD12	10	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2857)	1:44:A:LEU:H	1:44:A:LEU:HD22	4	0.9
(1,2857)	1:44:A:LEU:H	1:44:A:LEU:HD21	16	0.9
(1,2075)	1:61:A:ILE:HG23	1:33:A:PRO:HD2	8	0.9
(1,1859)	1:64:A:THR:HG23	1:60:A:GLU:HA	17	0.9
(1,1102)	1:56:A:GLN:HB3	1:58:A:ALA:H	16	0.9
(1,376)	1:73:A:ALA:HB1	1:77:A:PHE:H	10	0.9
(1,232)	1:74:A:LEU:HB3	1:76:A:MET:H	2	0.9
(1,232)	1:73:A:ALA:HB1	1:76:A:MET:H	14	0.9
(1,179)	1:38:A:ALA:HB1	1:40:A:VAL:H	15	0.9
(1,3645)	1:40:A:VAL:HA	1:35:A:LEU:HD12	2	0.89
(1,3568)	1:114:A:ALA:HB2	1:102:A:ALA:HB3	14	0.89
(1,3558)	1:118:A:ASN:HB3	1:114:A:ALA:HB1	3	0.89
(1,3504)	1:31:A:MET:HE2	1:86:A:LEU:HD23	16	0.89
(1,3239)	1:34:A:ILE:HD12	1:90:A:MET:HE1	18	0.89
(1,3238)	1:89:A:LEU:HD23	1:90:A:MET:HE3	1	0.89
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD22	7	0.89
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD23	17	0.89
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD11	15	0.89
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	13	0.89
(1,2699)	1:93:A:PHE:HD2	1:34:A:ILE:HG13	11	0.89
(1,1734)	1:44:A:LEU:HD12	1:76:A:MET:HA	15	0.89
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	6	0.89
(1,1095)	1:23:A:ALA:HB3	1:22:A:LEU:H	5	0.89
(1,1014)	1:86:A:LEU:HD13	1:40:A:VAL:H	6	0.89
(1,1014)	1:86:A:LEU:HD13	1:40:A:VAL:H	11	0.89
(1,906)	1:36:A:ALA:HB3	1:41:A:GLN:HE22	7	0.89
(1,298)	1:112:A:ALA:HB3	1:116:A:GLN:H	14	0.89
(1,232)	1:74:A:LEU:HB3	1:76:A:MET:H	3	0.89
(1,232)	1:73:A:ALA:HB3	1:76:A:MET:H	4	0.89
(1,232)	1:73:A:ALA:HB2	1:76:A:MET:H	16	0.89
(1,3627)	1:33:A:PRO:HG2	1:93:A:PHE:HB2	1	0.88
(1,3627)	1:33:A:PRO:HG2	1:93:A:PHE:HB2	10	0.88
(1,3627)	1:33:A:PRO:HG2	1:93:A:PHE:HB2	15	0.88
(1,3568)	1:114:A:ALA:HB2	1:102:A:ALA:HB2	3	0.88
(1,3380)	1:80:A:ALA:HB2	1:43:A:ARG:HD2	3	0.88
(1,3238)	1:89:A:LEU:HD21	1:90:A:MET:HE3	3	0.88
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD21	3	0.88
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD21	4	0.88
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD22	14	0.88
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD23	19	0.88
(1,2075)	1:61:A:ILE:HG23	1:33:A:PRO:HD2	11	0.88
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	14	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1135)	1:74:A:LEU:HD12	1:79:A:ALA:H	13	0.88
(1,1014)	1:86:A:LEU:HD12	1:40:A:VAL:H	3	0.88
(1,1014)	1:86:A:LEU:HD11	1:40:A:VAL:H	17	0.88
(1,932)	1:103:A:ALA:HB2	1:106:A:GLY:H	19	0.88
(1,795)	1:65:A:LEU:HD23	1:64:A:THR:H	13	0.88
(1,637)	1:40:A:VAL:HG22	1:43:A:ARG:H	9	0.88
(1,3568)	1:99:A:ALA:HB1	1:102:A:ALA:HB3	12	0.87
(1,3561)	1:31:A:MET:HG3	1:34:A:ILE:HG21	3	0.87
(1,3498)	1:102:A:ALA:HB2	1:81:A:LEU:HD13	10	0.87
(1,3498)	1:31:A:MET:HE3	1:81:A:LEU:HD11	12	0.87
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	8	0.87
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE1	14	0.87
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD22	12	0.87
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD22	13	0.87
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD23	3	0.87
(1,2915)	1:54:A:LEU:HA	1:54:A:LEU:HD11	20	0.87
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	13	0.87
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	11	0.87
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	18	0.87
(1,1246)	1:44:A:LEU:HD12	1:42:A:GLU:H	1	0.87
(1,1170)	1:74:A:LEU:HG	1:23:A:ALA:H	9	0.87
(1,1095)	1:23:A:ALA:HB3	1:22:A:LEU:H	2	0.87
(1,1027)	1:100:A:VAL:HG21	1:92:A:GLN:H	5	0.87
(1,1018)	1:77:A:PHE:HD2	1:81:A:LEU:H	1	0.87
(1,803)	1:46:A:PRO:HG2	1:85:A:GLN:HE21	11	0.87
(1,795)	1:65:A:LEU:HD23	1:64:A:THR:H	12	0.87
(1,365)	1:101:A:GLU:HG3	1:103:A:ALA:H	10	0.87
(1,338)	1:61:A:ILE:HG22	1:65:A:LEU:H	18	0.87
(1,232)	1:73:A:ALA:HB2	1:76:A:MET:H	5	0.87
(1,3734)	1:90:A:MET:HE1	1:93:A:PHE:HZ	7	0.86
(1,3733)	1:90:A:MET:HE1	1:93:A:PHE:HZ	7	0.86
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG21	17	0.86
(1,3504)	1:43:A:ARG:HG3	1:86:A:LEU:HD21	7	0.86
(1,3498)	1:102:A:ALA:HB1	1:81:A:LEU:HD12	13	0.86
(1,3498)	1:31:A:MET:HE3	1:81:A:LEU:HD13	14	0.86
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD12	15	0.86
(1,3253)	1:32:A:ALA:H	1:61:A:ILE:HD12	6	0.86
(1,3117)	1:116:A:GLN:H	1:115:A:MET:HE2	16	0.86
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD23	2	0.86
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD21	18	0.86
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD22	7	0.86
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD21	9	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD23	15	0.86
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD23	6	0.86
(1,2857)	1:44:A:LEU:H	1:44:A:LEU:HD23	19	0.86
(1,1734)	1:44:A:LEU:HD11	1:76:A:MET:HA	19	0.86
(1,1558)	1:30:A:ILE:HG13	1:28:A:PRO:HA	4	0.86
(1,1345)	1:35:A:LEU:HD11	1:31:A:MET:H	2	0.86
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	2	0.86
(1,1170)	1:74:A:LEU:HG	1:23:A:ALA:H	5	0.86
(1,1135)	1:44:A:LEU:HD13	1:79:A:ALA:H	9	0.86
(1,1027)	1:100:A:VAL:HG22	1:92:A:GLN:H	2	0.86
(1,1027)	1:100:A:VAL:HG22	1:92:A:GLN:H	18	0.86
(1,1014)	1:86:A:LEU:HD13	1:40:A:VAL:H	4	0.86
(1,1014)	1:86:A:LEU:HD13	1:40:A:VAL:H	9	0.86
(1,1014)	1:86:A:LEU:HD12	1:40:A:VAL:H	13	0.86
(1,1014)	1:86:A:LEU:HD11	1:40:A:VAL:H	18	0.86
(1,932)	1:103:A:ALA:HB1	1:106:A:GLY:H	9	0.86
(1,885)	1:80:A:ALA:HB2	1:83:A:SER:H	13	0.86
(1,795)	1:65:A:LEU:HD23	1:64:A:THR:H	10	0.86
(1,795)	1:65:A:LEU:HD21	1:64:A:THR:H	14	0.86
(1,637)	1:40:A:VAL:HG23	1:43:A:ARG:H	2	0.86
(1,637)	1:40:A:VAL:HG23	1:43:A:ARG:H	19	0.86
(1,523)	1:54:A:LEU:HD11	1:44:A:LEU:H	14	0.86
(1,425)	1:57:A:THR:HG22	1:60:A:GLU:H	13	0.86
(1,338)	1:65:A:LEU:HD12	1:65:A:LEU:H	13	0.86
(1,179)	1:38:A:ALA:HB1	1:40:A:VAL:H	3	0.86
(1,82)	1:61:A:ILE:HD12	1:32:A:ALA:H	6	0.86
(1,3734)	1:90:A:MET:HE2	1:93:A:PHE:HZ	10	0.85
(1,3733)	1:90:A:MET:HE2	1:93:A:PHE:HZ	10	0.85
(1,3673)	1:114:A:ALA:H	1:111:A:PHE:HD1	9	0.85
(1,3673)	1:114:A:ALA:H	1:111:A:PHE:HD1	13	0.85
(1,3627)	1:90:A:MET:HE2	1:93:A:PHE:HB2	13	0.85
(1,3627)	1:33:A:PRO:HG2	1:93:A:PHE:HB2	14	0.85
(1,3565)	1:90:A:MET:HE1	1:31:A:MET:HE1	7	0.85
(1,3551)	1:57:A:THR:HB	1:36:A:ALA:HB1	4	0.85
(1,3551)	1:57:A:THR:HB	1:36:A:ALA:HB1	11	0.85
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB1	15	0.85
(1,3267)	1:31:A:MET:HG3	1:34:A:ILE:HD11	4	0.85
(1,3253)	1:32:A:ALA:H	1:34:A:ILE:HD11	14	0.85
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE3	2	0.85
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE2	9	0.85
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG12	14	0.85
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD22	8	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2915)	1:21:A:ASP:HA	1:22:A:LEU:HD11	19	0.85
(1,2875)	1:93:A:PHE:HZ	1:86:A:LEU:HD13	1	0.85
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD13	14	0.85
(1,1734)	1:44:A:LEU:HD11	1:76:A:MET:HA	2	0.85
(1,1734)	1:44:A:LEU:HD12	1:76:A:MET:HA	18	0.85
(1,1719)	1:100:A:VAL:HG11	1:96:A:PRO:HA	1	0.85
(1,1135)	1:44:A:LEU:HD13	1:79:A:ALA:H	6	0.85
(1,1116)	1:96:A:PRO:HA	1:119:A:ALA:H	12	0.85
(1,1027)	1:100:A:VAL:HG23	1:92:A:GLN:H	8	0.85
(1,1027)	1:100:A:VAL:HG23	1:92:A:GLN:H	10	0.85
(1,1014)	1:86:A:LEU:HD13	1:40:A:VAL:H	8	0.85
(1,868)	1:65:A:LEU:HD23	1:69:A:GLN:HE21	3	0.85
(1,425)	1:57:A:THR:HG22	1:60:A:GLU:H	11	0.85
(1,425)	1:57:A:THR:HG22	1:60:A:GLU:H	12	0.85
(1,307)	1:26:A:LEU:HD21	1:114:A:ALA:H	6	0.85
(1,232)	1:73:A:ALA:HB3	1:76:A:MET:H	11	0.85
(1,232)	1:73:A:ALA:HB3	1:76:A:MET:H	13	0.85
(1,82)	1:34:A:ILE:HD11	1:32:A:ALA:H	14	0.85
(1,3734)	1:90:A:MET:HE3	1:93:A:PHE:HZ	12	0.84
(1,3733)	1:90:A:MET:HE3	1:93:A:PHE:HZ	12	0.84
(1,3673)	1:107:A:ASP:H	1:111:A:PHE:HD1	4	0.84
(1,3673)	1:114:A:ALA:H	1:111:A:PHE:HD2	7	0.84
(1,3645)	1:40:A:VAL:HA	1:35:A:LEU:HD12	3	0.84
(1,3627)	1:33:A:PRO:HG2	1:93:A:PHE:HB2	5	0.84
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG22	3	0.84
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB1	1	0.84
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB1	3	0.84
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB2	11	0.84
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD13	12	0.84
(1,3383)	1:42:A:GLU:HG3	1:43:A:ARG:HD2	12	0.84
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE2	14	0.84
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE2	10	0.84
(1,2952)	1:40:A:VAL:HA	1:86:A:LEU:HD21	19	0.84
(1,2915)	1:21:A:ASP:HA	1:22:A:LEU:HD12	7	0.84
(1,2915)	1:21:A:ASP:HA	1:22:A:LEU:HD13	13	0.84
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD12	5	0.84
(1,2857)	1:44:A:LEU:H	1:44:A:LEU:HD22	13	0.84
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	1	0.84
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	12	0.84
(1,2293)	1:34:A:ILE:HB	1:37:A:ASN:HB3	9	0.84
(1,2075)	1:61:A:ILE:HG21	1:33:A:PRO:HD2	5	0.84
(1,1345)	1:35:A:LEU:HD11	1:31:A:MET:H	3	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1027)	1:100:A:VAL:HG21	1:92:A:GLN:H	16	0.84
(1,932)	1:103:A:ALA:HB2	1:106:A:GLY:H	8	0.84
(1,909)	1:54:A:LEU:HD13	1:41:A:GLN:HE22	1	0.84
(1,885)	1:80:A:ALA:HB3	1:83:A:SER:H	6	0.84
(1,523)	1:44:A:LEU:HD22	1:44:A:LEU:H	13	0.84
(1,365)	1:101:A:GLU:HG3	1:104:A:ASN:H	4	0.84
(1,307)	1:25:A:VAL:HG22	1:114:A:ALA:H	16	0.84
(1,179)	1:38:A:ALA:HB2	1:40:A:VAL:H	4	0.84
(1,179)	1:38:A:ALA:HB2	1:40:A:VAL:H	11	0.84
(1,179)	1:38:A:ALA:HB3	1:40:A:VAL:H	13	0.84
(1,3734)	1:90:A:MET:HE2	1:93:A:PHE:HZ	13	0.83
(1,3734)	1:90:A:MET:HE3	1:93:A:PHE:HZ	15	0.83
(1,3733)	1:90:A:MET:HE2	1:93:A:PHE:HZ	13	0.83
(1,3733)	1:90:A:MET:HE3	1:93:A:PHE:HZ	15	0.83
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG23	7	0.83
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB2	4	0.83
(1,3383)	1:42:A:GLU:HG3	1:43:A:ARG:HD2	8	0.83
(1,3380)	1:40:A:VAL:HG11	1:43:A:ARG:HD3	11	0.83
(1,3239)	1:86:A:LEU:HD13	1:90:A:MET:HE2	15	0.83
(1,3232)	1:31:A:MET:HG2	1:30:A:ILE:HG23	4	0.83
(1,3027)	1:81:A:LEU:HB2	1:81:A:LEU:HD23	1	0.83
(1,3027)	1:103:A:ALA:HB1	1:81:A:LEU:HD22	6	0.83
(1,3027)	1:103:A:ALA:HB2	1:81:A:LEU:HD23	16	0.83
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD22	12	0.83
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD12	13	0.83
(1,2699)	1:93:A:PHE:HD2	1:34:A:ILE:HG13	5	0.83
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	10	0.83
(1,1345)	1:35:A:LEU:HD13	1:31:A:MET:H	18	0.83
(1,1213)	1:34:A:ILE:HG21	1:41:A:GLN:H	1	0.83
(1,1135)	1:74:A:LEU:HD13	1:79:A:ALA:H	1	0.83
(1,1095)	1:23:A:ALA:HB1	1:22:A:LEU:H	19	0.83
(1,1014)	1:86:A:LEU:HD12	1:40:A:VAL:H	12	0.83
(1,868)	1:65:A:LEU:HD21	1:72:A:GLN:HE21	7	0.83
(1,683)	1:128:A:THR:HG21	1:128:A:THR:H	18	0.83
(1,523)	1:44:A:LEU:HD23	1:44:A:LEU:H	15	0.83
(1,425)	1:57:A:THR:HG21	1:60:A:GLU:H	1	0.83
(1,305)	1:25:A:VAL:HG21	1:116:A:GLN:H	15	0.83
(1,232)	1:73:A:ALA:HB2	1:76:A:MET:H	18	0.83
(1,179)	1:38:A:ALA:HB3	1:40:A:VAL:H	5	0.83
(1,114)	1:81:A:LEU:HB2	1:79:A:ALA:H	2	0.83
(1,3561)	1:90:A:MET:HB3	1:34:A:ILE:HG23	18	0.82
(1,3239)	1:86:A:LEU:HD11	1:90:A:MET:HE3	14	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE1	18	0.82
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG23	11	0.82
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	16	0.82
(1,2640)	1:65:A:LEU:HD13	1:55:A:PRO:HB2	6	0.82
(1,2640)	1:30:A:ILE:HD12	1:115:A:MET:HG3	14	0.82
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	3	0.82
(1,1734)	1:44:A:LEU:HD13	1:76:A:MET:HA	7	0.82
(1,1734)	1:44:A:LEU:HD13	1:76:A:MET:HA	12	0.82
(1,1345)	1:35:A:LEU:HD12	1:31:A:MET:H	12	0.82
(1,1135)	1:44:A:LEU:HD13	1:79:A:ALA:H	15	0.82
(1,1095)	1:23:A:ALA:HB1	1:22:A:LEU:H	8	0.82
(1,1095)	1:23:A:ALA:HB3	1:22:A:LEU:H	9	0.82
(1,1095)	1:23:A:ALA:HB3	1:22:A:LEU:H	11	0.82
(1,1007)	1:30:A:ILE:HD11	1:119:A:ALA:H	3	0.82
(1,932)	1:103:A:ALA:HB1	1:106:A:GLY:H	1	0.82
(1,932)	1:103:A:ALA:HB1	1:106:A:GLY:H	3	0.82
(1,885)	1:80:A:ALA:HB1	1:83:A:SER:H	14	0.82
(1,885)	1:80:A:ALA:HB2	1:83:A:SER:H	18	0.82
(1,523)	1:44:A:LEU:HD23	1:44:A:LEU:H	20	0.82
(1,505)	1:25:A:VAL:HG21	1:117:A:ASN:H	18	0.82
(1,376)	1:73:A:ALA:HB1	1:77:A:PHE:H	8	0.82
(1,298)	1:119:A:ALA:HB1	1:116:A:GLN:H	10	0.82
(1,234)	1:44:A:LEU:HD22	1:76:A:MET:H	1	0.82
(1,179)	1:38:A:ALA:HB2	1:40:A:VAL:H	9	0.82
(1,3673)	1:114:A:ALA:H	1:111:A:PHE:HD1	18	0.81
(1,3645)	1:40:A:VAL:HA	1:35:A:LEU:HD13	12	0.81
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG22	16	0.81
(1,3519)	1:109:A:GLU:HG3	1:20:A:VAL:HG12	18	0.81
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB1	6	0.81
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB2	16	0.81
(1,3498)	1:102:A:ALA:HB3	1:81:A:LEU:HD12	4	0.81
(1,3142)	1:93:A:PHE:HD2	1:90:A:MET:HE2	19	0.81
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG22	6	0.81
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG22	15	0.81
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG12	12	0.81
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD21	4	0.81
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD22	7	0.81
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD11	11	0.81
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	2	0.81
(1,1719)	1:100:A:VAL:HG13	1:96:A:PRO:HA	5	0.81
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	8	0.81
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	19	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1102)	1:60:A:GLU:HG2	1:58:A:ALA:H	20	0.81
(1,1014)	1:86:A:LEU:HD13	1:40:A:VAL:H	15	0.81
(1,932)	1:103:A:ALA:HB3	1:106:A:GLY:H	17	0.81
(1,885)	1:80:A:ALA:HB1	1:83:A:SER:H	16	0.81
(1,404)	1:96:A:PRO:HG2	1:118:A:ASN:H	18	0.81
(1,338)	1:61:A:ILE:HG21	1:65:A:LEU:H	6	0.81
(1,307)	1:26:A:LEU:HD21	1:114:A:ALA:H	5	0.81
(1,179)	1:38:A:ALA:HB1	1:40:A:VAL:H	1	0.81
(1,179)	1:38:A:ALA:HB2	1:40:A:VAL:H	7	0.81
(1,179)	1:38:A:ALA:HB2	1:40:A:VAL:H	16	0.81
(1,179)	1:38:A:ALA:HB2	1:40:A:VAL:H	19	0.81
(1,3673)	1:114:A:ALA:H	1:111:A:PHE:HD1	12	0.8
(1,3627)	1:33:A:PRO:HG2	1:93:A:PHE:HB2	18	0.8
(1,3561)	1:90:A:MET:HB3	1:34:A:ILE:HG21	2	0.8
(1,3561)	1:90:A:MET:HB3	1:34:A:ILE:HG22	12	0.8
(1,3551)	1:56:A:GLN:HA	1:36:A:ALA:HB1	13	0.8
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB2	9	0.8
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB2	19	0.8
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD13	11	0.8
(1,3441)	1:114:A:ALA:HB2	1:96:A:PRO:HB3	18	0.8
(1,3253)	1:32:A:ALA:H	1:34:A:ILE:HD11	8	0.8
(1,3239)	1:86:A:LEU:HD12	1:90:A:MET:HE2	5	0.8
(1,3239)	1:34:A:ILE:HD12	1:90:A:MET:HE1	7	0.8
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB2	4	0.8
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD23	6	0.8
(1,2912)	1:85:A:GLN:HA	1:89:A:LEU:HD23	2	0.8
(1,2912)	1:50:A:SER:HA	1:48:A:LEU:HD22	16	0.8
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD13	6	0.8
(1,2617)	1:95:A:LEU:HD21	1:90:A:MET:HB2	1	0.8
(1,2293)	1:38:A:ALA:HB2	1:37:A:ASN:HB3	16	0.8
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	5	0.8
(1,2075)	1:61:A:ILE:HG21	1:33:A:PRO:HD2	13	0.8
(1,1975)	1:27:A:THR:HG21	1:26:A:LEU:HA	10	0.8
(1,1975)	1:27:A:THR:HG21	1:26:A:LEU:HA	19	0.8
(1,1859)	1:64:A:THR:HG23	1:60:A:GLU:HA	12	0.8
(1,1170)	1:74:A:LEU:HG	1:23:A:ALA:H	4	0.8
(1,1170)	1:114:A:ALA:HB1	1:112:A:ALA:H	14	0.8
(1,906)	1:58:A:ALA:HB1	1:62:A:GLN:HE22	18	0.8
(1,578)	1:23:A:ALA:HB1	1:25:A:VAL:H	16	0.8
(1,523)	1:54:A:LEU:HD12	1:44:A:LEU:H	19	0.8
(1,505)	1:25:A:VAL:HG21	1:117:A:ASN:H	9	0.8
(1,365)	1:101:A:GLU:HG3	1:104:A:ASN:H	6	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:25:A:VAL:HG21	1:116:A:GLN:H	1	0.8
(1,232)	1:73:A:ALA:HB3	1:76:A:MET:H	12	0.8
(1,179)	1:38:A:ALA:HB1	1:40:A:VAL:H	20	0.8
(1,114)	1:81:A:LEU:HB2	1:79:A:ALA:H	10	0.8
(1,82)	1:34:A:ILE:HD11	1:32:A:ALA:H	8	0.8
(1,3568)	1:114:A:ALA:HB2	1:102:A:ALA:HB3	16	0.79
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG23	15	0.79
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB3	2	0.79
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB2	7	0.79
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB2	8	0.79
(1,3504)	1:31:A:MET:HE3	1:86:A:LEU:HD22	20	0.79
(1,3498)	1:102:A:ALA:HB2	1:81:A:LEU:HD13	3	0.79
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD11	16	0.79
(1,3441)	1:114:A:ALA:HB2	1:96:A:PRO:HB3	7	0.79
(1,3239)	1:86:A:LEU:HD13	1:90:A:MET:HE2	2	0.79
(1,3238)	1:40:A:VAL:HG22	1:90:A:MET:HE1	8	0.79
(1,3080)	1:116:A:GLN:HA	1:25:A:VAL:HG21	3	0.79
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD22	13	0.79
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD13	16	0.79
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD22	16	0.79
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD21	17	0.79
(1,2868)	1:43:A:ARG:H	1:86:A:LEU:HD21	18	0.79
(1,2857)	1:44:A:LEU:H	1:44:A:LEU:HD22	8	0.79
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	17	0.79
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	16	0.79
(1,1883)	1:74:A:LEU:HD21	1:74:A:LEU:HA	4	0.79
(1,1734)	1:44:A:LEU:HD13	1:76:A:MET:HA	11	0.79
(1,1734)	1:44:A:LEU:HD11	1:76:A:MET:HA	17	0.79
(1,1572)	1:48:A:LEU:HD12	1:53:A:SER:HB2	5	0.79
(1,1558)	1:64:A:THR:HG23	1:53:A:SER:HB3	12	0.79
(1,1170)	1:114:A:ALA:HB1	1:112:A:ALA:H	11	0.79
(1,1170)	1:114:A:ALA:HB1	1:112:A:ALA:H	17	0.79
(1,1027)	1:100:A:VAL:HG21	1:92:A:GLN:H	7	0.79
(1,932)	1:103:A:ALA:HB2	1:106:A:GLY:H	11	0.79
(1,906)	1:58:A:ALA:HB3	1:62:A:GLN:HE22	11	0.79
(1,906)	1:36:A:ALA:HB2	1:41:A:GLN:HE22	15	0.79
(1,885)	1:80:A:ALA:HB1	1:83:A:SER:H	15	0.79
(1,849)	1:36:A:ALA:HB1	1:41:A:GLN:HE21	13	0.79
(1,523)	1:44:A:LEU:HD22	1:44:A:LEU:H	8	0.79
(1,305)	1:25:A:VAL:HG21	1:116:A:GLN:H	3	0.79
(1,298)	1:119:A:ALA:HB1	1:116:A:GLN:H	4	0.79
(1,232)	1:73:A:ALA:HB3	1:76:A:MET:H	7	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,179)	1:38:A:ALA:HB1	1:40:A:VAL:H	6	0.79
(1,114)	1:81:A:LEU:HB2	1:79:A:ALA:H	4	0.79
(1,114)	1:82:A:ALA:HB2	1:79:A:ALA:H	9	0.79
(1,3584)	1:48:A:LEU:HD12	1:49:A:PRO:HA	13	0.78
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB3	5	0.78
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB1	10	0.78
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB1	20	0.78
(1,3498)	1:102:A:ALA:HB2	1:81:A:LEU:HD12	17	0.78
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD11	2	0.78
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD13	7	0.78
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD13	2	0.78
(1,3441)	1:99:A:ALA:HB2	1:96:A:PRO:HB3	1	0.78
(1,3253)	1:32:A:ALA:H	1:61:A:ILE:HD13	12	0.78
(1,3239)	1:86:A:LEU:HD12	1:90:A:MET:HE2	20	0.78
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG11	1	0.78
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD11	14	0.78
(1,3027)	1:103:A:ALA:HB3	1:81:A:LEU:HD22	5	0.78
(1,3015)	1:97:A:ALA:HB1	1:100:A:VAL:HG11	7	0.78
(1,3015)	1:97:A:ALA:HB1	1:100:A:VAL:HG12	9	0.78
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD22	11	0.78
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD21	17	0.78
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD13	4	0.78
(1,2857)	1:44:A:LEU:H	1:44:A:LEU:HD23	3	0.78
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	5	0.78
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	6	0.78
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	13	0.78
(1,2293)	1:38:A:ALA:HB3	1:37:A:ASN:HB3	2	0.78
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	16	0.78
(1,1883)	1:74:A:LEU:HD23	1:74:A:LEU:HA	10	0.78
(1,1719)	1:100:A:VAL:HG12	1:96:A:PRO:HA	4	0.78
(1,1719)	1:100:A:VAL:HG13	1:96:A:PRO:HA	12	0.78
(1,1345)	1:35:A:LEU:HD12	1:31:A:MET:H	1	0.78
(1,1345)	1:35:A:LEU:HD12	1:31:A:MET:H	4	0.78
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	18	0.78
(1,1135)	1:44:A:LEU:HD12	1:79:A:ALA:H	2	0.78
(1,1135)	1:44:A:LEU:HD11	1:79:A:ALA:H	7	0.78
(1,1095)	1:23:A:ALA:HB3	1:22:A:LEU:H	6	0.78
(1,1095)	1:23:A:ALA:HB2	1:22:A:LEU:H	7	0.78
(1,932)	1:103:A:ALA:HB2	1:106:A:GLY:H	12	0.78
(1,932)	1:103:A:ALA:HB3	1:106:A:GLY:H	14	0.78
(1,906)	1:36:A:ALA:HB1	1:41:A:GLN:HE22	1	0.78
(1,885)	1:80:A:ALA:HB2	1:83:A:SER:H	12	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,795)	1:65:A:LEU:HD23	1:64:A:THR:H	20	0.78
(1,523)	1:44:A:LEU:HD23	1:44:A:LEU:H	3	0.78
(1,425)	1:57:A:THR:HG21	1:60:A:GLU:H	17	0.78
(1,376)	1:73:A:ALA:HB3	1:77:A:PHE:H	4	0.78
(1,365)	1:101:A:GLU:HG3	1:104:A:ASN:H	11	0.78
(1,365)	1:101:A:GLU:HG3	1:104:A:ASN:H	14	0.78
(1,305)	1:25:A:VAL:HG22	1:116:A:GLN:H	13	0.78
(1,179)	1:38:A:ALA:HB3	1:40:A:VAL:H	2	0.78
(1,114)	1:82:A:ALA:HB1	1:79:A:ALA:H	3	0.78
(1,82)	1:61:A:ILE:HD13	1:32:A:ALA:H	12	0.78
(1,3673)	1:114:A:ALA:H	1:111:A:PHE:HD1	2	0.77
(1,3673)	1:107:A:ASP:H	1:111:A:PHE:HD1	3	0.77
(1,3645)	1:40:A:VAL:HA	1:35:A:LEU:HD13	6	0.77
(1,3627)	1:33:A:PRO:HG2	1:93:A:PHE:HB2	16	0.77
(1,3584)	1:48:A:LEU:HD11	1:49:A:PRO:HA	18	0.77
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG23	13	0.77
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG21	18	0.77
(1,3519)	1:109:A:GLU:HG3	1:20:A:VAL:HG12	12	0.77
(1,3519)	1:109:A:GLU:HG3	1:20:A:VAL:HG12	19	0.77
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB3	13	0.77
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB1	17	0.77
(1,3441)	1:99:A:ALA:HB3	1:96:A:PRO:HB3	8	0.77
(1,3441)	1:99:A:ALA:HB1	1:96:A:PRO:HB3	14	0.77
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB2	16	0.77
(1,3080)	1:116:A:GLN:HA	1:25:A:VAL:HG22	4	0.77
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG21	7	0.77
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD22	5	0.77
(1,2874)	1:44:A:LEU:H	1:44:A:LEU:HD12	1	0.77
(1,2857)	1:44:A:LEU:H	1:44:A:LEU:HD22	5	0.77
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD11	7	0.77
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD12	9	0.77
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	12	0.77
(1,2699)	1:93:A:PHE:HD2	1:34:A:ILE:HG13	9	0.77
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	8	0.77
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	11	0.77
(1,1975)	1:27:A:THR:HG23	1:26:A:LEU:HA	2	0.77
(1,1975)	1:27:A:THR:HG23	1:26:A:LEU:HA	14	0.77
(1,1734)	1:44:A:LEU:HD12	1:76:A:MET:HA	9	0.77
(1,1345)	1:35:A:LEU:HD12	1:31:A:MET:H	6	0.77
(1,1232)	1:57:A:THR:HG22	1:59:A:ASP:H	12	0.77
(1,1225)	1:72:A:GLN:HG2	1:74:A:LEU:H	18	0.77
(1,1170)	1:74:A:LEU:HG	1:23:A:ALA:H	20	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1116)	1:96:A:PRO:HA	1:119:A:ALA:H	5	0.77
(1,1095)	1:23:A:ALA:HB1	1:22:A:LEU:H	10	0.77
(1,932)	1:103:A:ALA:HB1	1:106:A:GLY:H	7	0.77
(1,906)	1:36:A:ALA:HB1	1:41:A:GLN:HE22	8	0.77
(1,885)	1:80:A:ALA:HB2	1:83:A:SER:H	5	0.77
(1,795)	1:65:A:LEU:HD23	1:64:A:THR:H	11	0.77
(1,523)	1:44:A:LEU:HD22	1:44:A:LEU:H	5	0.77
(1,376)	1:73:A:ALA:HB2	1:77:A:PHE:H	1	0.77
(1,298)	1:119:A:ALA:HB2	1:116:A:GLN:H	8	0.77
(1,232)	1:73:A:ALA:HB2	1:76:A:MET:H	20	0.77
(1,179)	1:38:A:ALA:HB3	1:40:A:VAL:H	18	0.77
(1,114)	1:82:A:ALA:HB2	1:79:A:ALA:H	6	0.77
(1,3673)	1:114:A:ALA:H	1:111:A:PHE:HD1	14	0.76
(1,3642)	1:74:A:LEU:HD21	1:70:A:PHE:HA	4	0.76
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG21	12	0.76
(1,3484)	1:85:A:GLN:HB3	1:86:A:LEU:HD11	8	0.76
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD12	13	0.76
(1,3441)	1:99:A:ALA:HB3	1:96:A:PRO:HB3	5	0.76
(1,3253)	1:32:A:ALA:H	1:61:A:ILE:HD12	2	0.76
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG13	9	0.76
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG13	16	0.76
(1,3059)	1:111:A:PHE:HD2	1:108:A:VAL:HG11	18	0.76
(1,3015)	1:97:A:ALA:HB3	1:100:A:VAL:HG12	19	0.76
(1,2994)	1:31:A:MET:HG3	1:35:A:LEU:HD23	12	0.76
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD13	20	0.76
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD23	4	0.76
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	9	0.76
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	19	0.76
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	3	0.76
(1,2116)	1:86:A:LEU:HD13	1:43:A:ARG:HD2	3	0.76
(1,2075)	1:61:A:ILE:HG22	1:33:A:PRO:HD2	3	0.76
(1,1734)	1:44:A:LEU:HD12	1:76:A:MET:HA	6	0.76
(1,1345)	1:35:A:LEU:HD13	1:31:A:MET:H	9	0.76
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	3	0.76
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	10	0.76
(1,1232)	1:57:A:THR:HG23	1:59:A:ASP:H	1	0.76
(1,1145)	1:85:A:GLN:HB2	1:81:A:LEU:H	20	0.76
(1,1135)	1:44:A:LEU:HD11	1:79:A:ALA:H	10	0.76
(1,1116)	1:96:A:PRO:HA	1:119:A:ALA:H	3	0.76
(1,1116)	1:95:A:LEU:HA	1:119:A:ALA:H	8	0.76
(1,1095)	1:23:A:ALA:HB3	1:22:A:LEU:H	13	0.76
(1,1095)	1:23:A:ALA:HB2	1:22:A:LEU:H	15	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1027)	1:100:A:VAL:HG22	1:92:A:GLN:H	6	0.76
(1,1014)	1:86:A:LEU:HD13	1:40:A:VAL:H	1	0.76
(1,932)	1:103:A:ALA:HB1	1:106:A:GLY:H	5	0.76
(1,932)	1:103:A:ALA:HB2	1:106:A:GLY:H	15	0.76
(1,885)	1:80:A:ALA:HB1	1:83:A:SER:H	19	0.76
(1,849)	1:36:A:ALA:HB2	1:41:A:GLN:HE21	6	0.76
(1,849)	1:35:A:LEU:HB2	1:41:A:GLN:HE21	11	0.76
(1,637)	1:89:A:LEU:HD21	1:43:A:ARG:H	17	0.76
(1,523)	1:44:A:LEU:HD23	1:44:A:LEU:H	17	0.76
(1,505)	1:25:A:VAL:HG22	1:117:A:ASN:H	11	0.76
(1,376)	1:73:A:ALA:HB1	1:77:A:PHE:H	3	0.76
(1,338)	1:65:A:LEU:HD11	1:65:A:LEU:H	3	0.76
(1,338)	1:65:A:LEU:HD13	1:65:A:LEU:H	9	0.76
(1,305)	1:25:A:VAL:HG21	1:116:A:GLN:H	2	0.76
(1,305)	1:25:A:VAL:HG23	1:116:A:GLN:H	14	0.76
(1,232)	1:73:A:ALA:HB1	1:76:A:MET:H	15	0.76
(1,114)	1:82:A:ALA:HB2	1:79:A:ALA:H	16	0.76
(1,82)	1:61:A:ILE:HD12	1:32:A:ALA:H	2	0.76
(1,3645)	1:40:A:VAL:HA	1:35:A:LEU:HD11	20	0.75
(1,3558)	1:118:A:ASN:HB3	1:99:A:ALA:HB2	10	0.75
(1,3253)	1:32:A:ALA:H	1:34:A:ILE:HD12	11	0.75
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG13	5	0.75
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG12	11	0.75
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD12	7	0.75
(1,2857)	1:44:A:LEU:H	1:44:A:LEU:HD23	9	0.75
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD13	18	0.75
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD23	1	0.75
(1,2699)	1:93:A:PHE:HD2	1:34:A:ILE:HG13	18	0.75
(1,2075)	1:61:A:ILE:HG23	1:33:A:PRO:HD2	18	0.75
(1,1170)	1:114:A:ALA:HB3	1:112:A:ALA:H	18	0.75
(1,1095)	1:23:A:ALA:HB1	1:22:A:LEU:H	16	0.75
(1,932)	1:103:A:ALA:HB3	1:106:A:GLY:H	16	0.75
(1,906)	1:36:A:ALA:HB2	1:41:A:GLN:HE22	5	0.75
(1,885)	1:80:A:ALA:HB2	1:83:A:SER:H	3	0.75
(1,523)	1:44:A:LEU:HD23	1:44:A:LEU:H	9	0.75
(1,376)	1:73:A:ALA:HB2	1:77:A:PHE:H	5	0.75
(1,365)	1:101:A:GLU:HG3	1:104:A:ASN:H	2	0.75
(1,338)	1:65:A:LEU:HD11	1:65:A:LEU:H	15	0.75
(1,179)	1:38:A:ALA:HB3	1:40:A:VAL:H	12	0.75
(1,82)	1:34:A:ILE:HD12	1:32:A:ALA:H	11	0.75
(1,3734)	1:90:A:MET:HE2	1:93:A:PHE:HZ	11	0.74
(1,3733)	1:90:A:MET:HE2	1:93:A:PHE:HZ	11	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3673)	1:114:A:ALA:H	1:111:A:PHE:HD1	5	0.74
(1,3634)	1:65:A:LEU:HD11	1:70:A:PHE:HB3	7	0.74
(1,3380)	1:40:A:VAL:HG11	1:43:A:ARG:HD3	12	0.74
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE3	13	0.74
(1,3267)	1:31:A:MET:HG2	1:34:A:ILE:HD13	18	0.74
(1,3253)	1:32:A:ALA:H	1:34:A:ILE:HD11	13	0.74
(1,3194)	1:44:A:LEU:HA	1:79:A:ALA:HB1	13	0.74
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB2	7	0.74
(1,3015)	1:97:A:ALA:HB2	1:100:A:VAL:HG12	10	0.74
(1,2857)	1:44:A:LEU:H	1:44:A:LEU:HD23	18	0.74
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	5	0.74
(1,2640)	1:30:A:ILE:HD11	1:115:A:MET:HG3	13	0.74
(1,2618)	1:36:A:ALA:HB2	1:33:A:PRO:HB2	10	0.74
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	17	0.74
(1,2293)	1:34:A:ILE:HB	1:37:A:ASN:HB3	11	0.74
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	1	0.74
(1,1883)	1:74:A:LEU:HD23	1:74:A:LEU:HA	13	0.74
(1,1883)	1:35:A:LEU:HD22	1:74:A:LEU:HA	16	0.74
(1,1719)	1:100:A:VAL:HG13	1:96:A:PRO:HA	2	0.74
(1,1719)	1:100:A:VAL:HG12	1:96:A:PRO:HA	14	0.74
(1,1345)	1:35:A:LEU:HD12	1:31:A:MET:H	5	0.74
(1,1345)	1:35:A:LEU:HD13	1:31:A:MET:H	13	0.74
(1,1345)	1:35:A:LEU:HD13	1:31:A:MET:H	20	0.74
(1,1193)	1:108:A:VAL:HG13	1:107:A:ASP:H	17	0.74
(1,1158)	1:119:A:ALA:HB2	1:120:A:LYS:H	9	0.74
(1,1116)	1:95:A:LEU:HA	1:119:A:ALA:H	9	0.74
(1,1102)	1:56:A:GLN:HB3	1:58:A:ALA:H	15	0.74
(1,1095)	1:23:A:ALA:HB2	1:22:A:LEU:H	18	0.74
(1,1095)	1:23:A:ALA:HB3	1:22:A:LEU:H	20	0.74
(1,932)	1:103:A:ALA:HB3	1:106:A:GLY:H	20	0.74
(1,885)	1:80:A:ALA:HB3	1:83:A:SER:H	2	0.74
(1,827)	1:4:A:ILE:HD12	1:2:A:ASN:HD21	3	0.74
(1,795)	1:65:A:LEU:HD23	1:64:A:THR:H	1	0.74
(1,523)	1:44:A:LEU:HD23	1:44:A:LEU:H	18	0.74
(1,375)	1:99:A:ALA:HB2	1:103:A:ALA:H	7	0.74
(1,365)	1:101:A:GLU:HG3	1:104:A:ASN:H	13	0.74
(1,365)	1:101:A:GLU:HG3	1:104:A:ASN:H	16	0.74
(1,298)	1:112:A:ALA:HB2	1:116:A:GLN:H	5	0.74
(1,234)	1:44:A:LEU:HD23	1:76:A:MET:H	2	0.74
(1,232)	1:73:A:ALA:HB1	1:76:A:MET:H	10	0.74
(1,114)	1:81:A:LEU:HB2	1:79:A:ALA:H	13	0.74
(1,82)	1:34:A:ILE:HD11	1:32:A:ALA:H	13	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3673)	1:107:A:ASP:H	1:111:A:PHE:HD1	6	0.73
(1,3673)	1:114:A:ALA:H	1:111:A:PHE:HD1	8	0.73
(1,3673)	1:107:A:ASP:H	1:111:A:PHE:HD1	17	0.73
(1,3561)	1:90:A:MET:HB3	1:34:A:ILE:HG23	9	0.73
(1,3551)	1:56:A:GLN:HA	1:36:A:ALA:HB3	20	0.73
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG21	4	0.73
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB3	18	0.73
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD11	14	0.73
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD11	19	0.73
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD11	20	0.73
(1,3441)	1:99:A:ALA:HB1	1:96:A:PRO:HB3	3	0.73
(1,3441)	1:99:A:ALA:HB1	1:96:A:PRO:HB3	19	0.73
(1,3272)	1:96:A:PRO:HD3	1:115:A:MET:HE2	18	0.73
(1,3253)	1:32:A:ALA:H	1:34:A:ILE:HD12	16	0.73
(1,3239)	1:86:A:LEU:HD12	1:90:A:MET:HE3	12	0.73
(1,3239)	1:34:A:ILE:HD12	1:90:A:MET:HE2	19	0.73
(1,3106)	1:40:A:VAL:HG23	1:35:A:LEU:HD11	18	0.73
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG13	4	0.73
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG13	19	0.73
(1,3015)	1:97:A:ALA:HB1	1:100:A:VAL:HG13	15	0.73
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD23	14	0.73
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD11	13	0.73
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD13	19	0.73
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD11	6	0.73
(1,2801)	1:81:A:LEU:H	1:86:A:LEU:HD11	1	0.73
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD12	14	0.73
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD11	2	0.73
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	1	0.73
(1,2699)	1:93:A:PHE:HD2	1:34:A:ILE:HG13	2	0.73
(1,2699)	1:93:A:PHE:HD1	1:34:A:ILE:HG13	7	0.73
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	10	0.73
(1,2456)	1:63:A:ASN:H	1:55:A:PRO:HB3	1	0.73
(1,2293)	1:38:A:ALA:HB3	1:37:A:ASN:HB3	5	0.73
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	7	0.73
(1,1719)	1:100:A:VAL:HG12	1:96:A:PRO:HA	20	0.73
(1,1310)	1:89:A:LEU:HD23	1:86:A:LEU:H	10	0.73
(1,1193)	1:108:A:VAL:HG11	1:107:A:ASP:H	5	0.73
(1,1170)	1:74:A:LEU:HG	1:23:A:ALA:H	8	0.73
(1,1158)	1:119:A:ALA:HB1	1:120:A:LYS:H	13	0.73
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	10	0.73
(1,1116)	1:96:A:PRO:HA	1:119:A:ALA:H	6	0.73
(1,906)	1:58:A:ALA:HB2	1:62:A:GLN:HE22	9	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:36:A:ALA:HB3	1:41:A:GLN:HE21	9	0.73
(1,578)	1:112:A:ALA:HB1	1:25:A:VAL:H	2	0.73
(1,562)	1:95:A:LEU:HD21	1:93:A:PHE:H	6	0.73
(1,523)	1:44:A:LEU:HD22	1:44:A:LEU:H	11	0.73
(1,425)	1:57:A:THR:HG22	1:60:A:GLU:H	14	0.73
(1,376)	1:73:A:ALA:HB3	1:77:A:PHE:H	11	0.73
(1,376)	1:73:A:ALA:HB3	1:77:A:PHE:H	12	0.73
(1,375)	1:99:A:ALA:HB2	1:103:A:ALA:H	19	0.73
(1,365)	1:101:A:GLU:HG3	1:104:A:ASN:H	1	0.73
(1,338)	1:61:A:ILE:HG21	1:65:A:LEU:H	2	0.73
(1,338)	1:65:A:LEU:HD11	1:65:A:LEU:H	11	0.73
(1,338)	1:65:A:LEU:HD11	1:65:A:LEU:H	19	0.73
(1,305)	1:25:A:VAL:HG22	1:116:A:GLN:H	4	0.73
(1,305)	1:25:A:VAL:HG23	1:116:A:GLN:H	11	0.73
(1,298)	1:119:A:ALA:HB3	1:116:A:GLN:H	19	0.73
(1,234)	1:44:A:LEU:HD21	1:76:A:MET:H	7	0.73
(1,82)	1:34:A:ILE:HD12	1:32:A:ALA:H	16	0.73
(1,3734)	1:90:A:MET:HE2	1:93:A:PHE:HZ	9	0.72
(1,3733)	1:90:A:MET:HE2	1:93:A:PHE:HZ	9	0.72
(1,3634)	1:65:A:LEU:HD12	1:70:A:PHE:HB3	4	0.72
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD11	20	0.72
(1,3551)	1:56:A:GLN:HA	1:36:A:ALA:HB3	7	0.72
(1,3498)	1:102:A:ALA:HB1	1:81:A:LEU:HD12	2	0.72
(1,3441)	1:99:A:ALA:HB1	1:96:A:PRO:HB3	4	0.72
(1,3253)	1:32:A:ALA:H	1:61:A:ILE:HD12	10	0.72
(1,3239)	1:86:A:LEU:HD13	1:90:A:MET:HE2	11	0.72
(1,3239)	1:34:A:ILE:HD11	1:90:A:MET:HE1	17	0.72
(1,3238)	1:40:A:VAL:HG21	1:90:A:MET:HE2	6	0.72
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD22	1	0.72
(1,2912)	1:85:A:GLN:HA	1:89:A:LEU:HD23	7	0.72
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD22	3	0.72
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD22	8	0.72
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD23	14	0.72
(1,2857)	1:44:A:LEU:H	1:44:A:LEU:HD22	7	0.72
(1,2618)	1:36:A:ALA:HB2	1:33:A:PRO:HB2	1	0.72
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	14	0.72
(1,2293)	1:38:A:ALA:HB1	1:37:A:ASN:HB3	3	0.72
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	4	0.72
(1,2075)	1:61:A:ILE:HG22	1:33:A:PRO:HD2	10	0.72
(1,1345)	1:35:A:LEU:HD11	1:31:A:MET:H	14	0.72
(1,1344)	1:30:A:ILE:HD12	1:31:A:MET:H	1	0.72
(1,1344)	1:30:A:ILE:HD11	1:31:A:MET:H	16	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1158)	1:119:A:ALA:HB2	1:120:A:LYS:H	19	0.72
(1,1116)	1:96:A:PRO:HA	1:119:A:ALA:H	2	0.72
(1,1018)	1:77:A:PHE:HD2	1:81:A:LEU:H	7	0.72
(1,906)	1:58:A:ALA:HB3	1:62:A:GLN:HE22	6	0.72
(1,906)	1:36:A:ALA:HB3	1:41:A:GLN:HE22	20	0.72
(1,885)	1:80:A:ALA:HB3	1:83:A:SER:H	8	0.72
(1,885)	1:80:A:ALA:HB2	1:83:A:SER:H	17	0.72
(1,885)	1:80:A:ALA:HB3	1:83:A:SER:H	20	0.72
(1,849)	1:35:A:LEU:HB2	1:41:A:GLN:HE21	18	0.72
(1,578)	1:112:A:ALA:HB2	1:25:A:VAL:H	8	0.72
(1,523)	1:44:A:LEU:HD22	1:44:A:LEU:H	7	0.72
(1,505)	1:30:A:ILE:HD13	1:117:A:ASN:H	7	0.72
(1,376)	1:73:A:ALA:HB2	1:77:A:PHE:H	16	0.72
(1,375)	1:99:A:ALA:HB1	1:103:A:ALA:H	8	0.72
(1,307)	1:25:A:VAL:HG22	1:114:A:ALA:H	17	0.72
(1,305)	1:26:A:LEU:HD22	1:116:A:GLN:H	12	0.72
(1,298)	1:112:A:ALA:HB1	1:116:A:GLN:H	17	0.72
(1,234)	1:44:A:LEU:HD21	1:76:A:MET:H	5	0.72
(1,234)	1:44:A:LEU:HD23	1:76:A:MET:H	16	0.72
(1,232)	1:73:A:ALA:HB1	1:76:A:MET:H	6	0.72
(1,179)	1:38:A:ALA:HB1	1:40:A:VAL:H	10	0.72
(1,114)	1:82:A:ALA:HB1	1:79:A:ALA:H	12	0.72
(1,82)	1:61:A:ILE:HD12	1:32:A:ALA:H	10	0.72
(1,3673)	1:107:A:ASP:H	1:111:A:PHE:HD1	16	0.71
(1,3642)	1:74:A:LEU:HD23	1:70:A:PHE:HA	7	0.71
(1,3498)	1:31:A:MET:HE3	1:81:A:LEU:HD13	15	0.71
(1,3497)	1:85:A:GLN:HB3	1:86:A:LEU:HD22	11	0.71
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD12	18	0.71
(1,3377)	1:45:A:LEU:HD23	1:46:A:PRO:HD2	20	0.71
(1,3253)	1:32:A:ALA:H	1:61:A:ILE:HD13	1	0.71
(1,3253)	1:32:A:ALA:H	1:61:A:ILE:HD13	15	0.71
(1,3239)	1:86:A:LEU:HD12	1:90:A:MET:HE1	3	0.71
(1,3126)	1:111:A:PHE:H	1:114:A:ALA:HB3	8	0.71
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB3	10	0.71
(1,3106)	1:40:A:VAL:HG22	1:35:A:LEU:HD12	2	0.71
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG13	10	0.71
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG12	17	0.71
(1,3015)	1:97:A:ALA:HB2	1:100:A:VAL:HG13	8	0.71
(1,2994)	1:41:A:GLN:HG2	1:35:A:LEU:HD23	3	0.71
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD13	17	0.71
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD21	9	0.71
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD23	13	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD13	10	0.71
(1,2699)	1:93:A:PHE:HD2	1:34:A:ILE:HG13	16	0.71
(1,1719)	1:100:A:VAL:HG13	1:96:A:PRO:HA	3	0.71
(1,1345)	1:35:A:LEU:HD12	1:31:A:MET:H	11	0.71
(1,1345)	1:35:A:LEU:HD11	1:31:A:MET:H	16	0.71
(1,1345)	1:35:A:LEU:HD12	1:31:A:MET:H	19	0.71
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	15	0.71
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	12	0.71
(1,1144)	1:90:A:MET:HE3	1:81:A:LEU:H	1	0.71
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	19	0.71
(1,683)	1:40:A:VAL:HG12	1:37:A:ASN:HD21	9	0.71
(1,523)	1:44:A:LEU:HD22	1:44:A:LEU:H	12	0.71
(1,505)	1:25:A:VAL:HG22	1:117:A:ASN:H	14	0.71
(1,375)	1:99:A:ALA:HB3	1:103:A:ALA:H	10	0.71
(1,338)	1:65:A:LEU:HD13	1:65:A:LEU:H	4	0.71
(1,307)	1:25:A:VAL:HG22	1:114:A:ALA:H	2	0.71
(1,234)	1:44:A:LEU:HD22	1:76:A:MET:H	3	0.71
(1,234)	1:44:A:LEU:HD23	1:76:A:MET:H	6	0.71
(1,114)	1:81:A:LEU:HB2	1:79:A:ALA:H	14	0.71
(1,114)	1:82:A:ALA:HB3	1:79:A:ALA:H	20	0.71
(1,82)	1:61:A:ILE:HD13	1:32:A:ALA:H	1	0.71
(1,82)	1:61:A:ILE:HD13	1:32:A:ALA:H	15	0.71
(1,3673)	1:114:A:ALA:H	1:111:A:PHE:HD2	1	0.7
(1,3642)	1:74:A:LEU:HD23	1:70:A:PHE:HA	8	0.7
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD13	6	0.7
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG23	5	0.7
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD11	17	0.7
(1,3441)	1:114:A:ALA:HB3	1:96:A:PRO:HB3	17	0.7
(1,3380)	1:40:A:VAL:HG11	1:43:A:ARG:HD3	7	0.7
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE1	1	0.7
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE1	13	0.7
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB3	6	0.7
(1,3106)	1:40:A:VAL:HG22	1:35:A:LEU:HD13	5	0.7
(1,3106)	1:40:A:VAL:HG23	1:35:A:LEU:HD12	7	0.7
(1,3106)	1:40:A:VAL:HG21	1:35:A:LEU:HD11	9	0.7
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD13	18	0.7
(1,2871)	1:87:A:GLY:H	1:86:A:LEU:HD12	1	0.7
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD12	4	0.7
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD12	19	0.7
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD13	13	0.7
(1,2617)	1:99:A:ALA:HB3	1:100:A:VAL:HB	14	0.7
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	2	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	8	0.7
(1,1719)	1:100:A:VAL:HG12	1:96:A:PRO:HA	11	0.7
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	11	0.7
(1,1429)	1:116:A:GLN:HB3	1:119:A:ALA:H	10	0.7
(1,1429)	1:116:A:GLN:HB3	1:119:A:ALA:H	11	0.7
(1,1429)	1:116:A:GLN:HB3	1:119:A:ALA:H	14	0.7
(1,1345)	1:35:A:LEU:HD13	1:31:A:MET:H	15	0.7
(1,1275)	1:88:A:PRO:HB2	1:91:A:CYS:H	8	0.7
(1,1232)	1:57:A:THR:HG22	1:59:A:ASP:H	9	0.7
(1,1158)	1:119:A:ALA:HB3	1:120:A:LYS:H	12	0.7
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	6	0.7
(1,1145)	1:43:A:ARG:HB3	1:81:A:LEU:H	4	0.7
(1,1116)	1:96:A:PRO:HA	1:119:A:ALA:H	16	0.7
(1,1027)	1:100:A:VAL:HG23	1:92:A:GLN:H	1	0.7
(1,1014)	1:86:A:LEU:HD12	1:40:A:VAL:H	7	0.7
(1,932)	1:103:A:ALA:HB2	1:106:A:GLY:H	4	0.7
(1,906)	1:36:A:ALA:HB3	1:41:A:GLN:HE22	16	0.7
(1,885)	1:80:A:ALA:HB2	1:83:A:SER:H	1	0.7
(1,849)	1:36:A:ALA:HB1	1:41:A:GLN:HE21	4	0.7
(1,578)	1:23:A:ALA:HB2	1:25:A:VAL:H	3	0.7
(1,578)	1:23:A:ALA:HB3	1:25:A:VAL:H	5	0.7
(1,578)	1:112:A:ALA:HB1	1:25:A:VAL:H	11	0.7
(1,578)	1:23:A:ALA:HB1	1:25:A:VAL:H	17	0.7
(1,375)	1:99:A:ALA:HB3	1:103:A:ALA:H	6	0.7
(1,307)	1:26:A:LEU:HD21	1:114:A:ALA:H	7	0.7
(1,236)	1:74:A:LEU:HD11	1:76:A:MET:H	12	0.7
(1,179)	1:38:A:ALA:HB1	1:40:A:VAL:H	17	0.7
(1,3734)	1:90:A:MET:HE1	1:93:A:PHE:HZ	3	0.69
(1,3733)	1:90:A:MET:HE1	1:93:A:PHE:HZ	3	0.69
(1,3642)	1:74:A:LEU:HD21	1:70:A:PHE:HA	20	0.69
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD11	18	0.69
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB3	12	0.69
(1,3504)	1:31:A:MET:HE2	1:86:A:LEU:HD21	13	0.69
(1,3388)	1:20:A:VAL:HA	1:21:A:ASP:HB2	3	0.69
(1,3377)	1:45:A:LEU:HD21	1:46:A:PRO:HD2	11	0.69
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB2	2	0.69
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE2	11	0.69
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG11	18	0.69
(1,2921)	1:32:A:ALA:HA	1:35:A:LEU:HD21	18	0.69
(1,2857)	1:44:A:LEU:H	1:44:A:LEU:HD21	2	0.69
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD12	16	0.69
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	18	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2293)	1:38:A:ALA:HB2	1:37:A:ASN:HB3	7	0.69
(1,2293)	1:38:A:ALA:HB1	1:37:A:ASN:HB3	17	0.69
(1,2252)	1:41:A:GLN:HA	1:54:A:LEU:HB3	15	0.69
(1,1883)	1:35:A:LEU:HD22	1:74:A:LEU:HA	9	0.69
(1,1719)	1:100:A:VAL:HG11	1:96:A:PRO:HA	17	0.69
(1,1572)	1:48:A:LEU:HD11	1:53:A:SER:HB2	8	0.69
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	1	0.69
(1,1345)	1:35:A:LEU:HD11	1:31:A:MET:H	7	0.69
(1,1345)	1:35:A:LEU:HD12	1:31:A:MET:H	8	0.69
(1,1345)	1:35:A:LEU:HD13	1:31:A:MET:H	17	0.69
(1,1344)	1:30:A:ILE:HD12	1:31:A:MET:H	3	0.69
(1,1344)	1:30:A:ILE:HD13	1:31:A:MET:H	18	0.69
(1,1320)	1:61:A:ILE:HD12	1:35:A:LEU:H	10	0.69
(1,1275)	1:88:A:PRO:HB2	1:91:A:CYS:H	2	0.69
(1,1275)	1:89:A:LEU:HB3	1:91:A:CYS:H	18	0.69
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	2	0.69
(1,1027)	1:100:A:VAL:HG21	1:92:A:GLN:H	14	0.69
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	13	0.69
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	18	0.69
(1,885)	1:80:A:ALA:HB1	1:83:A:SER:H	4	0.69
(1,849)	1:36:A:ALA:HB2	1:41:A:GLN:HE21	14	0.69
(1,523)	1:44:A:LEU:HD21	1:44:A:LEU:H	2	0.69
(1,338)	1:65:A:LEU:HD12	1:65:A:LEU:H	16	0.69
(1,298)	1:119:A:ALA:HB2	1:116:A:GLN:H	13	0.69
(1,234)	1:44:A:LEU:HD21	1:76:A:MET:H	4	0.69
(1,234)	1:44:A:LEU:HD22	1:76:A:MET:H	19	0.69
(1,179)	1:38:A:ALA:HB2	1:40:A:VAL:H	8	0.69
(1,114)	1:82:A:ALA:HB1	1:79:A:ALA:H	5	0.69
(1,114)	1:82:A:ALA:HB3	1:79:A:ALA:H	8	0.69
(1,60)	1:54:A:LEU:HD13	1:54:A:LEU:H	6	0.69
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD13	11	0.68
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD11	12	0.68
(1,3551)	1:56:A:GLN:HA	1:36:A:ALA:HB2	5	0.68
(1,3504)	1:31:A:MET:HE2	1:86:A:LEU:HD23	5	0.68
(1,3504)	1:31:A:MET:HE3	1:86:A:LEU:HD23	15	0.68
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD12	18	0.68
(1,3377)	1:45:A:LEU:HD23	1:46:A:PRO:HD2	5	0.68
(1,3377)	1:45:A:LEU:HD23	1:46:A:PRO:HD2	12	0.68
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD11	11	0.68
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB3	9	0.68
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE2	4	0.68
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB3	15	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB2	9	0.68
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD13	13	0.68
(1,3015)	1:97:A:ALA:HB1	1:100:A:VAL:HG13	6	0.68
(1,3015)	1:97:A:ALA:HB2	1:100:A:VAL:HG11	13	0.68
(1,3015)	1:97:A:ALA:HB2	1:100:A:VAL:HG11	17	0.68
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD12	3	0.68
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD21	7	0.68
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD11	11	0.68
(1,2857)	1:44:A:LEU:H	1:44:A:LEU:HD21	10	0.68
(1,1975)	1:27:A:THR:HG21	1:26:A:LEU:HA	18	0.68
(1,1719)	1:100:A:VAL:HG13	1:96:A:PRO:HA	8	0.68
(1,1563)	1:112:A:ALA:HB2	1:108:A:VAL:HA	14	0.68
(1,1558)	1:30:A:ILE:HG13	1:28:A:PRO:HA	2	0.68
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	2	0.68
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	6	0.68
(1,1344)	1:30:A:ILE:HD12	1:31:A:MET:H	8	0.68
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	18	0.68
(1,1193)	1:108:A:VAL:HG11	1:107:A:ASP:H	16	0.68
(1,1170)	1:74:A:LEU:HG	1:23:A:ALA:H	10	0.68
(1,1027)	1:100:A:VAL:HG21	1:92:A:GLN:H	3	0.68
(1,921)	1:72:A:GLN:HB3	1:75:A:GLY:H	1	0.68
(1,849)	1:36:A:ALA:HB3	1:41:A:GLN:HE21	2	0.68
(1,578)	1:23:A:ALA:HB2	1:25:A:VAL:H	7	0.68
(1,523)	1:44:A:LEU:HD21	1:44:A:LEU:H	10	0.68
(1,523)	1:54:A:LEU:HD11	1:44:A:LEU:H	16	0.68
(1,376)	1:73:A:ALA:HB1	1:77:A:PHE:H	15	0.68
(1,375)	1:99:A:ALA:HB3	1:103:A:ALA:H	15	0.68
(1,338)	1:65:A:LEU:HD12	1:65:A:LEU:H	17	0.68
(1,236)	1:74:A:LEU:HD13	1:76:A:MET:H	2	0.68
(1,232)	1:73:A:ALA:HB2	1:76:A:MET:H	1	0.68
(1,3504)	1:31:A:MET:HE1	1:86:A:LEU:HD21	6	0.67
(1,3498)	1:102:A:ALA:HB1	1:81:A:LEU:HD13	18	0.67
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD12	6	0.67
(1,3377)	1:45:A:LEU:HD23	1:46:A:PRO:HD2	1	0.67
(1,3377)	1:45:A:LEU:HD21	1:46:A:PRO:HD2	6	0.67
(1,3377)	1:45:A:LEU:HD21	1:46:A:PRO:HD2	9	0.67
(1,3253)	1:32:A:ALA:H	1:34:A:ILE:HD13	19	0.67
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB3	13	0.67
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD13	15	0.67
(1,3015)	1:97:A:ALA:HB1	1:100:A:VAL:HG13	3	0.67
(1,2921)	1:32:A:ALA:HA	1:35:A:LEU:HD21	16	0.67
(1,2920)	1:87:A:GLY:HA3	1:86:A:LEU:HD23	9	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD22	5	0.67
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD21	19	0.67
(1,2699)	1:93:A:PHE:HD1	1:34:A:ILE:HG13	14	0.67
(1,2630)	1:34:A:ILE:HD12	1:90:A:MET:HG3	19	0.67
(1,2622)	1:30:A:ILE:HG13	1:115:A:MET:HG3	7	0.67
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	15	0.67
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	15	0.67
(1,2075)	1:61:A:ILE:HG22	1:33:A:PRO:HD2	9	0.67
(1,2075)	1:61:A:ILE:HG22	1:33:A:PRO:HD2	12	0.67
(1,1975)	1:27:A:THR:HG22	1:26:A:LEU:HA	5	0.67
(1,1572)	1:48:A:LEU:HD13	1:53:A:SER:HB2	16	0.67
(1,1558)	1:30:A:ILE:HG13	1:28:A:PRO:HA	8	0.67
(1,1344)	1:30:A:ILE:HD11	1:31:A:MET:H	9	0.67
(1,1275)	1:89:A:LEU:HB3	1:91:A:CYS:H	12	0.67
(1,1275)	1:89:A:LEU:HB3	1:91:A:CYS:H	19	0.67
(1,1165)	1:70:A:PHE:HD2	1:23:A:ALA:H	8	0.67
(1,1138)	1:87:A:GLY:HA2	1:81:A:LEU:H	8	0.67
(1,1042)	1:30:A:ILE:HD11	1:29:A:GLU:H	7	0.67
(1,1014)	1:86:A:LEU:HD13	1:40:A:VAL:H	19	0.67
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	15	0.67
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	20	0.67
(1,849)	1:36:A:ALA:HB1	1:41:A:GLN:HE21	3	0.67
(1,578)	1:23:A:ALA:HB3	1:25:A:VAL:H	13	0.67
(1,376)	1:73:A:ALA:HB3	1:77:A:PHE:H	7	0.67
(1,376)	1:73:A:ALA:HB2	1:77:A:PHE:H	19	0.67
(1,375)	1:99:A:ALA:HB3	1:103:A:ALA:H	13	0.67
(1,375)	1:99:A:ALA:HB2	1:103:A:ALA:H	14	0.67
(1,365)	1:101:A:GLU:HG3	1:104:A:ASN:H	19	0.67
(1,305)	1:26:A:LEU:HD21	1:116:A:GLN:H	5	0.67
(1,298)	1:119:A:ALA:HB3	1:116:A:GLN:H	18	0.67
(1,234)	1:44:A:LEU:HD22	1:76:A:MET:H	9	0.67
(1,232)	1:73:A:ALA:HB1	1:76:A:MET:H	17	0.67
(1,114)	1:82:A:ALA:HB2	1:79:A:ALA:H	17	0.67
(1,82)	1:34:A:ILE:HD13	1:32:A:ALA:H	19	0.67
(1,3645)	1:55:A:PRO:HD2	1:35:A:LEU:HD11	7	0.66
(1,3615)	1:29:A:GLU:HG3	1:30:A:ILE:HD13	17	0.66
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD13	16	0.66
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD11	19	0.66
(1,3561)	1:31:A:MET:HG3	1:34:A:ILE:HG23	16	0.66
(1,3551)	1:57:A:THR:HB	1:36:A:ALA:HB1	8	0.66
(1,3551)	1:57:A:THR:HB	1:36:A:ALA:HB2	14	0.66
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG21	8	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3377)	1:45:A:LEU:HD21	1:46:A:PRO:HD2	8	0.66
(1,3377)	1:45:A:LEU:HD22	1:46:A:PRO:HD2	10	0.66
(1,3377)	1:45:A:LEU:HD23	1:46:A:PRO:HD2	17	0.66
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB1	19	0.66
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE1	3	0.66
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG22	1	0.66
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD12	6	0.66
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD12	19	0.66
(1,3015)	1:97:A:ALA:HB1	1:100:A:VAL:HG13	2	0.66
(1,2921)	1:32:A:ALA:HA	1:35:A:LEU:HD23	19	0.66
(1,2920)	1:87:A:GLY:HA3	1:86:A:LEU:HD21	11	0.66
(1,2920)	1:87:A:GLY:HA3	1:86:A:LEU:HD21	15	0.66
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD13	5	0.66
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD21	20	0.66
(1,2618)	1:36:A:ALA:HB3	1:33:A:PRO:HB2	14	0.66
(1,2618)	1:36:A:ALA:HB1	1:33:A:PRO:HB2	18	0.66
(1,2617)	1:95:A:LEU:HD22	1:90:A:MET:HB2	9	0.66
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	9	0.66
(1,2293)	1:34:A:ILE:HB	1:37:A:ASN:HB3	8	0.66
(1,1975)	1:27:A:THR:HG21	1:26:A:LEU:HA	12	0.66
(1,1734)	1:44:A:LEU:HD13	1:76:A:MET:HA	10	0.66
(1,1563)	1:112:A:ALA:HB1	1:108:A:VAL:HA	1	0.66
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	9	0.66
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	10	0.66
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	16	0.66
(1,1429)	1:116:A:GLN:HB3	1:119:A:ALA:H	4	0.66
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	20	0.66
(1,1361)	1:88:A:PRO:HA	1:104:A:ASN:HD21	19	0.66
(1,1344)	1:30:A:ILE:HD11	1:31:A:MET:H	5	0.66
(1,1344)	1:30:A:ILE:HD12	1:31:A:MET:H	17	0.66
(1,1232)	1:57:A:THR:HG22	1:59:A:ASP:H	11	0.66
(1,1193)	1:108:A:VAL:HG13	1:107:A:ASP:H	7	0.66
(1,1170)	1:74:A:LEU:HG	1:23:A:ALA:H	1	0.66
(1,1168)	1:131:A:LYS:HB3	1:134:A:GLU:H	16	0.66
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	5	0.66
(1,906)	1:36:A:ALA:HB2	1:41:A:GLN:HE22	14	0.66
(1,885)	1:80:A:ALA:HB3	1:83:A:SER:H	11	0.66
(1,827)	1:4:A:ILE:HD12	1:2:A:ASN:HD21	12	0.66
(1,827)	1:4:A:ILE:HD13	1:2:A:ASN:HD21	20	0.66
(1,578)	1:23:A:ALA:HB3	1:25:A:VAL:H	6	0.66
(1,578)	1:23:A:ALA:HB2	1:25:A:VAL:H	12	0.66
(1,578)	1:23:A:ALA:HB1	1:25:A:VAL:H	15	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,578)	1:23:A:ALA:HB3	1:25:A:VAL:H	20	0.66
(1,522)	1:114:A:ALA:HB3	1:113:A:LYS:H	9	0.66
(1,376)	1:73:A:ALA:HB1	1:77:A:PHE:H	6	0.66
(1,365)	1:101:A:GLU:HG3	1:104:A:ASN:H	3	0.66
(1,365)	1:101:A:GLU:HG2	1:104:A:ASN:H	12	0.66
(1,338)	1:61:A:ILE:HG23	1:65:A:LEU:H	12	0.66
(1,338)	1:65:A:LEU:HD12	1:65:A:LEU:H	20	0.66
(1,236)	1:74:A:LEU:HD12	1:76:A:MET:H	19	0.66
(1,234)	1:44:A:LEU:HD21	1:76:A:MET:H	8	0.66
(1,232)	1:73:A:ALA:HB3	1:76:A:MET:H	9	0.66
(1,60)	1:54:A:LEU:HD11	1:54:A:LEU:H	15	0.66
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	2	0.65
(1,3766)	1:83:A:SER:H	1:47:A:TYR:HE2	19	0.65
(1,3645)	1:55:A:PRO:HD2	1:35:A:LEU:HD12	5	0.65
(1,3645)	1:40:A:VAL:HA	1:35:A:LEU:HD12	16	0.65
(1,3615)	1:29:A:GLU:HG3	1:30:A:ILE:HD13	13	0.65
(1,3568)	1:114:A:ALA:HB2	1:102:A:ALA:HB1	19	0.65
(1,3498)	1:102:A:ALA:HB1	1:81:A:LEU:HD12	8	0.65
(1,3497)	1:76:A:MET:HB2	1:86:A:LEU:HD22	15	0.65
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD12	9	0.65
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	18	0.65
(1,3441)	1:114:A:ALA:HB1	1:96:A:PRO:HB3	6	0.65
(1,3441)	1:99:A:ALA:HB2	1:96:A:PRO:HB3	11	0.65
(1,3380)	1:40:A:VAL:HG11	1:43:A:ARG:HD3	19	0.65
(1,3377)	1:45:A:LEU:HD23	1:46:A:PRO:HD2	2	0.65
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB2	18	0.65
(1,3106)	1:40:A:VAL:HG22	1:35:A:LEU:HD12	3	0.65
(1,2920)	1:87:A:GLY:HA3	1:86:A:LEU:HD23	20	0.65
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD12	8	0.65
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD12	11	0.65
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD23	10	0.65
(1,2857)	1:44:A:LEU:H	1:44:A:LEU:HD21	6	0.65
(1,2617)	1:95:A:LEU:HD22	1:90:A:MET:HB2	18	0.65
(1,2296)	1:102:A:ALA:HB1	1:111:A:PHE:HB3	15	0.65
(1,2075)	1:61:A:ILE:HG23	1:33:A:PRO:HD2	6	0.65
(1,1883)	1:35:A:LEU:HD21	1:74:A:LEU:HA	11	0.65
(1,1558)	1:30:A:ILE:HG13	1:28:A:PRO:HA	10	0.65
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	18	0.65
(1,1429)	1:116:A:GLN:HB3	1:119:A:ALA:H	18	0.65
(1,1193)	1:108:A:VAL:HG11	1:107:A:ASP:H	6	0.65
(1,1170)	1:74:A:LEU:HG	1:23:A:ALA:H	2	0.65
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1135)	1:44:A:LEU:HD12	1:79:A:ALA:H	19	0.65
(1,1063)	1:95:A:LEU:HD23	1:94:A:GLY:H	10	0.65
(1,932)	1:103:A:ALA:HB3	1:106:A:GLY:H	10	0.65
(1,795)	1:65:A:LEU:HD21	1:64:A:THR:H	18	0.65
(1,759)	1:60:A:GLU:HB3	1:63:A:ASN:HD21	20	0.65
(1,578)	1:23:A:ALA:HB1	1:25:A:VAL:H	19	0.65
(1,523)	1:44:A:LEU:HD21	1:44:A:LEU:H	6	0.65
(1,505)	1:25:A:VAL:HG22	1:117:A:ASN:H	13	0.65
(1,376)	1:73:A:ALA:HB3	1:77:A:PHE:H	2	0.65
(1,376)	1:73:A:ALA:HB1	1:77:A:PHE:H	17	0.65
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	8	0.65
(1,365)	1:101:A:GLU:HG2	1:104:A:ASN:H	9	0.65
(1,307)	1:25:A:VAL:HG23	1:114:A:ALA:H	4	0.65
(1,307)	1:25:A:VAL:HG22	1:114:A:ALA:H	9	0.65
(1,305)	1:25:A:VAL:HG21	1:116:A:GLN:H	9	0.65
(1,303)	1:73:A:ALA:HB3	1:72:A:GLN:H	18	0.65
(1,234)	1:44:A:LEU:HD21	1:76:A:MET:H	12	0.65
(1,231)	1:97:A:ALA:HB1	1:99:A:ALA:H	14	0.65
(1,114)	1:81:A:LEU:HB2	1:79:A:ALA:H	15	0.65
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	4	0.64
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	6	0.64
(1,3673)	1:114:A:ALA:H	1:111:A:PHE:HD1	11	0.64
(1,3673)	1:107:A:ASP:H	1:111:A:PHE:HD1	20	0.64
(1,3634)	1:65:A:LEU:HD11	1:70:A:PHE:HB3	16	0.64
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD11	9	0.64
(1,3568)	1:114:A:ALA:HB3	1:102:A:ALA:HB3	10	0.64
(1,3565)	1:90:A:MET:HE1	1:31:A:MET:HE2	1	0.64
(1,3561)	1:90:A:MET:HB3	1:34:A:ILE:HG23	4	0.64
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE1	6	0.64
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG23	6	0.64
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD11	4	0.64
(1,3377)	1:45:A:LEU:HD21	1:46:A:PRO:HD2	7	0.64
(1,3377)	1:45:A:LEU:HD22	1:46:A:PRO:HD2	15	0.64
(1,3253)	1:32:A:ALA:H	1:61:A:ILE:HD11	17	0.64
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG12	7	0.64
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD11	16	0.64
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD22	16	0.64
(1,2921)	1:73:A:ALA:HA	1:35:A:LEU:HD22	5	0.64
(1,2915)	1:21:A:ASP:HA	1:22:A:LEU:HD13	11	0.64
(1,2622)	1:99:A:ALA:HB3	1:115:A:MET:HG3	10	0.64
(1,2618)	1:36:A:ALA:HB2	1:33:A:PRO:HB2	12	0.64
(1,2293)	1:34:A:ILE:HB	1:37:A:ASN:HB3	12	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	14	0.64
(1,1975)	1:27:A:THR:HG21	1:26:A:LEU:HA	9	0.64
(1,1975)	1:27:A:THR:HG23	1:26:A:LEU:HA	20	0.64
(1,1859)	1:64:A:THR:HG22	1:60:A:GLU:HA	5	0.64
(1,1737)	1:54:A:LEU:HD13	1:41:A:GLN:HA	15	0.64
(1,1558)	1:30:A:ILE:HG13	1:28:A:PRO:HA	11	0.64
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	3	0.64
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	7	0.64
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	12	0.64
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	15	0.64
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	20	0.64
(1,1232)	1:57:A:THR:HG21	1:59:A:ASP:H	7	0.64
(1,1193)	1:108:A:VAL:HG11	1:107:A:ASP:H	4	0.64
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	2	0.64
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	5	0.64
(1,921)	1:72:A:GLN:HB3	1:75:A:GLY:H	10	0.64
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	16	0.64
(1,885)	1:80:A:ALA:HB1	1:83:A:SER:H	7	0.64
(1,827)	1:4:A:ILE:HD11	1:2:A:ASN:HD21	4	0.64
(1,505)	1:25:A:VAL:HG21	1:117:A:ASN:H	6	0.64
(1,376)	1:73:A:ALA:HB1	1:77:A:PHE:H	14	0.64
(1,365)	1:101:A:GLU:HG3	1:104:A:ASN:H	20	0.64
(1,338)	1:65:A:LEU:HD12	1:65:A:LEU:H	7	0.64
(1,338)	1:65:A:LEU:HD11	1:65:A:LEU:H	10	0.64
(1,338)	1:61:A:ILE:HG22	1:65:A:LEU:H	14	0.64
(1,307)	1:25:A:VAL:HG21	1:114:A:ALA:H	14	0.64
(1,307)	1:26:A:LEU:HD23	1:114:A:ALA:H	20	0.64
(1,234)	1:44:A:LEU:HD22	1:76:A:MET:H	15	0.64
(1,231)	1:97:A:ALA:HB2	1:99:A:ALA:H	9	0.64
(1,114)	1:82:A:ALA:HB1	1:79:A:ALA:H	18	0.64
(1,82)	1:61:A:ILE:HD11	1:32:A:ALA:H	17	0.64
(1,3645)	1:40:A:VAL:HA	1:35:A:LEU:HD13	8	0.63
(1,3497)	1:76:A:MET:HB2	1:86:A:LEU:HD23	10	0.63
(1,3497)	1:76:A:MET:HB2	1:86:A:LEU:HD21	17	0.63
(1,3441)	1:114:A:ALA:HB2	1:96:A:PRO:HB3	9	0.63
(1,3441)	1:99:A:ALA:HB2	1:96:A:PRO:HB3	10	0.63
(1,3380)	1:40:A:VAL:HG13	1:43:A:ARG:HD3	9	0.63
(1,3272)	1:96:A:PRO:HD3	1:115:A:MET:HE1	15	0.63
(1,3253)	1:32:A:ALA:H	1:61:A:ILE:HD11	9	0.63
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE1	8	0.63
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB2	3	0.63
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB1	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB1	10	0.63
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD11	3	0.63
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG12	8	0.63
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD21	2	0.63
(1,2618)	1:36:A:ALA:HB1	1:33:A:PRO:HB2	17	0.63
(1,2296)	1:102:A:ALA:HB3	1:111:A:PHE:HB3	13	0.63
(1,2293)	1:34:A:ILE:HB	1:37:A:ASN:HB3	6	0.63
(1,1975)	1:27:A:THR:HG22	1:26:A:LEU:HA	11	0.63
(1,1883)	1:35:A:LEU:HD23	1:74:A:LEU:HA	15	0.63
(1,1719)	1:100:A:VAL:HG11	1:96:A:PRO:HA	18	0.63
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	17	0.63
(1,1344)	1:30:A:ILE:HD11	1:31:A:MET:H	2	0.63
(1,1275)	1:88:A:PRO:HB2	1:91:A:CYS:H	6	0.63
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	12	0.63
(1,1232)	1:57:A:THR:HG23	1:59:A:ASP:H	4	0.63
(1,1232)	1:57:A:THR:HG21	1:59:A:ASP:H	14	0.63
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	1	0.63
(1,922)	1:86:A:LEU:HB2	1:84:A:GLY:H	17	0.63
(1,906)	1:36:A:ALA:HB1	1:41:A:GLN:HE22	12	0.63
(1,906)	1:58:A:ALA:HB2	1:62:A:GLN:HE22	13	0.63
(1,795)	1:65:A:LEU:HD22	1:64:A:THR:H	17	0.63
(1,563)	1:40:A:VAL:HG23	1:42:A:GLU:H	14	0.63
(1,376)	1:73:A:ALA:HB2	1:77:A:PHE:H	18	0.63
(1,375)	1:99:A:ALA:HB2	1:103:A:ALA:H	3	0.63
(1,375)	1:99:A:ALA:HB1	1:103:A:ALA:H	5	0.63
(1,365)	1:101:A:GLU:HG3	1:104:A:ASN:H	7	0.63
(1,338)	1:65:A:LEU:HD12	1:65:A:LEU:H	5	0.63
(1,307)	1:26:A:LEU:HD23	1:114:A:ALA:H	11	0.63
(1,236)	1:74:A:LEU:HD12	1:76:A:MET:H	16	0.63
(1,234)	1:44:A:LEU:HD22	1:76:A:MET:H	18	0.63
(1,82)	1:61:A:ILE:HD11	1:32:A:ALA:H	9	0.63
(1,3734)	1:90:A:MET:HE2	1:93:A:PHE:HZ	4	0.62
(1,3733)	1:90:A:MET:HE2	1:93:A:PHE:HZ	4	0.62
(1,3712)	1:65:A:LEU:HD11	1:70:A:PHE:HD1	13	0.62
(1,3645)	1:40:A:VAL:HA	1:35:A:LEU:HD11	17	0.62
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD12	5	0.62
(1,3561)	1:31:A:MET:HG2	1:34:A:ILE:HG21	14	0.62
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD12	13	0.62
(1,3377)	1:45:A:LEU:HD22	1:46:A:PRO:HD2	18	0.62
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	1	0.62
(1,3314)	1:40:A:VAL:HB	1:34:A:ILE:HA	6	0.62
(1,3253)	1:32:A:ALA:H	1:34:A:ILE:HD11	5	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3126)	1:111:A:PHE:H	1:114:A:ALA:HB1	14	0.62
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG23	14	0.62
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD12	11	0.62
(1,3015)	1:97:A:ALA:HB3	1:100:A:VAL:HG11	18	0.62
(1,2921)	1:32:A:ALA:HA	1:35:A:LEU:HD23	6	0.62
(1,2912)	1:85:A:GLN:HA	1:89:A:LEU:HD22	6	0.62
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD23	2	0.62
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD22	12	0.62
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD11	3	0.62
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD13	20	0.62
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD13	5	0.62
(1,2832)	1:108:A:VAL:H	1:81:A:LEU:HD12	15	0.62
(1,2699)	1:93:A:PHE:HD2	1:34:A:ILE:HG13	10	0.62
(1,2699)	1:93:A:PHE:HD1	1:34:A:ILE:HG13	13	0.62
(1,2630)	1:34:A:ILE:HD13	1:90:A:MET:HG3	14	0.62
(1,2617)	1:95:A:LEU:HD22	1:90:A:MET:HB2	19	0.62
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	14	0.62
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	17	0.62
(1,2296)	1:102:A:ALA:HB1	1:111:A:PHE:HB3	2	0.62
(1,2296)	1:102:A:ALA:HB2	1:111:A:PHE:HB3	4	0.62
(1,2296)	1:102:A:ALA:HB2	1:111:A:PHE:HB3	12	0.62
(1,2081)	1:95:A:LEU:HD12	1:96:A:PRO:HD2	10	0.62
(1,1719)	1:100:A:VAL:HG12	1:96:A:PRO:HA	19	0.62
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	13	0.62
(1,1344)	1:30:A:ILE:HD11	1:31:A:MET:H	10	0.62
(1,1335)	1:95:A:LEU:HD22	1:90:A:MET:H	3	0.62
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	5	0.62
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	12	0.62
(1,1135)	1:44:A:LEU:HD11	1:79:A:ALA:H	11	0.62
(1,1095)	1:23:A:ALA:HB2	1:22:A:LEU:H	12	0.62
(1,921)	1:72:A:GLN:HB3	1:75:A:GLY:H	6	0.62
(1,683)	1:40:A:VAL:HG13	1:37:A:ASN:HD21	3	0.62
(1,614)	1:95:A:LEU:HB2	1:91:A:CYS:H	4	0.62
(1,578)	1:23:A:ALA:HB1	1:25:A:VAL:H	14	0.62
(1,425)	1:57:A:THR:HG23	1:60:A:GLU:H	6	0.62
(1,425)	1:57:A:THR:HG21	1:60:A:GLU:H	7	0.62
(1,298)	1:112:A:ALA:HB3	1:116:A:GLN:H	7	0.62
(1,236)	1:74:A:LEU:HD12	1:76:A:MET:H	3	0.62
(1,234)	1:44:A:LEU:HD23	1:76:A:MET:H	10	0.62
(1,179)	1:38:A:ALA:HB3	1:40:A:VAL:H	14	0.62
(1,82)	1:34:A:ILE:HD11	1:32:A:ALA:H	5	0.62
(1,3663)	1:46:A:PRO:HB3	1:47:A:TYR:HD2	1	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3634)	1:65:A:LEU:HD11	1:70:A:PHE:HB3	13	0.61
(1,3561)	1:31:A:MET:HG3	1:34:A:ILE:HG23	8	0.61
(1,3551)	1:56:A:GLN:HA	1:36:A:ALA:HB3	17	0.61
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD11	8	0.61
(1,3272)	1:30:A:ILE:HA	1:115:A:MET:HE3	6	0.61
(1,3267)	1:31:A:MET:HG2	1:34:A:ILE:HD11	2	0.61
(1,3239)	1:34:A:ILE:HD12	1:90:A:MET:HE2	10	0.61
(1,3187)	1:115:A:MET:HA	1:99:A:ALA:HB2	18	0.61
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB3	18	0.61
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB2	2	0.61
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB3	9	0.61
(1,3059)	1:111:A:PHE:HD2	1:108:A:VAL:HG12	8	0.61
(1,3015)	1:97:A:ALA:HB3	1:100:A:VAL:HG12	11	0.61
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD22	20	0.61
(1,2923)	1:43:A:ARG:HA	1:86:A:LEU:HD11	1	0.61
(1,2920)	1:87:A:GLY:HA3	1:86:A:LEU:HD21	8	0.61
(1,2913)	1:23:A:ALA:HA	1:74:A:LEU:HD13	20	0.61
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD11	6	0.61
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD12	17	0.61
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	15	0.61
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	18	0.61
(1,2293)	1:34:A:ILE:HB	1:37:A:ASN:HB3	14	0.61
(1,2281)	1:61:A:ILE:HB	1:35:A:LEU:HB2	4	0.61
(1,1975)	1:27:A:THR:HG21	1:26:A:LEU:HA	7	0.61
(1,1859)	1:64:A:THR:HG23	1:60:A:GLU:HA	9	0.61
(1,1558)	1:30:A:ILE:HG13	1:28:A:PRO:HA	1	0.61
(1,1429)	1:116:A:GLN:HB2	1:119:A:ALA:H	8	0.61
(1,1344)	1:30:A:ILE:HD12	1:31:A:MET:H	12	0.61
(1,1344)	1:30:A:ILE:HD12	1:31:A:MET:H	20	0.61
(1,1275)	1:88:A:PRO:HB2	1:91:A:CYS:H	20	0.61
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	5	0.61
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	7	0.61
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	16	0.61
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	20	0.61
(1,1095)	1:23:A:ALA:HB2	1:22:A:LEU:H	4	0.61
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	4	0.61
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	17	0.61
(1,849)	1:36:A:ALA:HB3	1:41:A:GLN:HE21	7	0.61
(1,849)	1:35:A:LEU:HB2	1:41:A:GLN:HE21	8	0.61
(1,578)	1:23:A:ALA:HB1	1:25:A:VAL:H	10	0.61
(1,505)	1:25:A:VAL:HG23	1:117:A:ASN:H	20	0.61
(1,425)	1:57:A:THR:HG21	1:60:A:GLU:H	16	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:99:A:ALA:HB2	1:103:A:ALA:H	2	0.61
(1,375)	1:99:A:ALA:HB3	1:103:A:ALA:H	9	0.61
(1,338)	1:61:A:ILE:HG23	1:65:A:LEU:H	1	0.61
(1,307)	1:26:A:LEU:HD21	1:114:A:ALA:H	15	0.61
(1,298)	1:119:A:ALA:HB3	1:116:A:GLN:H	1	0.61
(1,236)	1:74:A:LEU:HD11	1:76:A:MET:H	14	0.61
(1,234)	1:44:A:LEU:HD22	1:76:A:MET:H	17	0.61
(1,115)	1:80:A:ALA:HB3	1:79:A:ALA:H	18	0.61
(1,36)	1:106:A:GLY:HA2	1:108:A:VAL:H	3	0.61
(1,36)	1:109:A:GLU:HA	1:108:A:VAL:H	12	0.61
(1,36)	1:109:A:GLU:HA	1:108:A:VAL:H	14	0.61
(1,3734)	1:90:A:MET:HE1	1:93:A:PHE:HZ	1	0.6
(1,3733)	1:90:A:MET:HE1	1:93:A:PHE:HZ	1	0.6
(1,3673)	1:114:A:ALA:H	1:111:A:PHE:HD1	15	0.6
(1,3634)	1:22:A:LEU:HD12	1:70:A:PHE:HB3	3	0.6
(1,3634)	1:65:A:LEU:HD11	1:70:A:PHE:HB3	17	0.6
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD11	7	0.6
(1,3551)	1:56:A:GLN:HA	1:36:A:ALA:HB3	19	0.6
(1,3533)	1:111:A:PHE:HD2	1:115:A:MET:HE1	6	0.6
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD11	12	0.6
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	3	0.6
(1,3232)	1:31:A:MET:HG2	1:30:A:ILE:HG21	13	0.6
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB3	17	0.6
(1,3106)	1:40:A:VAL:HG23	1:35:A:LEU:HD13	12	0.6
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD12	5	0.6
(1,3015)	1:97:A:ALA:HB1	1:100:A:VAL:HG12	4	0.6
(1,2912)	1:50:A:SER:HA	1:48:A:LEU:HD23	19	0.6
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD12	10	0.6
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD12	12	0.6
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD12	4	0.6
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD11	12	0.6
(1,2617)	1:95:A:LEU:HD21	1:90:A:MET:HB2	4	0.6
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	2	0.6
(1,2562)	1:50:A:SER:HB3	1:49:A:PRO:HB3	8	0.6
(1,2296)	1:102:A:ALA:HB2	1:111:A:PHE:HB3	5	0.6
(1,2296)	1:102:A:ALA:HB3	1:111:A:PHE:HB3	11	0.6
(1,2296)	1:102:A:ALA:HB1	1:111:A:PHE:HB3	14	0.6
(1,1563)	1:112:A:ALA:HB2	1:108:A:VAL:HA	13	0.6
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	4	0.6
(1,1275)	1:88:A:PRO:HB2	1:91:A:CYS:H	14	0.6
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	15	0.6
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	2	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1095)	1:23:A:ALA:HB2	1:22:A:LEU:H	3	0.6
(1,1042)	1:30:A:ILE:HD12	1:29:A:GLU:H	20	0.6
(1,1027)	1:100:A:VAL:HG22	1:92:A:GLN:H	9	0.6
(1,1007)	1:30:A:ILE:HD12	1:119:A:ALA:H	11	0.6
(1,922)	1:82:A:ALA:HB3	1:84:A:GLY:H	19	0.6
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	11	0.6
(1,868)	1:65:A:LEU:HD23	1:72:A:GLN:HE21	4	0.6
(1,849)	1:36:A:ALA:HB2	1:41:A:GLN:HE21	5	0.6
(1,849)	1:36:A:ALA:HB2	1:41:A:GLN:HE21	15	0.6
(1,425)	1:57:A:THR:HG23	1:60:A:GLU:H	19	0.6
(1,404)	1:96:A:PRO:HG2	1:118:A:ASN:H	4	0.6
(1,376)	1:73:A:ALA:HB3	1:77:A:PHE:H	9	0.6
(1,375)	1:99:A:ALA:HB3	1:103:A:ALA:H	17	0.6
(1,298)	1:119:A:ALA:HB3	1:116:A:GLN:H	15	0.6
(1,231)	1:97:A:ALA:HB2	1:99:A:ALA:H	15	0.6
(1,114)	1:81:A:LEU:HB2	1:79:A:ALA:H	1	0.6
(1,114)	1:81:A:LEU:HB2	1:79:A:ALA:H	7	0.6
(1,114)	1:82:A:ALA:HB3	1:79:A:ALA:H	19	0.6
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	11	0.59
(1,3631)	1:135:A:GLU:H	1:134:A:GLU:HG2	17	0.59
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD12	3	0.59
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD12	4	0.59
(1,3568)	1:114:A:ALA:HB1	1:102:A:ALA:HB1	11	0.59
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD22	1	0.59
(1,3497)	1:85:A:GLN:HB3	1:86:A:LEU:HD22	1	0.59
(1,3497)	1:85:A:GLN:HB3	1:86:A:LEU:HD22	5	0.59
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD12	6	0.59
(1,3441)	1:114:A:ALA:HB1	1:96:A:PRO:HB3	15	0.59
(1,3080)	1:22:A:LEU:HA	1:25:A:VAL:HG22	10	0.59
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD12	8	0.59
(1,2921)	1:73:A:ALA:HA	1:35:A:LEU:HD23	15	0.59
(1,2920)	1:87:A:GLY:HA3	1:86:A:LEU:HD23	17	0.59
(1,2912)	1:85:A:GLN:HA	1:89:A:LEU:HD22	9	0.59
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD11	16	0.59
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD11	5	0.59
(1,2618)	1:36:A:ALA:HB2	1:33:A:PRO:HB2	8	0.59
(1,2618)	1:36:A:ALA:HB1	1:33:A:PRO:HB2	20	0.59
(1,2617)	1:95:A:LEU:HD23	1:90:A:MET:HB2	11	0.59
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	20	0.59
(1,2296)	1:102:A:ALA:HB3	1:111:A:PHE:HB3	9	0.59
(1,2296)	1:102:A:ALA:HB1	1:111:A:PHE:HB3	16	0.59
(1,2293)	1:34:A:ILE:HB	1:37:A:ASN:HB3	4	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2293)	1:38:A:ALA:HB1	1:37:A:ASN:HB3	10	0.59
(1,1558)	1:30:A:ILE:HG13	1:28:A:PRO:HA	19	0.59
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	6	0.59
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	17	0.59
(1,1275)	1:88:A:PRO:HB2	1:91:A:CYS:H	10	0.59
(1,1275)	1:88:A:PRO:HB2	1:91:A:CYS:H	11	0.59
(1,1232)	1:57:A:THR:HG23	1:59:A:ASP:H	10	0.59
(1,1193)	1:108:A:VAL:HG13	1:107:A:ASP:H	11	0.59
(1,1193)	1:108:A:VAL:HG12	1:107:A:ASP:H	13	0.59
(1,1187)	1:116:A:GLN:HB2	1:118:A:ASN:H	8	0.59
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	4	0.59
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	15	0.59
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	17	0.59
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	9	0.59
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	20	0.59
(1,909)	1:61:A:ILE:HG23	1:62:A:GLN:HE22	20	0.59
(1,906)	1:58:A:ALA:HB1	1:62:A:GLN:HE22	19	0.59
(1,803)	1:46:A:PRO:HG2	1:85:A:GLN:HE21	10	0.59
(1,563)	1:40:A:VAL:HG21	1:42:A:GLU:H	12	0.59
(1,563)	1:54:A:LEU:HD12	1:42:A:GLU:H	16	0.59
(1,499)	1:115:A:MET:HB2	1:117:A:ASN:H	4	0.59
(1,307)	1:25:A:VAL:HG23	1:114:A:ALA:H	18	0.59
(1,234)	1:44:A:LEU:HD23	1:76:A:MET:H	14	0.59
(1,234)	1:44:A:LEU:HD22	1:76:A:MET:H	20	0.59
(1,36)	1:109:A:GLU:HA	1:108:A:VAL:H	5	0.59
(1,36)	1:109:A:GLU:HA	1:108:A:VAL:H	8	0.59
(1,36)	1:109:A:GLU:HA	1:108:A:VAL:H	17	0.59
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	10	0.58
(1,3615)	1:29:A:GLU:HG3	1:30:A:ILE:HD13	4	0.58
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD12	2	0.58
(1,3519)	1:109:A:GLU:HG3	1:20:A:VAL:HG13	4	0.58
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD23	18	0.58
(1,3497)	1:85:A:GLN:HB3	1:86:A:LEU:HD23	6	0.58
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	2	0.58
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	10	0.58
(1,3441)	1:114:A:ALA:HB1	1:96:A:PRO:HB3	2	0.58
(1,3441)	1:99:A:ALA:HB2	1:96:A:PRO:HB3	20	0.58
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	17	0.58
(1,3253)	1:32:A:ALA:H	1:61:A:ILE:HD13	4	0.58
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB1	6	0.58
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG13	6	0.58
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG12	20	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG13	1	0.58
(1,3015)	1:97:A:ALA:HB3	1:100:A:VAL:HG12	14	0.58
(1,3015)	1:97:A:ALA:HB2	1:100:A:VAL:HG13	16	0.58
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD11	9	0.58
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD12	2	0.58
(1,2618)	1:36:A:ALA:HB1	1:33:A:PRO:HB2	9	0.58
(1,2618)	1:36:A:ALA:HB3	1:33:A:PRO:HB2	15	0.58
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	8	0.58
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	6	0.58
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	6	0.58
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	10	0.58
(1,2081)	1:65:A:LEU:HD11	1:55:A:PRO:HD2	9	0.58
(1,1975)	1:27:A:THR:HG22	1:26:A:LEU:HA	16	0.58
(1,1719)	1:100:A:VAL:HG13	1:96:A:PRO:HA	6	0.58
(1,1572)	1:48:A:LEU:HD13	1:53:A:SER:HB2	19	0.58
(1,1429)	1:116:A:GLN:HB3	1:119:A:ALA:H	7	0.58
(1,1306)	1:49:A:PRO:HD2	1:53:A:SER:H	13	0.58
(1,1275)	1:88:A:PRO:HB2	1:91:A:CYS:H	16	0.58
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	8	0.58
(1,1193)	1:108:A:VAL:HG12	1:107:A:ASP:H	1	0.58
(1,1193)	1:108:A:VAL:HG11	1:107:A:ASP:H	10	0.58
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	1	0.58
(1,1102)	1:60:A:GLU:HG2	1:58:A:ALA:H	12	0.58
(1,922)	1:82:A:ALA:HB3	1:84:A:GLY:H	8	0.58
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	7	0.58
(1,906)	1:36:A:ALA:HB3	1:41:A:GLN:HE22	17	0.58
(1,760)	1:96:A:PRO:HB2	1:118:A:ASN:HD22	14	0.58
(1,563)	1:40:A:VAL:HG23	1:42:A:GLU:H	13	0.58
(1,562)	1:95:A:LEU:HD23	1:93:A:PHE:H	10	0.58
(1,562)	1:95:A:LEU:HD21	1:93:A:PHE:H	13	0.58
(1,522)	1:114:A:ALA:HB3	1:113:A:LYS:H	1	0.58
(1,522)	1:114:A:ALA:HB1	1:113:A:LYS:H	13	0.58
(1,307)	1:25:A:VAL:HG23	1:114:A:ALA:H	19	0.58
(1,298)	1:112:A:ALA:HB3	1:116:A:GLN:H	3	0.58
(1,298)	1:112:A:ALA:HB2	1:116:A:GLN:H	9	0.58
(1,236)	1:74:A:LEU:HD13	1:76:A:MET:H	5	0.58
(1,236)	1:74:A:LEU:HD12	1:76:A:MET:H	18	0.58
(1,234)	1:44:A:LEU:HD21	1:76:A:MET:H	11	0.58
(1,82)	1:61:A:ILE:HD13	1:32:A:ALA:H	4	0.58
(1,36)	1:106:A:GLY:HA2	1:108:A:VAL:H	20	0.58
(1,3782)	1:103:A:ALA:HA	1:111:A:PHE:HZ	1	0.57
(1,3712)	1:65:A:LEU:HD11	1:70:A:PHE:HD1	7	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3673)	1:107:A:ASP:H	1:111:A:PHE:HD1	19	0.57
(1,3645)	1:40:A:VAL:HA	1:35:A:LEU:HD13	19	0.57
(1,3634)	1:65:A:LEU:HD12	1:70:A:PHE:HB3	2	0.57
(1,3627)	1:33:A:PRO:HG2	1:93:A:PHE:HB2	4	0.57
(1,3561)	1:31:A:MET:HG2	1:34:A:ILE:HG23	15	0.57
(1,3556)	1:43:A:ARG:HD3	1:80:A:ALA:HB2	1	0.57
(1,3551)	1:56:A:GLN:HA	1:36:A:ALA:HB3	9	0.57
(1,3498)	1:102:A:ALA:HB1	1:81:A:LEU:HD11	1	0.57
(1,3497)	1:85:A:GLN:HB3	1:86:A:LEU:HD21	7	0.57
(1,3497)	1:76:A:MET:HB2	1:86:A:LEU:HD21	20	0.57
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD12	19	0.57
(1,3464)	1:31:A:MET:HG2	1:26:A:LEU:HD12	13	0.57
(1,3441)	1:114:A:ALA:HB3	1:96:A:PRO:HB3	13	0.57
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	13	0.57
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	17	0.57
(1,3377)	1:45:A:LEU:HD22	1:46:A:PRO:HD2	14	0.57
(1,3272)	1:96:A:PRO:HD3	1:115:A:MET:HE2	9	0.57
(1,3267)	1:31:A:MET:HG2	1:34:A:ILE:HD13	10	0.57
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB2	4	0.57
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB1	20	0.57
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB2	16	0.57
(1,3106)	1:40:A:VAL:HG22	1:35:A:LEU:HD11	17	0.57
(1,3015)	1:97:A:ALA:HB3	1:100:A:VAL:HG11	1	0.57
(1,3015)	1:97:A:ALA:HB1	1:100:A:VAL:HG13	5	0.57
(1,2995)	1:76:A:MET:HE2	1:35:A:LEU:HD21	13	0.57
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD12	7	0.57
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD21	9	0.57
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD12	2	0.57
(1,2694)	1:99:A:ALA:H	1:96:A:PRO:HG3	11	0.57
(1,2618)	1:36:A:ALA:HB1	1:33:A:PRO:HB2	16	0.57
(1,2618)	1:36:A:ALA:HB1	1:33:A:PRO:HB2	19	0.57
(1,2296)	1:102:A:ALA:HB3	1:111:A:PHE:HB3	1	0.57
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	17	0.57
(1,2075)	1:61:A:ILE:HG23	1:33:A:PRO:HD2	4	0.57
(1,2075)	1:61:A:ILE:HG22	1:33:A:PRO:HD2	7	0.57
(1,2075)	1:61:A:ILE:HG21	1:33:A:PRO:HD2	20	0.57
(1,1975)	1:27:A:THR:HG22	1:26:A:LEU:HA	3	0.57
(1,1719)	1:100:A:VAL:HG11	1:96:A:PRO:HA	13	0.57
(1,1719)	1:100:A:VAL:HG13	1:96:A:PRO:HA	16	0.57
(1,1558)	1:30:A:ILE:HG13	1:28:A:PRO:HA	13	0.57
(1,1232)	1:57:A:THR:HG21	1:59:A:ASP:H	15	0.57
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	16	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1146)	1:85:A:GLN:HB3	1:81:A:LEU:H	18	0.57
(1,1145)	1:85:A:GLN:HB2	1:81:A:LEU:H	3	0.57
(1,1145)	1:85:A:GLN:HB2	1:81:A:LEU:H	15	0.57
(1,1102)	1:60:A:GLU:HG2	1:58:A:ALA:H	4	0.57
(1,1042)	1:30:A:ILE:HD12	1:29:A:GLU:H	12	0.57
(1,922)	1:82:A:ALA:HB2	1:84:A:GLY:H	9	0.57
(1,827)	1:4:A:ILE:HD13	1:2:A:ASN:HD21	8	0.57
(1,563)	1:40:A:VAL:HG23	1:42:A:GLU:H	5	0.57
(1,562)	1:95:A:LEU:HD22	1:93:A:PHE:H	19	0.57
(1,562)	1:95:A:LEU:HD22	1:93:A:PHE:H	20	0.57
(1,425)	1:57:A:THR:HG22	1:60:A:GLU:H	9	0.57
(1,375)	1:99:A:ALA:HB2	1:103:A:ALA:H	16	0.57
(1,236)	1:74:A:LEU:HD12	1:76:A:MET:H	13	0.57
(1,234)	1:44:A:LEU:HD21	1:76:A:MET:H	13	0.57
(1,115)	1:80:A:ALA:HB2	1:79:A:ALA:H	4	0.57
(1,115)	1:80:A:ALA:HB1	1:79:A:ALA:H	20	0.57
(1,36)	1:109:A:GLU:HA	1:108:A:VAL:H	6	0.57
(1,36)	1:109:A:GLU:HA	1:108:A:VAL:H	10	0.57
(1,36)	1:109:A:GLU:HA	1:108:A:VAL:H	18	0.57
(1,3766)	1:45:A:LEU:H	1:47:A:TYR:HE2	10	0.56
(1,3645)	1:55:A:PRO:HD2	1:35:A:LEU:HD12	1	0.56
(1,3642)	1:35:A:LEU:HD21	1:70:A:PHE:HA	5	0.56
(1,3634)	1:65:A:LEU:HD13	1:70:A:PHE:HB3	15	0.56
(1,3627)	1:90:A:MET:HE2	1:93:A:PHE:HB2	19	0.56
(1,3584)	1:10:A:VAL:HG12	1:11:A:PRO:HA	7	0.56
(1,3561)	1:90:A:MET:HB3	1:34:A:ILE:HG23	10	0.56
(1,3561)	1:31:A:MET:HG3	1:34:A:ILE:HG22	20	0.56
(1,3504)	1:31:A:MET:HE3	1:86:A:LEU:HD23	8	0.56
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD22	19	0.56
(1,3498)	1:31:A:MET:HE1	1:81:A:LEU:HD13	6	0.56
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD13	1	0.56
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	1	0.56
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	12	0.56
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	20	0.56
(1,3377)	1:45:A:LEU:HD22	1:46:A:PRO:HD2	4	0.56
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	4	0.56
(1,3239)	1:86:A:LEU:HD13	1:90:A:MET:HE3	8	0.56
(1,3192)	1:33:A:PRO:HA	1:58:A:ALA:HB2	2	0.56
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB3	11	0.56
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB2	17	0.56
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB1	18	0.56
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD13	9	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD12	12	0.56
(1,2921)	1:32:A:ALA:HA	1:35:A:LEU:HD21	9	0.56
(1,2920)	1:43:A:ARG:HA	1:86:A:LEU:HD22	1	0.56
(1,2920)	1:87:A:GLY:HA3	1:86:A:LEU:HD22	10	0.56
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD11	16	0.56
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD13	2	0.56
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD23	17	0.56
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD13	14	0.56
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD12	2	0.56
(1,2782)	1:26:A:LEU:HD22	1:115:A:MET:HB3	14	0.56
(1,2770)	1:99:A:ALA:HB1	1:96:A:PRO:HG3	9	0.56
(1,2699)	1:93:A:PHE:HD1	1:34:A:ILE:HG13	17	0.56
(1,2694)	1:72:A:GLN:HE21	1:49:A:PRO:HG3	5	0.56
(1,2618)	1:36:A:ALA:HB1	1:33:A:PRO:HB2	2	0.56
(1,2296)	1:102:A:ALA:HB1	1:111:A:PHE:HB3	3	0.56
(1,2296)	1:102:A:ALA:HB3	1:111:A:PHE:HB3	20	0.56
(1,2075)	1:61:A:ILE:HG23	1:33:A:PRO:HD2	16	0.56
(1,1975)	1:27:A:THR:HG21	1:26:A:LEU:HA	6	0.56
(1,1975)	1:27:A:THR:HG22	1:26:A:LEU:HA	17	0.56
(1,1719)	1:100:A:VAL:HG13	1:96:A:PRO:HA	15	0.56
(1,1565)	1:64:A:THR:HG22	1:61:A:ILE:HA	17	0.56
(1,1543)	1:31:A:MET:HB3	1:28:A:PRO:HA	13	0.56
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	5	0.56
(1,1365)	1:88:A:PRO:HG3	1:104:A:ASN:HD22	10	0.56
(1,1276)	1:92:A:GLN:HB3	1:91:A:CYS:H	13	0.56
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	13	0.56
(1,1193)	1:108:A:VAL:HG13	1:107:A:ASP:H	12	0.56
(1,1193)	1:108:A:VAL:HG13	1:107:A:ASP:H	14	0.56
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	15	0.56
(1,1063)	1:95:A:LEU:HD21	1:94:A:GLY:H	8	0.56
(1,1042)	1:30:A:ILE:HD12	1:29:A:GLU:H	1	0.56
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	15	0.56
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	19	0.56
(1,921)	1:72:A:GLN:HB3	1:75:A:GLY:H	19	0.56
(1,849)	1:36:A:ALA:HB3	1:41:A:GLN:HE21	16	0.56
(1,759)	1:62:A:GLN:HB2	1:63:A:ASN:HD21	4	0.56
(1,614)	1:95:A:LEU:HB2	1:91:A:CYS:H	12	0.56
(1,563)	1:40:A:VAL:HG23	1:42:A:GLU:H	1	0.56
(1,449)	1:45:A:LEU:HD23	1:45:A:LEU:H	17	0.56
(1,375)	1:99:A:ALA:HB3	1:103:A:ALA:H	11	0.56
(1,307)	1:25:A:VAL:HG22	1:114:A:ALA:H	10	0.56
(1,36)	1:106:A:GLY:HA2	1:108:A:VAL:H	11	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:109:A:GLU:HA	1:108:A:VAL:H	16	0.56
(1,3645)	1:40:A:VAL:HA	1:35:A:LEU:HD12	14	0.55
(1,3565)	1:90:A:MET:HE2	1:31:A:MET:HE1	9	0.55
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG22	19	0.55
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD11	7	0.55
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD12	16	0.55
(1,3455)	1:104:A:ASN:H	1:105:A:LYS:HG3	10	0.55
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	3	0.55
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	19	0.55
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD13	3	0.55
(1,3238)	1:89:A:LEU:HD23	1:90:A:MET:HE2	2	0.55
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB3	17	0.55
(1,3106)	1:40:A:VAL:HG22	1:35:A:LEU:HD13	19	0.55
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD13	17	0.55
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG12	19	0.55
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD12	13	0.55
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD12	13	0.55
(1,2832)	1:103:A:ALA:H	1:81:A:LEU:HD13	18	0.55
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	20	0.55
(1,2482)	1:93:A:PHE:HZ	1:40:A:VAL:HB	19	0.55
(1,2456)	1:120:A:LYS:H	1:121:A:PRO:HB3	5	0.55
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	20	0.55
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	14	0.55
(1,2081)	1:65:A:LEU:HD13	1:55:A:PRO:HD2	5	0.55
(1,2030)	1:41:A:GLN:HE22	1:55:A:PRO:HD2	5	0.55
(1,1859)	1:64:A:THR:HG22	1:60:A:GLU:HA	14	0.55
(1,1558)	1:30:A:ILE:HG13	1:28:A:PRO:HA	5	0.55
(1,1558)	1:30:A:ILE:HG13	1:28:A:PRO:HA	16	0.55
(1,1457)	1:20:A:VAL:HG11	1:109:A:GLU:H	19	0.55
(1,1457)	1:20:A:VAL:HG12	1:109:A:GLU:H	19	0.55
(1,1457)	1:20:A:VAL:HG13	1:109:A:GLU:H	19	0.55
(1,1443)	1:41:A:GLN:HB2	1:37:A:ASN:H	19	0.55
(1,1429)	1:116:A:GLN:HB3	1:119:A:ALA:H	15	0.55
(1,1344)	1:26:A:LEU:HD21	1:31:A:MET:H	4	0.55
(1,1306)	1:49:A:PRO:HD2	1:53:A:SER:H	14	0.55
(1,1232)	1:57:A:THR:HG23	1:59:A:ASP:H	19	0.55
(1,1193)	1:108:A:VAL:HG12	1:107:A:ASP:H	3	0.55
(1,1183)	1:99:A:ALA:HB1	1:101:A:GLU:H	1	0.55
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	10	0.55
(1,1095)	1:23:A:ALA:HB2	1:22:A:LEU:H	17	0.55
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	4	0.55
(1,906)	1:58:A:ALA:HB3	1:62:A:GLN:HE22	3	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,889)	1:65:A:LEU:HA	1:69:A:GLN:HE22	1	0.55
(1,849)	1:36:A:ALA:HB1	1:41:A:GLN:HE21	1	0.55
(1,827)	1:4:A:ILE:HD12	1:2:A:ASN:HD21	10	0.55
(1,770)	1:64:A:THR:HB	1:63:A:ASN:HD22	8	0.55
(1,563)	1:40:A:VAL:HG22	1:42:A:GLU:H	15	0.55
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	8	0.55
(1,499)	1:115:A:MET:HB2	1:117:A:ASN:H	18	0.55
(1,316)	1:47:A:TYR:HE2	1:80:A:ALA:H	3	0.55
(1,236)	1:74:A:LEU:HD12	1:76:A:MET:H	11	0.55
(1,231)	1:97:A:ALA:HB3	1:99:A:ALA:H	16	0.55
(1,115)	1:80:A:ALA:HB3	1:79:A:ALA:H	17	0.55
(1,36)	1:109:A:GLU:HA	1:108:A:VAL:H	1	0.55
(1,36)	1:109:A:GLU:HA	1:108:A:VAL:H	19	0.55
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	16	0.54
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	20	0.54
(1,3646)	1:138:A:MET:HB2	1:137:A:ASP:HB3	16	0.54
(1,3615)	1:31:A:MET:HG2	1:30:A:ILE:HD12	8	0.54
(1,3504)	1:43:A:ARG:HG3	1:86:A:LEU:HD23	4	0.54
(1,3504)	1:31:A:MET:HE3	1:86:A:LEU:HD21	14	0.54
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD21	8	0.54
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD21	13	0.54
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD13	4	0.54
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD13	15	0.54
(1,3402)	1:25:A:VAL:HG12	1:21:A:ASP:HB2	7	0.54
(1,3402)	1:25:A:VAL:HG12	1:21:A:ASP:HB2	12	0.54
(1,3377)	1:45:A:LEU:HD21	1:46:A:PRO:HD2	3	0.54
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	1	0.54
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD12	15	0.54
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB1	3	0.54
(1,3059)	1:111:A:PHE:HD2	1:108:A:VAL:HG12	15	0.54
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD12	4	0.54
(1,2915)	1:21:A:ASP:HA	1:22:A:LEU:HD13	10	0.54
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD11	3	0.54
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD12	18	0.54
(1,2699)	1:93:A:PHE:HD1	1:34:A:ILE:HG13	8	0.54
(1,2694)	1:99:A:ALA:H	1:96:A:PRO:HG3	7	0.54
(1,2694)	1:72:A:GLN:HE21	1:49:A:PRO:HG3	16	0.54
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	4	0.54
(1,2296)	1:102:A:ALA:HB2	1:111:A:PHE:HB3	19	0.54
(1,2081)	1:95:A:LEU:HD13	1:96:A:PRO:HD2	1	0.54
(1,2030)	1:41:A:GLN:HE22	1:55:A:PRO:HD2	16	0.54
(1,1975)	1:27:A:THR:HG22	1:26:A:LEU:HA	13	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1296)	1:26:A:LEU:HD22	1:115:A:MET:H	4	0.54
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	11	0.54
(1,1232)	1:57:A:THR:HG23	1:59:A:ASP:H	6	0.54
(1,1170)	1:114:A:ALA:HB1	1:112:A:ALA:H	19	0.54
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	5	0.54
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	8	0.54
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	14	0.54
(1,1007)	1:30:A:ILE:HD11	1:119:A:ALA:H	1	0.54
(1,922)	1:82:A:ALA:HB2	1:84:A:GLY:H	7	0.54
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	2	0.54
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	12	0.54
(1,868)	1:65:A:LEU:HD23	1:69:A:GLN:HE21	8	0.54
(1,849)	1:36:A:ALA:HB3	1:41:A:GLN:HE21	19	0.54
(1,651)	1:34:A:ILE:HD12	1:34:A:ILE:H	15	0.54
(1,637)	1:44:A:LEU:HD21	1:43:A:ARG:H	1	0.54
(1,635)	1:40:A:VAL:HG22	1:36:A:ALA:H	11	0.54
(1,614)	1:95:A:LEU:HB2	1:91:A:CYS:H	10	0.54
(1,522)	1:114:A:ALA:HB2	1:113:A:LYS:H	6	0.54
(1,236)	1:74:A:LEU:HD11	1:76:A:MET:H	8	0.54
(1,231)	1:97:A:ALA:HB2	1:99:A:ALA:H	2	0.54
(1,221)	1:96:A:PRO:HD2	1:99:A:ALA:H	4	0.54
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	14	0.53
(1,3497)	1:76:A:MET:HB2	1:86:A:LEU:HD23	4	0.53
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD13	17	0.53
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD11	20	0.53
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	6	0.53
(1,3380)	1:40:A:VAL:HG11	1:43:A:ARG:HD3	20	0.53
(1,3377)	1:45:A:LEU:HD23	1:46:A:PRO:HD2	19	0.53
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD11	4	0.53
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD13	7	0.53
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD13	9	0.53
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD13	12	0.53
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD13	20	0.53
(1,3255)	1:41:A:GLN:HE21	1:61:A:ILE:HD11	10	0.53
(1,3253)	1:32:A:ALA:H	1:61:A:ILE:HD13	20	0.53
(1,3239)	1:34:A:ILE:HD12	1:90:A:MET:HE1	1	0.53
(1,3239)	1:34:A:ILE:HD13	1:90:A:MET:HE2	4	0.53
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB3	1	0.53
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB3	18	0.53
(1,3106)	1:40:A:VAL:HG21	1:35:A:LEU:HD13	6	0.53
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD11	2	0.53
(1,2972)	1:43:A:ARG:HD3	1:86:A:LEU:HD11	4	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2912)	1:50:A:SER:HA	1:48:A:LEU:HD21	13	0.53
(1,2872)	1:43:A:ARG:H	1:44:A:LEU:HD11	18	0.53
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD13	9	0.53
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	14	0.53
(1,2617)	1:95:A:LEU:HD21	1:90:A:MET:HB2	8	0.53
(1,2513)	1:70:A:PHE:HE1	1:28:A:PRO:HB2	7	0.53
(1,2293)	1:34:A:ILE:HB	1:37:A:ASN:HB3	15	0.53
(1,2293)	1:34:A:ILE:HB	1:37:A:ASN:HB3	20	0.53
(1,2116)	1:86:A:LEU:HD11	1:43:A:ARG:HD3	4	0.53
(1,1737)	1:44:A:LEU:HD23	1:41:A:GLN:HA	17	0.53
(1,1719)	1:100:A:VAL:HG11	1:96:A:PRO:HA	7	0.53
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	2	0.53
(1,1299)	1:40:A:VAL:HG22	1:34:A:ILE:H	11	0.53
(1,1275)	1:88:A:PRO:HB2	1:91:A:CYS:H	4	0.53
(1,1232)	1:57:A:THR:HG23	1:59:A:ASP:H	16	0.53
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	9	0.53
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	18	0.53
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	3	0.53
(1,1145)	1:85:A:GLN:HB2	1:81:A:LEU:H	16	0.53
(1,1145)	1:85:A:GLN:HB2	1:81:A:LEU:H	17	0.53
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	1	0.53
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	4	0.53
(1,1116)	1:95:A:LEU:HA	1:119:A:ALA:H	18	0.53
(1,1102)	1:60:A:GLU:HG2	1:58:A:ALA:H	14	0.53
(1,1095)	1:23:A:ALA:HB2	1:22:A:LEU:H	14	0.53
(1,1042)	1:30:A:ILE:HD12	1:29:A:GLU:H	17	0.53
(1,922)	1:82:A:ALA:HB3	1:84:A:GLY:H	2	0.53
(1,886)	1:89:A:LEU:HD13	1:92:A:GLN:HE21	7	0.53
(1,849)	1:36:A:ALA:HB1	1:41:A:GLN:HE21	12	0.53
(1,651)	1:34:A:ILE:HD11	1:34:A:ILE:H	4	0.53
(1,651)	1:34:A:ILE:HD13	1:34:A:ILE:H	7	0.53
(1,651)	1:34:A:ILE:HD13	1:34:A:ILE:H	9	0.53
(1,651)	1:34:A:ILE:HD13	1:34:A:ILE:H	12	0.53
(1,651)	1:34:A:ILE:HD13	1:34:A:ILE:H	20	0.53
(1,637)	1:89:A:LEU:HD12	1:43:A:ARG:H	20	0.53
(1,522)	1:114:A:ALA:HB1	1:113:A:LYS:H	4	0.53
(1,522)	1:114:A:ALA:HB1	1:113:A:LYS:H	12	0.53
(1,505)	1:25:A:VAL:HG21	1:117:A:ASN:H	10	0.53
(1,375)	1:99:A:ALA:HB3	1:103:A:ALA:H	1	0.53
(1,375)	1:99:A:ALA:HB3	1:103:A:ALA:H	18	0.53
(1,82)	1:61:A:ILE:HD13	1:32:A:ALA:H	20	0.53
(1,36)	1:109:A:GLU:HA	1:108:A:VAL:H	2	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:109:A:GLU:HA	1:108:A:VAL:H	9	0.53
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	17	0.52
(1,3646)	1:62:A:GLN:HB2	1:59:A:ASP:HB3	15	0.52
(1,3645)	1:40:A:VAL:HA	1:35:A:LEU:HD13	11	0.52
(1,3645)	1:55:A:PRO:HD2	1:35:A:LEU:HD13	15	0.52
(1,3561)	1:31:A:MET:HG3	1:34:A:ILE:HG21	19	0.52
(1,3519)	1:109:A:GLU:HG3	1:20:A:VAL:HG12	1	0.52
(1,3498)	1:31:A:MET:HE3	1:81:A:LEU:HD11	19	0.52
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD12	9	0.52
(1,3388)	1:20:A:VAL:HA	1:21:A:ASP:HB2	20	0.52
(1,3380)	1:40:A:VAL:HG13	1:43:A:ARG:HD3	10	0.52
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD12	10	0.52
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD12	19	0.52
(1,3192)	1:33:A:PRO:HA	1:58:A:ALA:HB3	4	0.52
(1,3015)	1:97:A:ALA:HB1	1:100:A:VAL:HG12	20	0.52
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD22	1	0.52
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD22	8	0.52
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD12	17	0.52
(1,2832)	1:103:A:ALA:H	1:81:A:LEU:HD12	8	0.52
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD12	12	0.52
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD13	6	0.52
(1,2694)	1:99:A:ALA:H	1:96:A:PRO:HG3	19	0.52
(1,2618)	1:36:A:ALA:HB3	1:33:A:PRO:HB2	5	0.52
(1,2617)	1:95:A:LEU:HD21	1:90:A:MET:HB2	12	0.52
(1,2456)	1:120:A:LYS:H	1:121:A:PRO:HB3	11	0.52
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	19	0.52
(1,1975)	1:27:A:THR:HG23	1:26:A:LEU:HA	8	0.52
(1,1975)	1:27:A:THR:HG21	1:26:A:LEU:HA	15	0.52
(1,1883)	1:35:A:LEU:HD21	1:74:A:LEU:HA	7	0.52
(1,1883)	1:35:A:LEU:HD21	1:74:A:LEU:HA	19	0.52
(1,1558)	1:30:A:ILE:HG13	1:28:A:PRO:HA	14	0.52
(1,1558)	1:30:A:ILE:HG13	1:28:A:PRO:HA	20	0.52
(1,1344)	1:30:A:ILE:HD12	1:31:A:MET:H	13	0.52
(1,1296)	1:26:A:LEU:HD22	1:115:A:MET:H	1	0.52
(1,1282)	1:91:A:CYS:HB3	1:89:A:LEU:H	1	0.52
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	1	0.52
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	8	0.52
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	6	0.52
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	19	0.52
(1,1042)	1:61:A:ILE:HG22	1:29:A:GLU:H	4	0.52
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	17	0.52
(1,905)	1:58:A:ALA:HB2	1:62:A:GLN:HE22	7	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:4:A:ILE:HD13	1:2:A:ASN:HD21	2	0.52
(1,578)	1:23:A:ALA:HB1	1:25:A:VAL:H	1	0.52
(1,563)	1:40:A:VAL:HG23	1:42:A:GLU:H	3	0.52
(1,562)	1:95:A:LEU:HD21	1:93:A:PHE:H	8	0.52
(1,517)	1:42:A:GLU:HB2	1:44:A:LEU:H	18	0.52
(1,425)	1:57:A:THR:HG22	1:60:A:GLU:H	2	0.52
(1,365)	1:101:A:GLU:HG3	1:104:A:ASN:H	15	0.52
(1,305)	1:25:A:VAL:HG22	1:116:A:GLN:H	18	0.52
(1,298)	1:119:A:ALA:HB3	1:116:A:GLN:H	2	0.52
(1,236)	1:74:A:LEU:HD13	1:76:A:MET:H	15	0.52
(1,231)	1:97:A:ALA:HB2	1:99:A:ALA:H	7	0.52
(1,231)	1:97:A:ALA:HB1	1:99:A:ALA:H	11	0.52
(1,172)	1:136:A:GLU:HB2	1:136:A:GLU:H	2	0.52
(1,75)	1:131:A:LYS:HB3	1:132:A:LYS:H	7	0.52
(1,3766)	1:83:A:SER:H	1:47:A:TYR:HE2	4	0.51
(1,3758)	1:26:A:LEU:HD11	1:77:A:PHE:HD1	8	0.51
(1,3642)	1:74:A:LEU:HD22	1:70:A:PHE:HA	17	0.51
(1,3634)	1:65:A:LEU:HD11	1:70:A:PHE:HB3	14	0.51
(1,3551)	1:56:A:GLN:HA	1:36:A:ALA:HB3	2	0.51
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD22	2	0.51
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD21	12	0.51
(1,3498)	1:31:A:MET:HE2	1:81:A:LEU:HD13	16	0.51
(1,3497)	1:85:A:GLN:HB3	1:86:A:LEU:HD22	16	0.51
(1,3402)	1:25:A:VAL:HG11	1:21:A:ASP:HB2	18	0.51
(1,3380)	1:40:A:VAL:HG13	1:43:A:ARG:HD3	5	0.51
(1,3375)	1:58:A:ALA:HB3	1:33:A:PRO:HD2	2	0.51
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD12	6	0.51
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD12	12	0.51
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB3	1	0.51
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB1	10	0.51
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB2	14	0.51
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG13	2	0.51
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD13	20	0.51
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG11	12	0.51
(1,2912)	1:43:A:ARG:HA	1:44:A:LEU:HD21	1	0.51
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD22	10	0.51
(1,2618)	1:36:A:ALA:HB3	1:33:A:PRO:HB2	6	0.51
(1,2369)	1:43:A:ARG:H	1:42:A:GLU:HG2	9	0.51
(1,2296)	1:102:A:ALA:HB3	1:111:A:PHE:HB3	6	0.51
(1,2296)	1:102:A:ALA:HB1	1:111:A:PHE:HB3	7	0.51
(1,2296)	1:102:A:ALA:HB1	1:111:A:PHE:HB3	10	0.51
(1,2293)	1:34:A:ILE:HB	1:37:A:ASN:HB3	18	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	10	0.51
(1,2081)	1:65:A:LEU:HD12	1:55:A:PRO:HD2	11	0.51
(1,2075)	1:61:A:ILE:HG21	1:33:A:PRO:HD2	14	0.51
(1,2067)	1:99:A:ALA:HB3	1:96:A:PRO:HD2	4	0.51
(1,1859)	1:64:A:THR:HG23	1:60:A:GLU:HA	19	0.51
(1,1563)	1:112:A:ALA:HB3	1:108:A:VAL:HA	11	0.51
(1,1344)	1:30:A:ILE:HD11	1:31:A:MET:H	7	0.51
(1,1276)	1:92:A:GLN:HB3	1:91:A:CYS:H	5	0.51
(1,1232)	1:57:A:THR:HG21	1:59:A:ASP:H	13	0.51
(1,1193)	1:108:A:VAL:HG11	1:107:A:ASP:H	9	0.51
(1,1183)	1:99:A:ALA:HB3	1:101:A:GLU:H	16	0.51
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	20	0.51
(1,1158)	1:119:A:ALA:HB3	1:120:A:LYS:H	7	0.51
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	11	0.51
(1,1042)	1:30:A:ILE:HD12	1:29:A:GLU:H	13	0.51
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	10	0.51
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	16	0.51
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	18	0.51
(1,909)	1:61:A:ILE:HG21	1:62:A:GLN:HE22	7	0.51
(1,905)	1:58:A:ALA:HB3	1:62:A:GLN:HE22	20	0.51
(1,849)	1:36:A:ALA:HB3	1:41:A:GLN:HE21	20	0.51
(1,792)	1:65:A:LEU:HB2	1:64:A:THR:H	8	0.51
(1,767)	1:100:A:VAL:HG22	1:90:A:MET:H	6	0.51
(1,683)	1:40:A:VAL:HG12	1:37:A:ASN:HD21	10	0.51
(1,651)	1:34:A:ILE:HD12	1:34:A:ILE:H	6	0.51
(1,614)	1:95:A:LEU:HB2	1:91:A:CYS:H	20	0.51
(1,578)	1:23:A:ALA:HB2	1:25:A:VAL:H	4	0.51
(1,563)	1:40:A:VAL:HG21	1:42:A:GLU:H	7	0.51
(1,518)	1:43:A:ARG:HB3	1:44:A:LEU:H	4	0.51
(1,449)	1:45:A:LEU:HD22	1:45:A:LEU:H	10	0.51
(1,425)	1:57:A:THR:HG23	1:60:A:GLU:H	5	0.51
(1,115)	1:80:A:ALA:HB3	1:79:A:ALA:H	1	0.51
(1,115)	1:80:A:ALA:HB1	1:79:A:ALA:H	10	0.51
(1,115)	1:80:A:ALA:HB2	1:79:A:ALA:H	14	0.51
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	9	0.5
(1,3737)	1:89:A:LEU:HG	1:93:A:PHE:HZ	8	0.5
(1,3561)	1:31:A:MET:HG3	1:34:A:ILE:HG21	5	0.5
(1,3558)	1:117:A:ASN:HB2	1:114:A:ALA:HB2	18	0.5
(1,3556)	1:77:A:PHE:HB3	1:80:A:ALA:HB1	9	0.5
(1,3498)	1:31:A:MET:HE2	1:81:A:LEU:HD12	5	0.5
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD13	5	0.5
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD11	14	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	8	0.5
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	18	0.5
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	8	0.5
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	19	0.5
(1,3314)	1:93:A:PHE:HB2	1:34:A:ILE:HA	20	0.5
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	20	0.5
(1,3272)	1:96:A:PRO:HD3	1:115:A:MET:HE3	3	0.5
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD11	14	0.5
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD12	17	0.5
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB1	8	0.5
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB2	16	0.5
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE3	20	0.5
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB2	4	0.5
(1,3106)	1:40:A:VAL:HG22	1:35:A:LEU:HD11	20	0.5
(1,2921)	1:73:A:ALA:HA	1:35:A:LEU:HD23	8	0.5
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD21	20	0.5
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD22	18	0.5
(1,2832)	1:108:A:VAL:H	1:81:A:LEU:HD13	4	0.5
(1,2617)	1:95:A:LEU:HD21	1:90:A:MET:HB2	2	0.5
(1,2297)	1:114:A:ALA:HB3	1:111:A:PHE:HB3	10	0.5
(1,2293)	1:34:A:ILE:HB	1:37:A:ASN:HB3	19	0.5
(1,2075)	1:61:A:ILE:HG23	1:33:A:PRO:HD2	17	0.5
(1,1883)	1:35:A:LEU:HD21	1:74:A:LEU:HA	1	0.5
(1,1859)	1:64:A:THR:HG21	1:60:A:GLU:HA	3	0.5
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	9	0.5
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	12	0.5
(1,1344)	1:30:A:ILE:HD13	1:31:A:MET:H	11	0.5
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	4	0.5
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	18	0.5
(1,1299)	1:40:A:VAL:HG22	1:34:A:ILE:H	3	0.5
(1,1276)	1:92:A:GLN:HB3	1:91:A:CYS:H	15	0.5
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	16	0.5
(1,1183)	1:99:A:ALA:HB1	1:101:A:GLU:H	20	0.5
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	2	0.5
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	7	0.5
(1,1095)	1:23:A:ALA:HB2	1:22:A:LEU:H	1	0.5
(1,1044)	1:108:A:VAL:HB	1:78:A:SER:H	1	0.5
(1,651)	1:34:A:ILE:HD11	1:34:A:ILE:H	14	0.5
(1,651)	1:34:A:ILE:HD12	1:34:A:ILE:H	17	0.5
(1,635)	1:40:A:VAL:HG22	1:36:A:ALA:H	20	0.5
(1,578)	1:23:A:ALA:HB3	1:25:A:VAL:H	9	0.5
(1,562)	1:95:A:LEU:HD21	1:93:A:PHE:H	16	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	8	0.5
(1,449)	1:45:A:LEU:HD22	1:45:A:LEU:H	18	0.5
(1,375)	1:99:A:ALA:HB2	1:103:A:ALA:H	4	0.5
(1,365)	1:101:A:GLU:HG2	1:104:A:ASN:H	18	0.5
(1,298)	1:119:A:ALA:HB1	1:116:A:GLN:H	12	0.5
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	1	0.5
(1,236)	1:74:A:LEU:HD13	1:76:A:MET:H	4	0.5
(1,236)	1:74:A:LEU:HD12	1:76:A:MET:H	6	0.5
(1,231)	1:97:A:ALA:HB3	1:99:A:ALA:H	13	0.5
(1,192)	1:108:A:VAL:HG11	1:82:A:ALA:H	19	0.5
(1,115)	1:80:A:ALA:HB2	1:79:A:ALA:H	16	0.5
(1,114)	1:81:A:LEU:HB2	1:79:A:ALA:H	11	0.5
(1,60)	1:54:A:LEU:HD12	1:54:A:LEU:H	7	0.5
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	12	0.49
(1,3766)	1:45:A:LEU:H	1:47:A:TYR:HE2	16	0.49
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	9	0.49
(1,3646)	1:62:A:GLN:HB2	1:59:A:ASP:HB3	17	0.49
(1,3634)	1:65:A:LEU:HD13	1:70:A:PHE:HB3	11	0.49
(1,3533)	1:111:A:PHE:HD2	1:115:A:MET:HE3	15	0.49
(1,3533)	1:93:A:PHE:HD2	1:115:A:MET:HE2	20	0.49
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD21	14	0.49
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD21	16	0.49
(1,3498)	1:31:A:MET:HE3	1:81:A:LEU:HD11	20	0.49
(1,3497)	1:85:A:GLN:HB3	1:86:A:LEU:HD22	12	0.49
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD12	3	0.49
(1,3464)	1:31:A:MET:HG3	1:26:A:LEU:HD11	14	0.49
(1,3449)	1:97:A:ALA:HA	1:91:A:CYS:HB2	19	0.49
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	11	0.49
(1,3434)	1:116:A:GLN:HA	1:120:A:LYS:HB2	6	0.49
(1,3407)	1:32:A:ALA:H	1:29:A:GLU:HG3	5	0.49
(1,3377)	1:45:A:LEU:HD22	1:46:A:PRO:HD2	16	0.49
(1,3272)	1:96:A:PRO:HD3	1:115:A:MET:HE3	7	0.49
(1,3267)	1:31:A:MET:HG2	1:34:A:ILE:HD12	17	0.49
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD11	8	0.49
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD12	16	0.49
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD11	6	0.49
(1,3253)	1:32:A:ALA:H	1:61:A:ILE:HD11	7	0.49
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB3	15	0.49
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB3	3	0.49
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB1	6	0.49
(1,3094)	1:56:A:GLN:HB3	1:57:A:THR:HG21	5	0.49
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD12	13	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG11	13	0.49
(1,2921)	1:32:A:ALA:HA	1:35:A:LEU:HD21	3	0.49
(1,2920)	1:43:A:ARG:HA	1:86:A:LEU:HD21	19	0.49
(1,2912)	1:50:A:SER:HA	1:48:A:LEU:HD22	3	0.49
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD13	18	0.49
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD21	6	0.49
(1,2832)	1:103:A:ALA:H	1:81:A:LEU:HD11	1	0.49
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD12	20	0.49
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD21	15	0.49
(1,2769)	1:99:A:ALA:HB2	1:115:A:MET:HB2	7	0.49
(1,2699)	1:93:A:PHE:HD2	1:34:A:ILE:HG13	1	0.49
(1,2618)	1:36:A:ALA:HB2	1:33:A:PRO:HB2	4	0.49
(1,2617)	1:95:A:LEU:HD22	1:90:A:MET:HB2	5	0.49
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	12	0.49
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	4	0.49
(1,2482)	1:93:A:PHE:HZ	1:40:A:VAL:HB	17	0.49
(1,2296)	1:102:A:ALA:HB3	1:111:A:PHE:HB3	8	0.49
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	2	0.49
(1,2066)	1:95:A:LEU:HB2	1:96:A:PRO:HD2	7	0.49
(1,2066)	1:54:A:LEU:HB3	1:55:A:PRO:HD2	17	0.49
(1,1719)	1:100:A:VAL:HG12	1:96:A:PRO:HA	10	0.49
(1,1562)	1:102:A:ALA:HB1	1:108:A:VAL:HA	3	0.49
(1,1562)	1:102:A:ALA:HB3	1:108:A:VAL:HA	11	0.49
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	12	0.49
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	15	0.49
(1,1276)	1:92:A:GLN:HB3	1:91:A:CYS:H	17	0.49
(1,1193)	1:108:A:VAL:HG11	1:107:A:ASP:H	15	0.49
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	9	0.49
(1,870)	1:25:A:VAL:HG11	1:24:A:SER:H	3	0.49
(1,651)	1:34:A:ILE:HD11	1:34:A:ILE:H	8	0.49
(1,651)	1:34:A:ILE:HD12	1:34:A:ILE:H	16	0.49
(1,617)	1:93:A:PHE:HZ	1:37:A:ASN:HD22	13	0.49
(1,578)	1:23:A:ALA:HB2	1:25:A:VAL:H	18	0.49
(1,563)	1:40:A:VAL:HG21	1:42:A:GLU:H	10	0.49
(1,563)	1:40:A:VAL:HG23	1:42:A:GLU:H	20	0.49
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	11	0.49
(1,517)	1:42:A:GLU:HB2	1:44:A:LEU:H	13	0.49
(1,517)	1:42:A:GLU:HB2	1:44:A:LEU:H	16	0.49
(1,494)	1:72:A:GLN:HB3	1:74:A:LEU:H	18	0.49
(1,449)	1:45:A:LEU:HD21	1:45:A:LEU:H	6	0.49
(1,236)	1:74:A:LEU:HD13	1:76:A:MET:H	17	0.49
(1,231)	1:97:A:ALA:HB3	1:99:A:ALA:H	17	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,105)	1:76:A:MET:HB3	1:48:A:LEU:H	3	0.49
(1,82)	1:61:A:ILE:HD11	1:32:A:ALA:H	7	0.49
(1,36)	1:106:A:GLY:HA2	1:108:A:VAL:H	7	0.49
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	7	0.48
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	18	0.48
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	20	0.48
(1,3642)	1:74:A:LEU:HD22	1:70:A:PHE:HA	9	0.48
(1,3565)	1:90:A:MET:HE2	1:31:A:MET:HE2	13	0.48
(1,3504)	1:31:A:MET:HE3	1:86:A:LEU:HD22	19	0.48
(1,3484)	1:76:A:MET:HB2	1:44:A:LEU:HD13	10	0.48
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	2	0.48
(1,3379)	1:86:A:LEU:HA	1:43:A:ARG:HD3	19	0.48
(1,3267)	1:31:A:MET:HG2	1:34:A:ILE:HD13	9	0.48
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD11	2	0.48
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD11	5	0.48
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD13	18	0.48
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB3	12	0.48
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB1	8	0.48
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB3	19	0.48
(1,3106)	1:40:A:VAL:HG23	1:35:A:LEU:HD13	4	0.48
(1,3106)	1:40:A:VAL:HG23	1:35:A:LEU:HD12	16	0.48
(1,2994)	1:31:A:MET:HG3	1:35:A:LEU:HD22	5	0.48
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD22	15	0.48
(1,2839)	1:70:A:PHE:HE1	1:28:A:PRO:HG2	18	0.48
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD11	9	0.48
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD13	11	0.48
(1,2768)	1:64:A:THR:HG22	1:60:A:GLU:HB2	5	0.48
(1,2620)	1:64:A:THR:HG22	1:60:A:GLU:HB2	5	0.48
(1,2618)	1:36:A:ALA:HB2	1:33:A:PRO:HB2	13	0.48
(1,2296)	1:102:A:ALA:HB3	1:111:A:PHE:HB3	18	0.48
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	6	0.48
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD2	4	0.48
(1,2030)	1:41:A:GLN:HE22	1:55:A:PRO:HD2	3	0.48
(1,1806)	1:36:A:ALA:HA	1:56:A:GLN:HA	18	0.48
(1,1562)	1:102:A:ALA:HB1	1:108:A:VAL:HA	7	0.48
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	13	0.48
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	19	0.48
(1,1365)	1:101:A:GLU:HB2	1:104:A:ASN:HD22	19	0.48
(1,1344)	1:30:A:ILE:HD13	1:31:A:MET:H	14	0.48
(1,1344)	1:30:A:ILE:HD13	1:31:A:MET:H	15	0.48
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	11	0.48
(1,1276)	1:92:A:GLN:HB3	1:91:A:CYS:H	9	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	9	0.48
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	20	0.48
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	1	0.48
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	2	0.48
(1,1183)	1:99:A:ALA:HB2	1:101:A:GLU:H	12	0.48
(1,1183)	1:99:A:ALA:HB1	1:101:A:GLU:H	13	0.48
(1,1168)	1:132:A:LYS:HB3	1:134:A:GLU:H	5	0.48
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	6	0.48
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	9	0.48
(1,1145)	1:85:A:GLN:HB2	1:81:A:LEU:H	14	0.48
(1,1116)	1:95:A:LEU:HA	1:119:A:ALA:H	17	0.48
(1,1027)	1:100:A:VAL:HG21	1:92:A:GLN:H	13	0.48
(1,905)	1:58:A:ALA:HB3	1:62:A:GLN:HE22	1	0.48
(1,870)	1:25:A:VAL:HG11	1:24:A:SER:H	13	0.48
(1,684)	1:65:A:LEU:HD22	1:53:A:SER:H	12	0.48
(1,651)	1:34:A:ILE:HD11	1:34:A:ILE:H	2	0.48
(1,651)	1:34:A:ILE:HD11	1:34:A:ILE:H	5	0.48
(1,651)	1:34:A:ILE:HD13	1:34:A:ILE:H	18	0.48
(1,635)	1:40:A:VAL:HG21	1:36:A:ALA:H	15	0.48
(1,614)	1:89:A:LEU:HB2	1:91:A:CYS:H	19	0.48
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	15	0.48
(1,517)	1:42:A:GLU:HB2	1:44:A:LEU:H	10	0.48
(1,425)	1:57:A:THR:HG23	1:60:A:GLU:H	3	0.48
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	14	0.48
(1,231)	1:97:A:ALA:HB2	1:99:A:ALA:H	12	0.48
(1,115)	1:80:A:ALA:HB3	1:79:A:ALA:H	12	0.48
(1,36)	1:109:A:GLU:HA	1:108:A:VAL:H	15	0.48
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	8	0.47
(1,3558)	1:117:A:ASN:HB2	1:114:A:ALA:HB1	6	0.47
(1,3556)	1:77:A:PHE:HB3	1:80:A:ALA:HB2	7	0.47
(1,3556)	1:77:A:PHE:HB3	1:80:A:ALA:HB1	20	0.47
(1,3498)	1:31:A:MET:HE1	1:81:A:LEU:HD12	11	0.47
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD12	11	0.47
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	16	0.47
(1,3380)	1:40:A:VAL:HG12	1:43:A:ARG:HD3	6	0.47
(1,3267)	1:31:A:MET:HG2	1:34:A:ILE:HD13	12	0.47
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD13	1	0.47
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD11	13	0.47
(1,3258)	1:111:A:PHE:HE2	1:34:A:ILE:HD13	1	0.47
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB1	10	0.47
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB2	10	0.47
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB3	10	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3228)	1:61:A:ILE:HB	1:32:A:ALA:HB1	5	0.47
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB3	17	0.47
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB1	9	0.47
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB1	12	0.47
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB3	4	0.47
(1,3054)	1:77:A:PHE:H	1:35:A:LEU:HD12	10	0.47
(1,3015)	1:97:A:ALA:HB1	1:100:A:VAL:HG13	12	0.47
(1,2921)	1:32:A:ALA:HA	1:35:A:LEU:HD21	17	0.47
(1,2920)	1:43:A:ARG:HA	1:86:A:LEU:HD23	6	0.47
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD23	5	0.47
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD21	11	0.47
(1,2694)	1:99:A:ALA:H	1:96:A:PRO:HG3	17	0.47
(1,2644)	1:89:A:LEU:HD21	1:92:A:GLN:HG3	4	0.47
(1,2644)	1:89:A:LEU:HD22	1:92:A:GLN:HG3	4	0.47
(1,2644)	1:89:A:LEU:HD23	1:92:A:GLN:HG3	4	0.47
(1,2622)	1:64:A:THR:HG22	1:55:A:PRO:HB2	1	0.47
(1,2618)	1:36:A:ALA:HB1	1:33:A:PRO:HB2	7	0.47
(1,2617)	1:95:A:LEU:HD21	1:90:A:MET:HB2	13	0.47
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	5	0.47
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	19	0.47
(1,2456)	1:63:A:ASN:H	1:55:A:PRO:HB3	4	0.47
(1,2417)	1:114:A:ALA:HB1	1:98:A:GLU:HG3	10	0.47
(1,2417)	1:114:A:ALA:HB2	1:98:A:GLU:HG3	10	0.47
(1,2417)	1:114:A:ALA:HB3	1:98:A:GLU:HG3	10	0.47
(1,2296)	1:102:A:ALA:HB1	1:111:A:PHE:HB3	17	0.47
(1,2293)	1:34:A:ILE:HB	1:37:A:ASN:HB3	13	0.47
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	9	0.47
(1,2277)	1:60:A:GLU:HB2	1:63:A:ASN:HB3	13	0.47
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	7	0.47
(1,1365)	1:88:A:PRO:HG3	1:104:A:ASN:HD22	20	0.47
(1,1361)	1:88:A:PRO:HA	1:104:A:ASN:HD21	17	0.47
(1,1344)	1:30:A:ILE:HD13	1:31:A:MET:H	6	0.47
(1,1344)	1:30:A:ILE:HD13	1:31:A:MET:H	19	0.47
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	14	0.47
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	16	0.47
(1,1299)	1:61:A:ILE:HG23	1:34:A:ILE:H	6	0.47
(1,1287)	1:33:A:PRO:HG2	1:36:A:ALA:H	4	0.47
(1,1287)	1:33:A:PRO:HG2	1:36:A:ALA:H	7	0.47
(1,1232)	1:57:A:THR:HG22	1:59:A:ASP:H	5	0.47
(1,1183)	1:99:A:ALA:HB3	1:101:A:GLU:H	7	0.47
(1,1183)	1:99:A:ALA:HB2	1:101:A:GLU:H	8	0.47
(1,1183)	1:99:A:ALA:HB3	1:101:A:GLU:H	14	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1145)	1:85:A:GLN:HB2	1:81:A:LEU:H	2	0.47
(1,1145)	1:43:A:ARG:HB3	1:81:A:LEU:H	7	0.47
(1,1063)	1:95:A:LEU:HD22	1:94:A:GLY:H	15	0.47
(1,1042)	1:30:A:ILE:HD11	1:29:A:GLU:H	5	0.47
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	6	0.47
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	14	0.47
(1,886)	1:61:A:ILE:HG22	1:62:A:GLN:HE21	4	0.47
(1,794)	1:5:A:LEU:HB3	1:7:A:THR:H	19	0.47
(1,775)	1:62:A:GLN:HB2	1:63:A:ASN:HD22	3	0.47
(1,651)	1:34:A:ILE:HD13	1:34:A:ILE:H	1	0.47
(1,651)	1:34:A:ILE:HD11	1:34:A:ILE:H	13	0.47
(1,614)	1:95:A:LEU:HB2	1:91:A:CYS:H	2	0.47
(1,614)	1:95:A:LEU:HB2	1:91:A:CYS:H	16	0.47
(1,563)	1:40:A:VAL:HG22	1:42:A:GLU:H	6	0.47
(1,563)	1:40:A:VAL:HG21	1:42:A:GLU:H	18	0.47
(1,522)	1:114:A:ALA:HB3	1:113:A:LYS:H	7	0.47
(1,517)	1:42:A:GLU:HB3	1:44:A:LEU:H	7	0.47
(1,504)	1:22:A:LEU:HD12	1:74:A:LEU:H	13	0.47
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	16	0.47
(1,449)	1:45:A:LEU:HD23	1:45:A:LEU:H	5	0.47
(1,449)	1:45:A:LEU:HD21	1:45:A:LEU:H	11	0.47
(1,376)	1:73:A:ALA:HB3	1:77:A:PHE:H	13	0.47
(1,375)	1:99:A:ALA:HB1	1:103:A:ALA:H	12	0.47
(1,221)	1:96:A:PRO:HD2	1:99:A:ALA:H	18	0.47
(1,115)	1:80:A:ALA:HB1	1:79:A:ALA:H	9	0.47
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	1	0.46
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	5	0.46
(1,3766)	1:83:A:SER:H	1:47:A:TYR:HE2	3	0.46
(1,3565)	1:90:A:MET:HE3	1:31:A:MET:HE2	10	0.46
(1,3558)	1:117:A:ASN:HB2	1:114:A:ALA:HB3	14	0.46
(1,3551)	1:56:A:GLN:HA	1:36:A:ALA:HB2	6	0.46
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE1	13	0.46
(1,3533)	1:93:A:PHE:HD2	1:115:A:MET:HE3	16	0.46
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB3	8	0.46
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG11	7	0.46
(1,3473)	1:55:A:PRO:HD2	1:65:A:LEU:HD22	11	0.46
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	19	0.46
(1,3441)	1:99:A:ALA:HB1	1:96:A:PRO:HB3	16	0.46
(1,3377)	1:45:A:LEU:HD21	1:46:A:PRO:HD2	13	0.46
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	17	0.46
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD12	11	0.46
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD13	19	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD12	20	0.46
(1,3242)	1:95:A:LEU:HD12	1:115:A:MET:HE3	13	0.46
(1,3229)	1:98:A:GLU:HG2	1:114:A:ALA:HB1	9	0.46
(1,3229)	1:98:A:GLU:HG2	1:114:A:ALA:HB2	9	0.46
(1,3229)	1:98:A:GLU:HG2	1:114:A:ALA:HB3	9	0.46
(1,3228)	1:61:A:ILE:HB	1:32:A:ALA:HB3	19	0.46
(1,3126)	1:103:A:ALA:H	1:99:A:ALA:HB3	20	0.46
(1,3080)	1:116:A:GLN:HA	1:25:A:VAL:HG22	18	0.46
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG11	11	0.46
(1,2921)	1:32:A:ALA:HA	1:35:A:LEU:HD21	20	0.46
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD13	7	0.46
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD13	15	0.46
(1,2617)	1:95:A:LEU:HD23	1:90:A:MET:HB2	7	0.46
(1,2617)	1:95:A:LEU:HD22	1:90:A:MET:HB2	17	0.46
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	20	0.46
(1,2482)	1:93:A:PHE:HZ	1:40:A:VAL:HB	15	0.46
(1,2467)	1:132:A:LYS:H	1:132:A:LYS:HB2	7	0.46
(1,2456)	1:120:A:LYS:H	1:121:A:PRO:HB3	19	0.46
(1,2417)	1:114:A:ALA:HB1	1:98:A:GLU:HG2	9	0.46
(1,2417)	1:114:A:ALA:HB2	1:98:A:GLU:HG2	9	0.46
(1,2417)	1:114:A:ALA:HB3	1:98:A:GLU:HG2	9	0.46
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	14	0.46
(1,2281)	1:61:A:ILE:HB	1:35:A:LEU:HB2	13	0.46
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	1	0.46
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	20	0.46
(1,2066)	1:95:A:LEU:HB2	1:96:A:PRO:HD2	9	0.46
(1,1563)	1:112:A:ALA:HB2	1:108:A:VAL:HA	19	0.46
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	18	0.46
(1,1429)	1:116:A:GLN:HB2	1:119:A:ALA:H	19	0.46
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	3	0.46
(1,1299)	1:61:A:ILE:HG21	1:34:A:ILE:H	13	0.46
(1,1296)	1:26:A:LEU:HD22	1:115:A:MET:H	14	0.46
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	16	0.46
(1,1193)	1:108:A:VAL:HG13	1:107:A:ASP:H	20	0.46
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	17	0.46
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	11	0.46
(1,922)	1:82:A:ALA:HB1	1:84:A:GLY:H	3	0.46
(1,870)	1:25:A:VAL:HG11	1:24:A:SER:H	6	0.46
(1,786)	1:30:A:ILE:HG23	1:31:A:MET:H	5	0.46
(1,760)	1:96:A:PRO:HB2	1:118:A:ASN:HD22	16	0.46
(1,651)	1:34:A:ILE:HD12	1:34:A:ILE:H	11	0.46
(1,651)	1:34:A:ILE:HD13	1:34:A:ILE:H	19	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:95:A:LEU:HB2	1:91:A:CYS:H	8	0.46
(1,614)	1:95:A:LEU:HB2	1:91:A:CYS:H	18	0.46
(1,522)	1:114:A:ALA:HB3	1:113:A:LYS:H	10	0.46
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	20	0.46
(1,499)	1:115:A:MET:HB2	1:117:A:ASN:H	11	0.46
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	15	0.46
(1,425)	1:57:A:THR:HG21	1:60:A:GLU:H	10	0.46
(1,375)	1:99:A:ALA:HB3	1:103:A:ALA:H	20	0.46
(1,305)	1:26:A:LEU:HD22	1:116:A:GLN:H	7	0.46
(1,60)	1:54:A:LEU:HD12	1:54:A:LEU:H	2	0.46
(1,36)	1:106:A:GLY:HA2	1:108:A:VAL:H	13	0.46
(1,3756)	1:22:A:LEU:HB3	1:77:A:PHE:HD1	17	0.45
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	18	0.45
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD12	8	0.45
(1,3565)	1:90:A:MET:HE2	1:31:A:MET:HE2	16	0.45
(1,3533)	1:111:A:PHE:HD2	1:115:A:MET:HE1	8	0.45
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD23	5	0.45
(1,3497)	1:85:A:GLN:HB3	1:86:A:LEU:HD22	3	0.45
(1,3473)	1:55:A:PRO:HD2	1:65:A:LEU:HD21	19	0.45
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	12	0.45
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	11	0.45
(1,3394)	1:33:A:PRO:HG2	1:93:A:PHE:HB3	6	0.45
(1,3388)	1:20:A:VAL:HA	1:21:A:ASP:HB2	7	0.45
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	4	0.45
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD11	3	0.45
(1,3261)	1:34:A:ILE:H	1:34:A:ILE:HD13	10	0.45
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD13	8	0.45
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD13	1	0.45
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB1	14	0.45
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB1	6	0.45
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB2	15	0.45
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB2	12	0.45
(1,3117)	1:116:A:GLN:H	1:115:A:MET:HE3	6	0.45
(1,3106)	1:40:A:VAL:HG22	1:35:A:LEU:HD13	8	0.45
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD11	1	0.45
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD12	4	0.45
(1,2832)	1:108:A:VAL:H	1:81:A:LEU:HD12	6	0.45
(1,2630)	1:34:A:ILE:HD11	1:90:A:MET:HG3	15	0.45
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	10	0.45
(1,2513)	1:92:A:GLN:HE22	1:88:A:PRO:HB2	1	0.45
(1,2482)	1:93:A:PHE:HZ	1:40:A:VAL:HB	6	0.45
(1,2369)	1:43:A:ARG:HE	1:42:A:GLU:HG3	3	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2066)	1:95:A:LEU:HB2	1:96:A:PRO:HD2	6	0.45
(1,1838)	1:18:A:GLN:HG2	1:18:A:GLN:HA	7	0.45
(1,1719)	1:100:A:VAL:HG13	1:96:A:PRO:HA	9	0.45
(1,1572)	1:65:A:LEU:HD22	1:53:A:SER:HB2	7	0.45
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	19	0.45
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	4	0.45
(1,1320)	1:61:A:ILE:HD13	1:35:A:LEU:H	1	0.45
(1,1299)	1:40:A:VAL:HG22	1:34:A:ILE:H	20	0.45
(1,1296)	1:26:A:LEU:HD22	1:115:A:MET:H	3	0.45
(1,1287)	1:33:A:PRO:HG2	1:36:A:ALA:H	17	0.45
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	5	0.45
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	17	0.45
(1,1193)	1:108:A:VAL:HG11	1:107:A:ASP:H	2	0.45
(1,1193)	1:108:A:VAL:HG11	1:107:A:ASP:H	8	0.45
(1,1183)	1:99:A:ALA:HB1	1:101:A:GLU:H	6	0.45
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	5	0.45
(1,1116)	1:95:A:LEU:HA	1:119:A:ALA:H	7	0.45
(1,1063)	1:95:A:LEU:HD22	1:94:A:GLY:H	19	0.45
(1,1042)	1:30:A:ILE:HD12	1:29:A:GLU:H	8	0.45
(1,922)	1:82:A:ALA:HB2	1:84:A:GLY:H	14	0.45
(1,922)	1:82:A:ALA:HB1	1:84:A:GLY:H	18	0.45
(1,922)	1:86:A:LEU:HB2	1:84:A:GLY:H	20	0.45
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	13	0.45
(1,786)	1:30:A:ILE:HG23	1:31:A:MET:H	7	0.45
(1,651)	1:34:A:ILE:HD11	1:34:A:ILE:H	3	0.45
(1,651)	1:34:A:ILE:HD13	1:34:A:ILE:H	10	0.45
(1,614)	1:95:A:LEU:HB2	1:91:A:CYS:H	14	0.45
(1,562)	1:95:A:LEU:HD22	1:93:A:PHE:H	15	0.45
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	9	0.45
(1,517)	1:42:A:GLU:HB2	1:44:A:LEU:H	14	0.45
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	20	0.45
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	12	0.45
(1,316)	1:47:A:TYR:HE2	1:80:A:ALA:H	16	0.45
(1,305)	1:26:A:LEU:HD23	1:116:A:GLN:H	20	0.45
(1,115)	1:80:A:ALA:HB1	1:79:A:ALA:H	6	0.45
(1,115)	1:80:A:ALA:HB2	1:79:A:ALA:H	15	0.45
(1,60)	1:54:A:LEU:HD11	1:54:A:LEU:H	1	0.45
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	13	0.44
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	15	0.44
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	5	0.44
(1,3642)	1:35:A:LEU:HD21	1:70:A:PHE:HA	11	0.44
(1,3642)	1:35:A:LEU:HD22	1:70:A:PHE:HA	15	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3561)	1:31:A:MET:HG3	1:34:A:ILE:HG21	6	0.44
(1,3557)	1:40:A:VAL:HA	1:80:A:ALA:HB3	10	0.44
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE2	2	0.44
(1,3497)	1:85:A:GLN:HB3	1:86:A:LEU:HD21	19	0.44
(1,3455)	1:104:A:ASN:H	1:105:A:LYS:HG3	5	0.44
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	16	0.44
(1,3337)	1:11:A:PRO:HD2	1:11:A:PRO:HA	14	0.44
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	2	0.44
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	16	0.44
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	18	0.44
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD12	2	0.44
(1,3231)	1:107:A:ASP:HB2	1:110:A:ALA:HB2	17	0.44
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB2	12	0.44
(1,3177)	1:27:A:THR:H	1:30:A:ILE:HG21	7	0.44
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB1	5	0.44
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB1	16	0.44
(1,3059)	1:79:A:ALA:H	1:108:A:VAL:HG11	3	0.44
(1,2920)	1:43:A:ARG:HA	1:86:A:LEU:HD23	4	0.44
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD13	11	0.44
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD11	14	0.44
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD12	17	0.44
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD12	20	0.44
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD12	17	0.44
(1,2770)	1:99:A:ALA:HB3	1:96:A:PRO:HG3	8	0.44
(1,2699)	1:93:A:PHE:HD2	1:34:A:ILE:HG13	4	0.44
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	1	0.44
(1,2456)	1:120:A:LYS:H	1:121:A:PRO:HB3	7	0.44
(1,2369)	1:43:A:ARG:H	1:42:A:GLU:HG3	11	0.44
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	3	0.44
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	13	0.44
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	5	0.44
(1,1975)	1:27:A:THR:HG23	1:26:A:LEU:HA	4	0.44
(1,1859)	1:64:A:THR:HG22	1:60:A:GLU:HA	6	0.44
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	16	0.44
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	11	0.44
(1,1320)	1:61:A:ILE:HD12	1:35:A:LEU:H	2	0.44
(1,1299)	1:40:A:VAL:HG22	1:34:A:ILE:H	8	0.44
(1,1299)	1:61:A:ILE:HG23	1:34:A:ILE:H	18	0.44
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	11	0.44
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	11	0.44
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	9	0.44
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	14	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	4	0.44
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	17	0.44
(1,1042)	1:30:A:ILE:HD13	1:29:A:GLU:H	18	0.44
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	12	0.44
(1,922)	1:82:A:ALA:HB2	1:84:A:GLY:H	6	0.44
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	3	0.44
(1,775)	1:62:A:GLN:HB2	1:63:A:ASN:HD22	18	0.44
(1,635)	1:61:A:ILE:HG21	1:36:A:ALA:H	13	0.44
(1,617)	1:92:A:GLN:HE22	1:37:A:ASN:HD22	3	0.44
(1,614)	1:95:A:LEU:HB2	1:91:A:CYS:H	11	0.44
(1,563)	1:54:A:LEU:HD12	1:42:A:GLU:H	11	0.44
(1,522)	1:114:A:ALA:HB2	1:113:A:LYS:H	16	0.44
(1,517)	1:42:A:GLU:HB3	1:44:A:LEU:H	4	0.44
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	4	0.44
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	7	0.44
(1,236)	1:74:A:LEU:HD11	1:76:A:MET:H	7	0.44
(1,236)	1:74:A:LEU:HD12	1:76:A:MET:H	9	0.44
(1,231)	1:97:A:ALA:HB1	1:99:A:ALA:H	19	0.44
(1,115)	1:108:A:VAL:HG11	1:79:A:ALA:H	3	0.44
(1,105)	1:76:A:MET:HB3	1:48:A:LEU:H	2	0.44
(1,3646)	1:62:A:GLN:HB2	1:59:A:ASP:HB3	3	0.43
(1,3634)	1:65:A:LEU:HD12	1:70:A:PHE:HB3	6	0.43
(1,3551)	1:57:A:THR:HB	1:36:A:ALA:HB2	15	0.43
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB2	7	0.43
(1,3464)	1:31:A:MET:HG2	1:26:A:LEU:HD13	15	0.43
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	7	0.43
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	15	0.43
(1,3402)	1:25:A:VAL:HG11	1:21:A:ASP:HB2	17	0.43
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	15	0.43
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB2	11	0.43
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB2	20	0.43
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB2	7	0.43
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB3	13	0.43
(1,2958)	1:103:A:ALA:HA	1:81:A:LEU:HD13	10	0.43
(1,2958)	1:103:A:ALA:HA	1:81:A:LEU:HD11	15	0.43
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD23	4	0.43
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD23	10	0.43
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD21	9	0.43
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD11	10	0.43
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD11	8	0.43
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	17	0.43
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2575)	1:14:A:PRO:HD3	1:14:A:PRO:HB2	1	0.43
(1,2283)	1:71:A:GLN:HB3	1:74:A:LEU:HB2	13	0.43
(1,2277)	1:60:A:GLU:HB2	1:63:A:ASN:HB3	2	0.43
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	18	0.43
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	19	0.43
(1,2038)	1:88:A:PRO:HA	1:88:A:PRO:HD3	1	0.43
(1,1883)	1:35:A:LEU:HD21	1:74:A:LEU:HA	14	0.43
(1,1849)	1:26:A:LEU:HG	1:112:A:ALA:HA	16	0.43
(1,1563)	1:112:A:ALA:HB2	1:108:A:VAL:HA	3	0.43
(1,1562)	1:102:A:ALA:HB1	1:108:A:VAL:HA	16	0.43
(1,1558)	1:64:A:THR:HG21	1:53:A:SER:HB3	18	0.43
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	1	0.43
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	7	0.43
(1,1299)	1:40:A:VAL:HG22	1:34:A:ILE:H	19	0.43
(1,1287)	1:33:A:PRO:HG2	1:36:A:ALA:H	12	0.43
(1,1282)	1:91:A:CYS:HB2	1:89:A:LEU:H	8	0.43
(1,1276)	1:92:A:GLN:HB3	1:91:A:CYS:H	7	0.43
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	3	0.43
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	7	0.43
(1,1183)	1:99:A:ALA:HB1	1:101:A:GLU:H	18	0.43
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	14	0.43
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	17	0.43
(1,1158)	1:119:A:ALA:HB2	1:120:A:LYS:H	17	0.43
(1,1146)	1:85:A:GLN:HB3	1:81:A:LEU:H	13	0.43
(1,1146)	1:76:A:MET:HB2	1:81:A:LEU:H	14	0.43
(1,1063)	1:95:A:LEU:HD21	1:94:A:GLY:H	14	0.43
(1,1063)	1:95:A:LEU:HD21	1:94:A:GLY:H	16	0.43
(1,1042)	1:30:A:ILE:HD11	1:29:A:GLU:H	2	0.43
(1,922)	1:82:A:ALA:HB2	1:84:A:GLY:H	15	0.43
(1,906)	1:58:A:ALA:HB3	1:62:A:GLN:HE22	2	0.43
(1,886)	1:61:A:ILE:HG21	1:62:A:GLN:HE21	12	0.43
(1,803)	1:46:A:PRO:HG2	1:85:A:GLN:HE21	2	0.43
(1,786)	1:30:A:ILE:HG23	1:31:A:MET:H	6	0.43
(1,775)	1:62:A:GLN:HB2	1:63:A:ASN:HD22	11	0.43
(1,563)	1:40:A:VAL:HG23	1:42:A:GLU:H	2	0.43
(1,562)	1:95:A:LEU:HD22	1:93:A:PHE:H	3	0.43
(1,522)	1:114:A:ALA:HB2	1:113:A:LYS:H	20	0.43
(1,517)	1:42:A:GLU:HB2	1:44:A:LEU:H	12	0.43
(1,517)	1:42:A:GLU:HB3	1:44:A:LEU:H	19	0.43
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	7	0.43
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	9	0.43
(1,449)	1:45:A:LEU:HD21	1:45:A:LEU:H	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	1:97:A:ALA:HB2	1:99:A:ALA:H	3	0.43
(1,231)	1:97:A:ALA:HB2	1:99:A:ALA:H	4	0.43
(1,231)	1:97:A:ALA:HB3	1:99:A:ALA:H	10	0.43
(1,231)	1:97:A:ALA:HB1	1:99:A:ALA:H	18	0.43
(1,115)	1:80:A:ALA:HB2	1:79:A:ALA:H	7	0.43
(1,115)	1:80:A:ALA:HB3	1:79:A:ALA:H	13	0.43
(1,3734)	1:90:A:MET:HE3	1:93:A:PHE:HZ	20	0.42
(1,3733)	1:90:A:MET:HE3	1:93:A:PHE:HZ	20	0.42
(1,3712)	1:65:A:LEU:HD12	1:70:A:PHE:HD1	2	0.42
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	8	0.42
(1,3642)	1:74:A:LEU:HD21	1:70:A:PHE:HA	16	0.42
(1,3584)	1:10:A:VAL:HG11	1:11:A:PRO:HA	6	0.42
(1,3547)	1:48:A:LEU:HG	1:76:A:MET:HE3	20	0.42
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB3	13	0.42
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB2	18	0.42
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB3	1	0.42
(1,3527)	1:82:A:ALA:HB1	1:108:A:VAL:HG23	1	0.42
(1,3519)	1:109:A:GLU:HG3	1:20:A:VAL:HG11	6	0.42
(1,3511)	1:39:A:ASP:HA	1:38:A:ALA:HB3	14	0.42
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD23	9	0.42
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG13	1	0.42
(1,3455)	1:104:A:ASN:H	1:105:A:LYS:HG3	17	0.42
(1,3388)	1:20:A:VAL:HA	1:21:A:ASP:HB2	17	0.42
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	6	0.42
(1,3314)	1:93:A:PHE:HB2	1:34:A:ILE:HA	19	0.42
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	6	0.42
(1,3267)	1:31:A:MET:HG2	1:34:A:ILE:HD13	7	0.42
(1,3258)	1:111:A:PHE:HE2	1:34:A:ILE:HD11	17	0.42
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD11	4	0.42
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG12	15	0.42
(1,2920)	1:43:A:ARG:HA	1:86:A:LEU:HD23	14	0.42
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD11	6	0.42
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD22	11	0.42
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD21	17	0.42
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD23	20	0.42
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD12	15	0.42
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD13	10	0.42
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD11	3	0.42
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD12	5	0.42
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG2	15	0.42
(1,2630)	1:34:A:ILE:HD13	1:90:A:MET:HG3	8	0.42
(1,2617)	1:95:A:LEU:HD22	1:90:A:MET:HB2	20	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	3	0.42
(1,2189)	1:92:A:GLN:HE22	1:89:A:LEU:HB2	20	0.42
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	5	0.42
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	19	0.42
(1,2081)	1:65:A:LEU:HD13	1:55:A:PRO:HD2	17	0.42
(1,2066)	1:54:A:LEU:HB3	1:55:A:PRO:HD2	8	0.42
(1,1915)	1:70:A:PHE:HE2	1:26:A:LEU:HA	14	0.42
(1,1562)	1:102:A:ALA:HB1	1:108:A:VAL:HA	15	0.42
(1,1534)	1:88:A:PRO:HG2	1:88:A:PRO:HA	15	0.42
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	12	0.42
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	20	0.42
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	5	0.42
(1,1299)	1:40:A:VAL:HG21	1:34:A:ILE:H	9	0.42
(1,1287)	1:33:A:PRO:HG2	1:36:A:ALA:H	9	0.42
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	13	0.42
(1,1183)	1:99:A:ALA:HB3	1:101:A:GLU:H	3	0.42
(1,1183)	1:99:A:ALA:HB1	1:101:A:GLU:H	17	0.42
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	15	0.42
(1,1146)	1:85:A:GLN:HB3	1:81:A:LEU:H	9	0.42
(1,1145)	1:85:A:GLN:HB2	1:81:A:LEU:H	10	0.42
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	16	0.42
(1,1042)	1:30:A:ILE:HD13	1:29:A:GLU:H	6	0.42
(1,922)	1:82:A:ALA:HB3	1:84:A:GLY:H	1	0.42
(1,922)	1:82:A:ALA:HB3	1:84:A:GLY:H	4	0.42
(1,922)	1:82:A:ALA:HB3	1:84:A:GLY:H	10	0.42
(1,870)	1:25:A:VAL:HG12	1:24:A:SER:H	5	0.42
(1,786)	1:30:A:ILE:HG21	1:31:A:MET:H	1	0.42
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	13	0.42
(1,635)	1:40:A:VAL:HG21	1:36:A:ALA:H	6	0.42
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	13	0.42
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	14	0.42
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	4	0.42
(1,449)	1:45:A:LEU:HD23	1:45:A:LEU:H	20	0.42
(1,316)	1:47:A:TYR:HE2	1:80:A:ALA:H	17	0.42
(1,298)	1:119:A:ALA:HB3	1:116:A:GLN:H	6	0.42
(1,231)	1:97:A:ALA:HB2	1:99:A:ALA:H	5	0.42
(1,60)	1:48:A:LEU:HD11	1:54:A:LEU:H	3	0.42
(1,3766)	1:83:A:SER:H	1:47:A:TYR:HE2	15	0.41
(1,3737)	1:89:A:LEU:HG	1:93:A:PHE:HZ	16	0.41
(1,3642)	1:35:A:LEU:HD21	1:70:A:PHE:HA	19	0.41
(1,3556)	1:77:A:PHE:HB3	1:80:A:ALA:HB2	19	0.41
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB2	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB1	14	0.41
(1,3473)	1:55:A:PRO:HD2	1:65:A:LEU:HD22	5	0.41
(1,3434)	1:116:A:GLN:HA	1:120:A:LYS:HB2	5	0.41
(1,3402)	1:22:A:LEU:HD11	1:21:A:ASP:HB2	9	0.41
(1,3380)	1:40:A:VAL:HG13	1:43:A:ARG:HD3	16	0.41
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	16	0.41
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE2	4	0.41
(1,3267)	1:31:A:MET:HG2	1:34:A:ILE:HD13	1	0.41
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB1	5	0.41
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB2	5	0.41
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB3	5	0.41
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB1	1	0.41
(1,3194)	1:44:A:LEU:HA	1:79:A:ALA:HB1	10	0.41
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB1	11	0.41
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB2	11	0.41
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG11	14	0.41
(1,2958)	1:103:A:ALA:HA	1:81:A:LEU:HD11	6	0.41
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD13	11	0.41
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD21	8	0.41
(1,2694)	1:99:A:ALA:H	1:96:A:PRO:HG3	4	0.41
(1,2630)	1:34:A:ILE:HD13	1:90:A:MET:HG3	3	0.41
(1,2630)	1:34:A:ILE:HD11	1:90:A:MET:HG3	11	0.41
(1,2617)	1:95:A:LEU:HD22	1:90:A:MET:HB2	15	0.41
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	7	0.41
(1,2417)	1:114:A:ALA:HB1	1:98:A:GLU:HG3	5	0.41
(1,2417)	1:114:A:ALA:HB2	1:98:A:GLU:HG3	5	0.41
(1,2417)	1:114:A:ALA:HB3	1:98:A:GLU:HG3	5	0.41
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	9	0.41
(1,2075)	1:61:A:ILE:HG21	1:33:A:PRO:HD2	1	0.41
(1,2075)	1:61:A:ILE:HG22	1:33:A:PRO:HD2	15	0.41
(1,2067)	1:99:A:ALA:HB1	1:96:A:PRO:HD2	9	0.41
(1,2066)	1:54:A:LEU:HB3	1:55:A:PRO:HD2	11	0.41
(1,1759)	1:137:A:ASP:H	1:136:A:GLU:HA	11	0.41
(1,1563)	1:112:A:ALA:HB3	1:108:A:VAL:HA	17	0.41
(1,1287)	1:33:A:PRO:HG2	1:36:A:ALA:H	19	0.41
(1,1232)	1:57:A:THR:HG21	1:59:A:ASP:H	18	0.41
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	20	0.41
(1,1193)	1:108:A:VAL:HG13	1:107:A:ASP:H	18	0.41
(1,1183)	1:99:A:ALA:HB3	1:101:A:GLU:H	4	0.41
(1,1183)	1:99:A:ALA:HB2	1:101:A:GLU:H	5	0.41
(1,1183)	1:99:A:ALA:HB1	1:101:A:GLU:H	10	0.41
(1,1183)	1:99:A:ALA:HB1	1:101:A:GLU:H	11	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	2	0.41
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	12	0.41
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	19	0.41
(1,1042)	1:30:A:ILE:HD11	1:29:A:GLU:H	9	0.41
(1,922)	1:82:A:ALA:HB2	1:84:A:GLY:H	16	0.41
(1,849)	1:36:A:ALA:HB3	1:41:A:GLN:HE21	17	0.41
(1,786)	1:30:A:ILE:HG23	1:31:A:MET:H	14	0.41
(1,563)	1:40:A:VAL:HG21	1:42:A:GLU:H	17	0.41
(1,523)	1:54:A:LEU:HD11	1:44:A:LEU:H	4	0.41
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	7	0.41
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	17	0.41
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	1	0.41
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	18	0.41
(1,468)	1:57:A:THR:HG22	1:56:A:GLN:H	13	0.41
(1,449)	1:45:A:LEU:HD21	1:45:A:LEU:H	8	0.41
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	1	0.41
(1,303)	1:73:A:ALA:HB2	1:72:A:GLN:H	10	0.41
(1,231)	1:97:A:ALA:HB3	1:99:A:ALA:H	8	0.41
(1,221)	1:96:A:PRO:HD2	1:99:A:ALA:H	10	0.41
(1,192)	1:108:A:VAL:HG12	1:82:A:ALA:H	8	0.41
(1,115)	1:80:A:ALA:HB1	1:79:A:ALA:H	11	0.41
(1,3766)	1:45:A:LEU:H	1:47:A:TYR:HE2	2	0.4
(1,3766)	1:83:A:SER:H	1:47:A:TYR:HE2	9	0.4
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	12	0.4
(1,3646)	1:62:A:GLN:HB2	1:59:A:ASP:HB2	12	0.4
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD11	10	0.4
(1,3565)	1:90:A:MET:HE3	1:31:A:MET:HE3	15	0.4
(1,3565)	1:90:A:MET:HE1	1:31:A:MET:HE1	17	0.4
(1,3561)	1:31:A:MET:HG3	1:34:A:ILE:HG21	11	0.4
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB2	15	0.4
(1,3526)	1:22:A:LEU:HB3	1:108:A:VAL:HG22	20	0.4
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD21	11	0.4
(1,3380)	1:40:A:VAL:HG12	1:43:A:ARG:HD3	18	0.4
(1,3337)	1:121:A:PRO:HD2	1:121:A:PRO:HA	15	0.4
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	14	0.4
(1,3231)	1:107:A:ASP:HB2	1:110:A:ALA:HB2	4	0.4
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB1	4	0.4
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB2	4	0.4
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB3	4	0.4
(1,2958)	1:78:A:SER:HB3	1:81:A:LEU:HD11	11	0.4
(1,2921)	1:32:A:ALA:HA	1:35:A:LEU:HD23	11	0.4
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD22	15	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD11	11	0.4
(1,2770)	1:99:A:ALA:HB2	1:96:A:PRO:HG3	13	0.4
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG3	9	0.4
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG2	11	0.4
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG2	14	0.4
(1,2644)	1:89:A:LEU:HD21	1:92:A:GLN:HG3	8	0.4
(1,2644)	1:89:A:LEU:HD22	1:92:A:GLN:HG3	8	0.4
(1,2644)	1:89:A:LEU:HD23	1:92:A:GLN:HG3	8	0.4
(1,2630)	1:34:A:ILE:HD13	1:90:A:MET:HG3	5	0.4
(1,2530)	1:56:A:GLN:HA	1:56:A:GLN:HG2	5	0.4
(1,2417)	1:114:A:ALA:HB1	1:98:A:GLU:HG3	4	0.4
(1,2417)	1:114:A:ALA:HB2	1:98:A:GLU:HG3	4	0.4
(1,2417)	1:114:A:ALA:HB3	1:98:A:GLU:HG3	4	0.4
(1,2369)	1:43:A:ARG:H	1:42:A:GLU:HG2	2	0.4
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	15	0.4
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	2	0.4
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	17	0.4
(1,2081)	1:65:A:LEU:HD12	1:55:A:PRO:HD2	12	0.4
(1,2075)	1:61:A:ILE:HG23	1:33:A:PRO:HD2	2	0.4
(1,2030)	1:62:A:GLN:HE22	1:28:A:PRO:HD3	20	0.4
(1,1563)	1:112:A:ALA:HB3	1:108:A:VAL:HA	6	0.4
(1,1563)	1:112:A:ALA:HB1	1:108:A:VAL:HA	8	0.4
(1,1562)	1:102:A:ALA:HB2	1:108:A:VAL:HA	5	0.4
(1,1562)	1:102:A:ALA:HB2	1:108:A:VAL:HA	12	0.4
(1,1534)	1:88:A:PRO:HG3	1:88:A:PRO:HA	9	0.4
(1,1534)	1:88:A:PRO:HG2	1:88:A:PRO:HA	11	0.4
(1,1534)	1:88:A:PRO:HG2	1:88:A:PRO:HA	14	0.4
(1,1510)	1:80:A:ALA:H	1:78:A:SER:HB2	1	0.4
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	10	0.4
(1,1429)	1:116:A:GLN:HB2	1:119:A:ALA:H	3	0.4
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	10	0.4
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	16	0.4
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	5	0.4
(1,1299)	1:40:A:VAL:HG22	1:34:A:ILE:H	17	0.4
(1,1276)	1:92:A:GLN:HB3	1:91:A:CYS:H	3	0.4
(1,1273)	1:80:A:ALA:HB1	1:85:A:GLN:H	4	0.4
(1,1273)	1:80:A:ALA:HB1	1:85:A:GLN:H	7	0.4
(1,1273)	1:80:A:ALA:HB1	1:85:A:GLN:H	16	0.4
(1,1273)	1:80:A:ALA:HB3	1:85:A:GLN:H	20	0.4
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	12	0.4
(1,1202)	1:40:A:VAL:HA	1:45:A:LEU:H	13	0.4
(1,1187)	1:116:A:GLN:HB2	1:118:A:ASN:H	20	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1183)	1:99:A:ALA:HB1	1:101:A:GLU:H	15	0.4
(1,1183)	1:99:A:ALA:HB3	1:101:A:GLU:H	19	0.4
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	3	0.4
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	10	0.4
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	16	0.4
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	11	0.4
(1,1153)	1:19:A:GLN:HB2	1:19:A:GLN:H	2	0.4
(1,1042)	1:30:A:ILE:HD11	1:29:A:GLU:H	10	0.4
(1,1042)	1:30:A:ILE:HD13	1:29:A:GLU:H	14	0.4
(1,905)	1:58:A:ALA:HB3	1:62:A:GLN:HE22	16	0.4
(1,870)	1:25:A:VAL:HG13	1:24:A:SER:H	8	0.4
(1,868)	1:65:A:LEU:HD22	1:69:A:GLN:HE21	19	0.4
(1,786)	1:30:A:ILE:HG22	1:31:A:MET:H	18	0.4
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	1	0.4
(1,505)	1:25:A:VAL:HG23	1:117:A:ASN:H	17	0.4
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	15	0.4
(1,499)	1:115:A:MET:HB3	1:117:A:ASN:H	14	0.4
(1,499)	1:115:A:MET:HB2	1:117:A:ASN:H	15	0.4
(1,449)	1:45:A:LEU:HD22	1:45:A:LEU:H	15	0.4
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	16	0.4
(1,307)	1:26:A:LEU:HD22	1:114:A:ALA:H	8	0.4
(1,305)	1:26:A:LEU:HD23	1:116:A:GLN:H	16	0.4
(1,303)	1:73:A:ALA:HB1	1:72:A:GLN:H	2	0.4
(1,231)	1:97:A:ALA:HB1	1:99:A:ALA:H	1	0.4
(1,231)	1:97:A:ALA:HB2	1:99:A:ALA:H	20	0.4
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	18	0.39
(1,3737)	1:89:A:LEU:HG	1:93:A:PHE:HZ	10	0.39
(1,3712)	1:65:A:LEU:HD13	1:70:A:PHE:HD1	3	0.39
(1,3556)	1:43:A:ARG:HD3	1:80:A:ALA:HB3	11	0.39
(1,3556)	1:77:A:PHE:HB3	1:80:A:ALA:HB3	18	0.39
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB3	4	0.39
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB3	10	0.39
(1,3497)	1:85:A:GLN:HB3	1:86:A:LEU:HD23	2	0.39
(1,3497)	1:76:A:MET:HB2	1:86:A:LEU:HD23	14	0.39
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	4	0.39
(1,3434)	1:114:A:ALA:HA	1:113:A:LYS:HB3	15	0.39
(1,3434)	1:116:A:GLN:HA	1:120:A:LYS:HB2	19	0.39
(1,3407)	1:32:A:ALA:H	1:29:A:GLU:HG3	20	0.39
(1,3402)	1:25:A:VAL:HG11	1:21:A:ASP:HB2	2	0.39
(1,3380)	1:40:A:VAL:HG12	1:43:A:ARG:HD3	2	0.39
(1,3379)	1:86:A:LEU:HA	1:43:A:ARG:HD3	8	0.39
(1,3337)	1:11:A:PRO:HD2	1:11:A:PRO:HA	12	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD13	2	0.39
(1,3239)	1:86:A:LEU:HD12	1:90:A:MET:HE1	13	0.39
(1,3228)	1:61:A:ILE:HB	1:32:A:ALA:HB1	18	0.39
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB1	5	0.39
(1,2920)	1:43:A:ARG:HA	1:86:A:LEU:HD22	5	0.39
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD23	2	0.39
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD21	7	0.39
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD21	7	0.39
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD23	9	0.39
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD22	10	0.39
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD21	12	0.39
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD21	16	0.39
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD11	8	0.39
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD12	19	0.39
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD11	12	0.39
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG3	2	0.39
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG2	3	0.39
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG2	5	0.39
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG2	6	0.39
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG2	7	0.39
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG2	8	0.39
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG3	17	0.39
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG2	18	0.39
(1,2644)	1:89:A:LEU:HD21	1:92:A:GLN:HG3	12	0.39
(1,2644)	1:89:A:LEU:HD22	1:92:A:GLN:HG3	12	0.39
(1,2644)	1:89:A:LEU:HD23	1:92:A:GLN:HG3	12	0.39
(1,2631)	1:100:A:VAL:HG23	1:90:A:MET:HB3	2	0.39
(1,2618)	1:36:A:ALA:HB2	1:33:A:PRO:HB2	11	0.39
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	6	0.39
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	13	0.39
(1,2575)	1:14:A:PRO:HD3	1:14:A:PRO:HB2	11	0.39
(1,2530)	1:56:A:GLN:HA	1:56:A:GLN:HG2	9	0.39
(1,2265)	1:37:A:ASN:HB3	1:89:A:LEU:HB3	4	0.39
(1,2189)	1:93:A:PHE:HZ	1:89:A:LEU:HB2	9	0.39
(1,1975)	1:27:A:THR:HG21	1:26:A:LEU:HA	1	0.39
(1,1849)	1:26:A:LEU:HG	1:112:A:ALA:HA	19	0.39
(1,1707)	1:30:A:ILE:HG13	1:30:A:ILE:HA	6	0.39
(1,1571)	1:61:A:ILE:HG23	1:28:A:PRO:HA	13	0.39
(1,1563)	1:112:A:ALA:HB1	1:108:A:VAL:HA	5	0.39
(1,1562)	1:102:A:ALA:HB1	1:108:A:VAL:HA	14	0.39
(1,1534)	1:88:A:PRO:HG3	1:88:A:PRO:HA	2	0.39
(1,1534)	1:88:A:PRO:HG2	1:88:A:PRO:HA	3	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1534)	1:88:A:PRO:HG2	1:88:A:PRO:HA	5	0.39
(1,1534)	1:88:A:PRO:HG2	1:88:A:PRO:HA	6	0.39
(1,1534)	1:88:A:PRO:HG2	1:88:A:PRO:HA	7	0.39
(1,1534)	1:88:A:PRO:HG2	1:88:A:PRO:HA	8	0.39
(1,1534)	1:88:A:PRO:HG3	1:88:A:PRO:HA	17	0.39
(1,1534)	1:88:A:PRO:HG2	1:88:A:PRO:HA	18	0.39
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	1	0.39
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	18	0.39
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	10	0.39
(1,1307)	1:51:A:GLY:HA3	1:53:A:SER:H	2	0.39
(1,1307)	1:51:A:GLY:HA3	1:53:A:SER:H	14	0.39
(1,1296)	1:26:A:LEU:HD23	1:115:A:MET:H	13	0.39
(1,1287)	1:33:A:PRO:HG2	1:36:A:ALA:H	8	0.39
(1,1287)	1:61:A:ILE:HB	1:36:A:ALA:H	13	0.39
(1,1287)	1:33:A:PRO:HG2	1:36:A:ALA:H	20	0.39
(1,1273)	1:80:A:ALA:HB3	1:85:A:GLN:H	2	0.39
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	14	0.39
(1,1222)	1:60:A:GLU:HB2	1:59:A:ASP:H	14	0.39
(1,1183)	1:99:A:ALA:HB3	1:101:A:GLU:H	2	0.39
(1,1183)	1:99:A:ALA:HB1	1:101:A:GLU:H	9	0.39
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	1	0.39
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	4	0.39
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	5	0.39
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	9	0.39
(1,1175)	1:113:A:LYS:HG2	1:114:A:ALA:H	12	0.39
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	16	0.39
(1,1042)	1:30:A:ILE:HD12	1:29:A:GLU:H	3	0.39
(1,1042)	1:30:A:ILE:HD11	1:29:A:GLU:H	16	0.39
(1,922)	1:82:A:ALA:HB1	1:84:A:GLY:H	13	0.39
(1,786)	1:30:A:ILE:HG23	1:31:A:MET:H	9	0.39
(1,635)	1:40:A:VAL:HG22	1:36:A:ALA:H	2	0.39
(1,562)	1:95:A:LEU:HD21	1:93:A:PHE:H	14	0.39
(1,522)	1:114:A:ALA:HB3	1:113:A:LYS:H	8	0.39
(1,522)	1:114:A:ALA:HB2	1:113:A:LYS:H	15	0.39
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	16	0.39
(1,517)	1:42:A:GLU:HB3	1:44:A:LEU:H	3	0.39
(1,517)	1:42:A:GLU:HB3	1:44:A:LEU:H	15	0.39
(1,452)	1:44:A:LEU:HD13	1:45:A:LEU:H	3	0.39
(1,449)	1:45:A:LEU:HD23	1:45:A:LEU:H	2	0.39
(1,449)	1:45:A:LEU:HD21	1:45:A:LEU:H	7	0.39
(1,303)	1:73:A:ALA:HB2	1:72:A:GLN:H	14	0.39
(1,236)	1:74:A:LEU:HD11	1:76:A:MET:H	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,236)	1:74:A:LEU:HD11	1:76:A:MET:H	20	0.39
(1,3758)	1:26:A:LEU:HD13	1:77:A:PHE:HD1	6	0.38
(1,3673)	1:107:A:ASP:H	1:111:A:PHE:HD1	10	0.38
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	19	0.38
(1,3642)	1:74:A:LEU:HD21	1:70:A:PHE:HA	1	0.38
(1,3584)	1:10:A:VAL:HG12	1:11:A:PRO:HA	8	0.38
(1,3558)	1:117:A:ASN:HB2	1:114:A:ALA:HB2	8	0.38
(1,3541)	1:103:A:ALA:HB3	1:90:A:MET:HE3	9	0.38
(1,3533)	1:111:A:PHE:HD2	1:115:A:MET:HE3	10	0.38
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB2	17	0.38
(1,3504)	1:31:A:MET:HE1	1:86:A:LEU:HD23	11	0.38
(1,3468)	1:77:A:PHE:HA	1:74:A:LEU:HD11	10	0.38
(1,3464)	1:31:A:MET:HG2	1:26:A:LEU:HD11	4	0.38
(1,3455)	1:104:A:ASN:H	1:105:A:LYS:HG3	16	0.38
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	7	0.38
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	13	0.38
(1,3402)	1:22:A:LEU:HD11	1:21:A:ASP:HB2	4	0.38
(1,3383)	1:42:A:GLU:HG3	1:43:A:ARG:HD2	7	0.38
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	6	0.38
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	19	0.38
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE2	6	0.38
(1,3272)	1:96:A:PRO:HD3	1:115:A:MET:HE2	17	0.38
(1,3231)	1:107:A:ASP:HB2	1:110:A:ALA:HB1	13	0.38
(1,3228)	1:61:A:ILE:HB	1:32:A:ALA:HB2	11	0.38
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB1	2	0.38
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB3	5	0.38
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB1	8	0.38
(1,3106)	1:40:A:VAL:HG22	1:35:A:LEU:HD13	1	0.38
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG12	5	0.38
(1,2994)	1:31:A:MET:HG3	1:35:A:LEU:HD23	1	0.38
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD23	2	0.38
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD23	4	0.38
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD21	8	0.38
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD21	11	0.38
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD22	17	0.38
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD21	20	0.38
(1,2782)	1:26:A:LEU:HD22	1:115:A:MET:HB3	19	0.38
(1,2770)	1:99:A:ALA:HB1	1:96:A:PRO:HG3	14	0.38
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	6	0.38
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG3	1	0.38
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG2	4	0.38
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG2	12	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG2	19	0.38
(1,2617)	1:95:A:LEU:HD21	1:90:A:MET:HB2	6	0.38
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	16	0.38
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	3	0.38
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	6	0.38
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	10	0.38
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	7	0.38
(1,2081)	1:54:A:LEU:HD21	1:55:A:PRO:HD2	19	0.38
(1,2081)	1:65:A:LEU:HD13	1:55:A:PRO:HD2	20	0.38
(1,2066)	1:54:A:LEU:HB3	1:55:A:PRO:HD2	12	0.38
(1,1849)	1:115:A:MET:HB3	1:112:A:ALA:HA	14	0.38
(1,1562)	1:102:A:ALA:HB1	1:108:A:VAL:HA	10	0.38
(1,1534)	1:88:A:PRO:HG3	1:88:A:PRO:HA	1	0.38
(1,1534)	1:88:A:PRO:HG2	1:88:A:PRO:HA	4	0.38
(1,1534)	1:88:A:PRO:HG2	1:88:A:PRO:HA	12	0.38
(1,1534)	1:88:A:PRO:HG2	1:88:A:PRO:HA	19	0.38
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	14	0.38
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	17	0.38
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	2	0.38
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	8	0.38
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	13	0.38
(1,1287)	1:33:A:PRO:HG2	1:36:A:ALA:H	10	0.38
(1,1275)	1:92:A:GLN:HB2	1:91:A:CYS:H	1	0.38
(1,1273)	1:80:A:ALA:HB2	1:85:A:GLN:H	18	0.38
(1,1222)	1:60:A:GLU:HB2	1:59:A:ASP:H	12	0.38
(1,1187)	1:116:A:GLN:HB2	1:118:A:ASN:H	9	0.38
(1,1187)	1:116:A:GLN:HB2	1:118:A:ASN:H	12	0.38
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	12	0.38
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	14	0.38
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	3	0.38
(1,1063)	1:95:A:LEU:HD22	1:94:A:GLY:H	3	0.38
(1,922)	1:82:A:ALA:HB1	1:84:A:GLY:H	11	0.38
(1,827)	1:4:A:ILE:HD12	1:2:A:ASN:HD21	16	0.38
(1,755)	1:116:A:GLN:HB3	1:115:A:MET:H	1	0.38
(1,563)	1:54:A:LEU:HD11	1:42:A:GLU:H	9	0.38
(1,522)	1:114:A:ALA:HB3	1:113:A:LYS:H	5	0.38
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	6	0.38
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	18	0.38
(1,517)	1:42:A:GLU:HB3	1:44:A:LEU:H	9	0.38
(1,499)	1:115:A:MET:HB3	1:117:A:ASN:H	3	0.38
(1,452)	1:44:A:LEU:HD13	1:45:A:LEU:H	12	0.38
(1,452)	1:44:A:LEU:HD11	1:45:A:LEU:H	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,297)	1:112:A:ALA:HB3	1:114:A:ALA:H	8	0.38
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	11	0.38
(1,231)	1:97:A:ALA:HB2	1:99:A:ALA:H	6	0.38
(1,115)	1:80:A:ALA:HB1	1:79:A:ALA:H	2	0.38
(1,115)	1:80:A:ALA:HB3	1:79:A:ALA:H	5	0.38
(1,115)	1:80:A:ALA:HB1	1:79:A:ALA:H	8	0.38
(1,36)	1:106:A:GLY:HA2	1:108:A:VAL:H	4	0.38
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	20	0.37
(1,3737)	1:92:A:GLN:HB3	1:93:A:PHE:HZ	3	0.37
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	1	0.37
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	14	0.37
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	15	0.37
(1,3634)	1:65:A:LEU:HD11	1:70:A:PHE:HB3	5	0.37
(1,3556)	1:77:A:PHE:HB3	1:80:A:ALA:HB2	14	0.37
(1,3556)	1:77:A:PHE:HB3	1:80:A:ALA:HB3	17	0.37
(1,3547)	1:54:A:LEU:HG	1:76:A:MET:HE3	8	0.37
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE1	9	0.37
(1,3536)	1:44:A:LEU:H	1:80:A:ALA:HB3	16	0.37
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB2	9	0.37
(1,3504)	1:31:A:MET:HE3	1:86:A:LEU:HD23	12	0.37
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG11	14	0.37
(1,3455)	1:104:A:ASN:H	1:105:A:LYS:HG3	4	0.37
(1,3441)	1:99:A:ALA:HB3	1:96:A:PRO:HB3	12	0.37
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	5	0.37
(1,3402)	1:25:A:VAL:HG13	1:21:A:ASP:HB2	14	0.37
(1,3402)	1:25:A:VAL:HG11	1:21:A:ASP:HB2	16	0.37
(1,3337)	1:14:A:PRO:HD2	1:14:A:PRO:HA	20	0.37
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE2	8	0.37
(1,3272)	1:96:A:PRO:HD3	1:115:A:MET:HE3	1	0.37
(1,3231)	1:107:A:ASP:HB2	1:110:A:ALA:HB2	16	0.37
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB1	1	0.37
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB2	1	0.37
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB3	1	0.37
(1,3192)	1:33:A:PRO:HA	1:58:A:ALA:HB1	13	0.37
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB2	3	0.37
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB3	14	0.37
(1,2972)	1:43:A:ARG:HD3	1:86:A:LEU:HD12	8	0.37
(1,2958)	1:103:A:ALA:HA	1:81:A:LEU:HD13	5	0.37
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD12	15	0.37
(1,2921)	1:73:A:ALA:HA	1:35:A:LEU:HD21	14	0.37
(1,2875)	1:47:A:TYR:HD2	1:44:A:LEU:HD12	13	0.37
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD23	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD23	1	0.37
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD23	12	0.37
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD12	1	0.37
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD11	16	0.37
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD23	3	0.37
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD21	13	0.37
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD21	14	0.37
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD23	15	0.37
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD12	17	0.37
(1,2785)	1:74:A:LEU:HD13	1:31:A:MET:HB2	14	0.37
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG2	10	0.37
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG2	16	0.37
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG2	20	0.37
(1,2618)	1:36:A:ALA:HB2	1:33:A:PRO:HB2	3	0.37
(1,2417)	1:114:A:ALA:HB1	1:98:A:GLU:HG3	1	0.37
(1,2417)	1:114:A:ALA:HB2	1:98:A:GLU:HG3	1	0.37
(1,2417)	1:114:A:ALA:HB3	1:98:A:GLU:HG3	1	0.37
(1,2252)	1:53:A:SER:HB3	1:54:A:LEU:HB2	6	0.37
(1,2116)	1:86:A:LEU:HD12	1:43:A:ARG:HD3	8	0.37
(1,1915)	1:70:A:PHE:HE2	1:26:A:LEU:HA	13	0.37
(1,1883)	1:35:A:LEU:HD22	1:74:A:LEU:HA	5	0.37
(1,1849)	1:115:A:MET:HB3	1:112:A:ALA:HA	13	0.37
(1,1676)	1:42:A:GLU:HG3	1:42:A:GLU:HA	17	0.37
(1,1563)	1:112:A:ALA:HB2	1:108:A:VAL:HA	4	0.37
(1,1562)	1:102:A:ALA:HB2	1:108:A:VAL:HA	9	0.37
(1,1534)	1:88:A:PRO:HG2	1:88:A:PRO:HA	10	0.37
(1,1534)	1:88:A:PRO:HG2	1:88:A:PRO:HA	16	0.37
(1,1534)	1:88:A:PRO:HG2	1:88:A:PRO:HA	20	0.37
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	4	0.37
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	8	0.37
(1,1340)	1:98:A:GLU:HG2	1:118:A:ASN:HD21	6	0.37
(1,1299)	1:40:A:VAL:HG23	1:34:A:ILE:H	10	0.37
(1,1296)	1:26:A:LEU:HD22	1:115:A:MET:H	17	0.37
(1,1282)	1:91:A:CYS:HB3	1:89:A:LEU:H	14	0.37
(1,1222)	1:62:A:GLN:HG2	1:59:A:ASP:H	2	0.37
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	8	0.37
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	20	0.37
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	7	0.37
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	15	0.37
(1,1063)	1:95:A:LEU:HD21	1:94:A:GLY:H	6	0.37
(1,1042)	1:30:A:ILE:HD13	1:29:A:GLU:H	11	0.37
(1,1042)	1:30:A:ILE:HD13	1:29:A:GLU:H	19	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1007)	1:30:A:ILE:HD11	1:119:A:ALA:H	8	0.37
(1,997)	1:123:A:GLN:HG2	1:124:A:LYS:H	11	0.37
(1,921)	1:71:A:GLN:HB3	1:75:A:GLY:H	8	0.37
(1,870)	1:25:A:VAL:HG13	1:24:A:SER:H	9	0.37
(1,786)	1:30:A:ILE:HG21	1:31:A:MET:H	19	0.37
(1,522)	1:114:A:ALA:HB1	1:113:A:LYS:H	17	0.37
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	12	0.37
(1,517)	1:42:A:GLU:HB3	1:44:A:LEU:H	2	0.37
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	17	0.37
(1,452)	1:44:A:LEU:HD13	1:45:A:LEU:H	5	0.37
(1,452)	1:44:A:LEU:HD12	1:45:A:LEU:H	15	0.37
(1,452)	1:44:A:LEU:HD11	1:45:A:LEU:H	16	0.37
(1,452)	1:44:A:LEU:HD11	1:45:A:LEU:H	17	0.37
(1,452)	1:44:A:LEU:HD11	1:45:A:LEU:H	20	0.37
(1,449)	1:45:A:LEU:HD23	1:45:A:LEU:H	1	0.37
(1,449)	1:45:A:LEU:HD23	1:45:A:LEU:H	12	0.37
(1,316)	1:47:A:TYR:HE2	1:80:A:ALA:H	7	0.37
(1,305)	1:26:A:LEU:HD22	1:116:A:GLN:H	8	0.37
(1,303)	1:73:A:ALA:HB2	1:72:A:GLN:H	6	0.37
(1,264)	1:110:A:ALA:HB3	1:109:A:GLU:H	11	0.37
(1,60)	1:48:A:LEU:HD12	1:54:A:LEU:H	17	0.37
(1,3766)	1:45:A:LEU:H	1:47:A:TYR:HE2	6	0.36
(1,3766)	1:83:A:SER:H	1:47:A:TYR:HE2	14	0.36
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	5	0.36
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	8	0.36
(1,3646)	1:62:A:GLN:HB2	1:59:A:ASP:HB3	18	0.36
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD12	13	0.36
(1,3556)	1:77:A:PHE:HB3	1:80:A:ALA:HB2	16	0.36
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB1	6	0.36
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB1	15	0.36
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB2	19	0.36
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB3	2	0.36
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB3	19	0.36
(1,3527)	1:82:A:ALA:HB2	1:108:A:VAL:HG22	13	0.36
(1,3493)	1:76:A:MET:HG2	1:74:A:LEU:HD12	13	0.36
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	4	0.36
(1,3402)	1:22:A:LEU:HD12	1:21:A:ASP:HB2	1	0.36
(1,3383)	1:42:A:GLU:HG3	1:43:A:ARG:HD2	13	0.36
(1,3271)	1:55:A:PRO:HB2	1:61:A:ILE:HD12	4	0.36
(1,3259)	1:77:A:PHE:HE1	1:34:A:ILE:HD12	7	0.36
(1,3258)	1:111:A:PHE:HE2	1:34:A:ILE:HD12	19	0.36
(1,3167)	1:70:A:PHE:HD1	1:61:A:ILE:HG22	13	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3106)	1:40:A:VAL:HG22	1:35:A:LEU:HD12	14	0.36
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD12	10	0.36
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD11	11	0.36
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD21	2	0.36
(1,2920)	1:43:A:ARG:HA	1:86:A:LEU:HD22	16	0.36
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD22	11	0.36
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD22	15	0.36
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD21	19	0.36
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD12	7	0.36
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD23	6	0.36
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD12	11	0.36
(1,2770)	1:99:A:ALA:HB1	1:96:A:PRO:HG3	6	0.36
(1,2770)	1:99:A:ALA:HB1	1:96:A:PRO:HG3	10	0.36
(1,2723)	1:88:A:PRO:HA	1:88:A:PRO:HG3	13	0.36
(1,2644)	1:89:A:LEU:HD21	1:92:A:GLN:HG3	11	0.36
(1,2644)	1:89:A:LEU:HD22	1:92:A:GLN:HG3	11	0.36
(1,2644)	1:89:A:LEU:HD23	1:92:A:GLN:HG3	11	0.36
(1,2456)	1:63:A:ASN:H	1:55:A:PRO:HB3	6	0.36
(1,2297)	1:114:A:ALA:HB3	1:111:A:PHE:HB3	7	0.36
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	16	0.36
(1,2081)	1:65:A:LEU:HD12	1:55:A:PRO:HD2	15	0.36
(1,2066)	1:54:A:LEU:HB3	1:55:A:PRO:HD2	16	0.36
(1,1737)	1:54:A:LEU:HD22	1:41:A:GLN:HA	1	0.36
(1,1737)	1:54:A:LEU:HD22	1:41:A:GLN:HA	5	0.36
(1,1707)	1:30:A:ILE:HG13	1:30:A:ILE:HA	13	0.36
(1,1703)	1:114:A:ALA:HB1	1:98:A:GLU:HA	15	0.36
(1,1569)	1:35:A:LEU:HD23	1:28:A:PRO:HA	1	0.36
(1,1562)	1:102:A:ALA:HB3	1:108:A:VAL:HA	20	0.36
(1,1534)	1:88:A:PRO:HG3	1:88:A:PRO:HA	13	0.36
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	7	0.36
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	11	0.36
(1,1276)	1:95:A:LEU:HB3	1:91:A:CYS:H	1	0.36
(1,1232)	1:57:A:THR:HG22	1:59:A:ASP:H	2	0.36
(1,1222)	1:62:A:GLN:HG2	1:59:A:ASP:H	5	0.36
(1,1187)	1:116:A:GLN:HB2	1:118:A:ASN:H	19	0.36
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	7	0.36
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	18	0.36
(1,1168)	1:131:A:LYS:HB3	1:134:A:GLU:H	8	0.36
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	5	0.36
(1,1067)	1:124:A:LYS:HB3	1:126:A:GLY:H	16	0.36
(1,1018)	1:77:A:PHE:HD1	1:81:A:LEU:H	3	0.36
(1,922)	1:82:A:ALA:HB1	1:84:A:GLY:H	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,922)	1:82:A:ALA:HB1	1:84:A:GLY:H	12	0.36
(1,786)	1:30:A:ILE:HG23	1:31:A:MET:H	10	0.36
(1,786)	1:30:A:ILE:HG22	1:31:A:MET:H	11	0.36
(1,786)	1:30:A:ILE:HG22	1:31:A:MET:H	15	0.36
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	4	0.36
(1,635)	1:40:A:VAL:HG21	1:36:A:ALA:H	9	0.36
(1,614)	1:89:A:LEU:HB2	1:91:A:CYS:H	6	0.36
(1,522)	1:114:A:ALA:HB1	1:113:A:LYS:H	14	0.36
(1,522)	1:114:A:ALA:HB3	1:113:A:LYS:H	18	0.36
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	10	0.36
(1,517)	1:42:A:GLU:HB3	1:44:A:LEU:H	5	0.36
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	13	0.36
(1,468)	1:57:A:THR:HG22	1:56:A:GLN:H	15	0.36
(1,452)	1:44:A:LEU:HD12	1:45:A:LEU:H	6	0.36
(1,452)	1:44:A:LEU:HD11	1:45:A:LEU:H	14	0.36
(1,303)	1:73:A:ALA:HB3	1:72:A:GLN:H	5	0.36
(1,303)	1:73:A:ALA:HB2	1:72:A:GLN:H	15	0.36
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	8	0.36
(1,221)	1:96:A:PRO:HD2	1:99:A:ALA:H	1	0.36
(1,192)	1:108:A:VAL:HG11	1:82:A:ALA:H	18	0.36
(1,60)	1:54:A:LEU:HD12	1:54:A:LEU:H	5	0.36
(1,60)	1:48:A:LEU:HD12	1:54:A:LEU:H	11	0.36
(1,60)	1:54:A:LEU:HD13	1:54:A:LEU:H	12	0.36
(1,3783)	1:26:A:LEU:HD11	1:77:A:PHE:HZ	5	0.35
(1,3782)	1:103:A:ALA:HA	1:111:A:PHE:HZ	14	0.35
(1,3734)	1:90:A:MET:HE1	1:93:A:PHE:HZ	8	0.35
(1,3733)	1:90:A:MET:HE1	1:93:A:PHE:HZ	8	0.35
(1,3712)	1:65:A:LEU:HD13	1:70:A:PHE:HD1	15	0.35
(1,3698)	1:90:A:MET:HE3	1:93:A:PHE:HD2	20	0.35
(1,3627)	1:90:A:MET:HE2	1:93:A:PHE:HB2	6	0.35
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	17	0.35
(1,3556)	1:77:A:PHE:HB3	1:80:A:ALA:HB3	5	0.35
(1,3554)	1:43:A:ARG:HA	1:80:A:ALA:HB3	9	0.35
(1,3541)	1:103:A:ALA:HB2	1:90:A:MET:HE3	8	0.35
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB3	8	0.35
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB3	12	0.35
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB2	16	0.35
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB1	20	0.35
(1,3527)	1:82:A:ALA:HB2	1:108:A:VAL:HG21	11	0.35
(1,3527)	1:82:A:ALA:HB3	1:108:A:VAL:HG22	14	0.35
(1,3504)	1:31:A:MET:HE1	1:86:A:LEU:HD21	2	0.35
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD23	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3464)	1:31:A:MET:HG3	1:26:A:LEU:HD11	11	0.35
(1,3455)	1:104:A:ASN:H	1:105:A:LYS:HG3	14	0.35
(1,3438)	1:35:A:LEU:HB2	1:41:A:GLN:HG3	9	0.35
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	20	0.35
(1,3258)	1:37:A:ASN:H	1:61:A:ILE:HD12	14	0.35
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD13	3	0.35
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD11	13	0.35
(1,3231)	1:107:A:ASP:HB2	1:110:A:ALA:HB3	5	0.35
(1,3231)	1:107:A:ASP:HB2	1:110:A:ALA:HB1	8	0.35
(1,3228)	1:61:A:ILE:HB	1:32:A:ALA:HB1	8	0.35
(1,3192)	1:33:A:PRO:HA	1:58:A:ALA:HB2	16	0.35
(1,3126)	1:111:A:PHE:H	1:114:A:ALA:HB1	19	0.35
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD13	16	0.35
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD11	19	0.35
(1,2746)	1:43:A:ARG:HD2	1:88:A:PRO:HG2	3	0.35
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	4	0.35
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	7	0.35
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	17	0.35
(1,2630)	1:34:A:ILE:HD12	1:90:A:MET:HG3	20	0.35
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	13	0.35
(1,2530)	1:56:A:GLN:HA	1:56:A:GLN:HG2	2	0.35
(1,2530)	1:56:A:GLN:HA	1:56:A:GLN:HG2	11	0.35
(1,2530)	1:56:A:GLN:HA	1:56:A:GLN:HG2	18	0.35
(1,2456)	1:63:A:ASN:H	1:55:A:PRO:HB3	2	0.35
(1,2297)	1:114:A:ALA:HB2	1:111:A:PHE:HB3	3	0.35
(1,2293)	1:34:A:ILE:HB	1:37:A:ASN:HB3	1	0.35
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	20	0.35
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD3	3	0.35
(1,2081)	1:95:A:LEU:HD11	1:96:A:PRO:HD2	18	0.35
(1,1703)	1:114:A:ALA:HB1	1:98:A:GLU:HA	16	0.35
(1,1572)	1:65:A:LEU:HD23	1:53:A:SER:HB2	6	0.35
(1,1563)	1:112:A:ALA:HB1	1:108:A:VAL:HA	15	0.35
(1,1543)	1:31:A:MET:HB3	1:28:A:PRO:HA	4	0.35
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	4	0.35
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	7	0.35
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	17	0.35
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	9	0.35
(1,1365)	1:101:A:GLU:HB2	1:104:A:ASN:HD22	17	0.35
(1,1320)	1:61:A:ILE:HD13	1:35:A:LEU:H	3	0.35
(1,1320)	1:61:A:ILE:HD11	1:35:A:LEU:H	13	0.35
(1,1299)	1:61:A:ILE:HG21	1:34:A:ILE:H	14	0.35
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	14	0.35
(1,1287)	1:33:A:PRO:HG2	1:36:A:ALA:H	2	0.35
(1,1255)	1:26:A:LEU:HG	1:25:A:VAL:H	7	0.35
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	19	0.35
(1,1222)	1:60:A:GLU:HB2	1:59:A:ASP:H	15	0.35
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	15	0.35
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	3	0.35
(1,870)	1:25:A:VAL:HG12	1:24:A:SER:H	20	0.35
(1,760)	1:96:A:PRO:HB2	1:118:A:ASN:HD22	10	0.35
(1,683)	1:40:A:VAL:HG13	1:37:A:ASN:HD21	7	0.35
(1,635)	1:40:A:VAL:HG22	1:36:A:ALA:H	1	0.35
(1,635)	1:40:A:VAL:HG23	1:36:A:ALA:H	4	0.35
(1,635)	1:40:A:VAL:HG23	1:36:A:ALA:H	18	0.35
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	5	0.35
(1,499)	1:115:A:MET:HB2	1:117:A:ASN:H	2	0.35
(1,499)	1:115:A:MET:HB2	1:117:A:ASN:H	8	0.35
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	3	0.35
(1,468)	1:57:A:THR:HG21	1:56:A:GLN:H	4	0.35
(1,452)	1:44:A:LEU:HD11	1:45:A:LEU:H	4	0.35
(1,452)	1:44:A:LEU:HD13	1:45:A:LEU:H	7	0.35
(1,452)	1:44:A:LEU:HD13	1:45:A:LEU:H	8	0.35
(1,452)	1:44:A:LEU:HD12	1:45:A:LEU:H	9	0.35
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	7	0.35
(1,365)	1:101:A:GLU:HG3	1:104:A:ASN:H	8	0.35
(1,172)	1:136:A:GLU:HB3	1:136:A:GLU:H	10	0.35
(1,105)	1:76:A:MET:HB3	1:48:A:LEU:H	16	0.35
(1,3737)	1:89:A:LEU:HG	1:93:A:PHE:HZ	4	0.34
(1,3734)	1:90:A:MET:HE2	1:93:A:PHE:HZ	6	0.34
(1,3733)	1:90:A:MET:HE2	1:93:A:PHE:HZ	6	0.34
(1,3591)	1:44:A:LEU:HA	1:76:A:MET:HE1	20	0.34
(1,3541)	1:89:A:LEU:HB2	1:90:A:MET:HE1	13	0.34
(1,3536)	1:44:A:LEU:H	1:80:A:ALA:HB3	4	0.34
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB2	2	0.34
(1,3504)	1:31:A:MET:HE1	1:86:A:LEU:HD22	18	0.34
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD23	4	0.34
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD23	15	0.34
(1,3470)	1:35:A:LEU:HA	1:44:A:LEU:HD22	11	0.34
(1,3434)	1:114:A:ALA:HA	1:113:A:LYS:HB3	14	0.34
(1,3407)	1:32:A:ALA:H	1:29:A:GLU:HG3	1	0.34
(1,3380)	1:40:A:VAL:HG12	1:43:A:ARG:HD3	14	0.34
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	18	0.34
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	4	0.34
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD11	17	0.34
(1,3258)	1:111:A:PHE:HE2	1:34:A:ILE:HD13	8	0.34
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD12	5	0.34
(1,3231)	1:109:A:GLU:HG3	1:110:A:ALA:HB2	9	0.34
(1,3231)	1:109:A:GLU:HG3	1:110:A:ALA:HB3	14	0.34
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG12	4	0.34
(1,2994)	1:31:A:MET:HG3	1:35:A:LEU:HD23	2	0.34
(1,2958)	1:78:A:SER:HB3	1:81:A:LEU:HD13	7	0.34
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD22	12	0.34
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD23	5	0.34
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD21	18	0.34
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD22	19	0.34
(1,2768)	1:64:A:THR:HG23	1:60:A:GLU:HB2	9	0.34
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	7	0.34
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	5	0.34
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	9	0.34
(1,2669)	1:86:A:LEU:H	1:43:A:ARG:HG3	11	0.34
(1,2669)	1:86:A:LEU:H	1:43:A:ARG:HG3	15	0.34
(1,2631)	1:100:A:VAL:HG21	1:90:A:MET:HB3	5	0.34
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	15	0.34
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	11	0.34
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	16	0.34
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	19	0.34
(1,2530)	1:56:A:GLN:HA	1:56:A:GLN:HG2	6	0.34
(1,2530)	1:56:A:GLN:HA	1:56:A:GLN:HG2	17	0.34
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	15	0.34
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD3	16	0.34
(1,2067)	1:99:A:ALA:HB1	1:96:A:PRO:HD2	1	0.34
(1,2066)	1:54:A:LEU:HB3	1:55:A:PRO:HD2	3	0.34
(1,1849)	1:26:A:LEU:HG	1:112:A:ALA:HA	15	0.34
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	16	0.34
(1,1759)	1:137:A:ASP:H	1:136:A:GLU:HA	13	0.34
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	5	0.34
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	9	0.34
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	15	0.34
(1,1320)	1:61:A:ILE:HD12	1:35:A:LEU:H	5	0.34
(1,1299)	1:40:A:VAL:HG23	1:34:A:ILE:H	7	0.34
(1,1193)	1:108:A:VAL:HG11	1:107:A:ASP:H	19	0.34
(1,1187)	1:116:A:GLN:HB2	1:118:A:ASN:H	1	0.34
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	13	0.34
(1,1145)	1:85:A:GLN:HB2	1:81:A:LEU:H	11	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	20	0.34
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	8	0.34
(1,1067)	1:124:A:LYS:HB3	1:126:A:GLY:H	8	0.34
(1,1042)	1:30:A:ILE:HD13	1:29:A:GLU:H	15	0.34
(1,866)	1:22:A:LEU:HG	1:24:A:SER:H	17	0.34
(1,786)	1:30:A:ILE:HG23	1:31:A:MET:H	8	0.34
(1,786)	1:30:A:ILE:HG22	1:31:A:MET:H	16	0.34
(1,760)	1:96:A:PRO:HB2	1:118:A:ASN:HD22	3	0.34
(1,760)	1:96:A:PRO:HB2	1:118:A:ASN:HD22	11	0.34
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	19	0.34
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	20	0.34
(1,635)	1:40:A:VAL:HG22	1:36:A:ALA:H	5	0.34
(1,522)	1:114:A:ALA:HB2	1:113:A:LYS:H	3	0.34
(1,504)	1:65:A:LEU:HD13	1:74:A:LEU:H	11	0.34
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	16	0.34
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	19	0.34
(1,452)	1:44:A:LEU:HD13	1:45:A:LEU:H	11	0.34
(1,316)	1:47:A:TYR:HE2	1:80:A:ALA:H	14	0.34
(1,303)	1:73:A:ALA:HB3	1:72:A:GLN:H	16	0.34
(1,297)	1:113:A:LYS:HG3	1:114:A:ALA:H	5	0.34
(1,264)	1:110:A:ALA:HB2	1:109:A:GLU:H	2	0.34
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	13	0.34
(1,221)	1:96:A:PRO:HD2	1:99:A:ALA:H	8	0.34
(1,60)	1:54:A:LEU:HD11	1:54:A:LEU:H	13	0.34
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	19	0.33
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	9	0.33
(1,3737)	1:89:A:LEU:HG	1:93:A:PHE:HZ	18	0.33
(1,3712)	1:65:A:LEU:HD12	1:70:A:PHE:HD1	6	0.33
(1,3556)	1:43:A:ARG:HD3	1:80:A:ALA:HB3	2	0.33
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE3	17	0.33
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE1	19	0.33
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB2	14	0.33
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG13	13	0.33
(1,3464)	1:31:A:MET:HG2	1:26:A:LEU:HD11	16	0.33
(1,3455)	1:104:A:ASN:H	1:105:A:LYS:HG3	7	0.33
(1,3455)	1:104:A:ASN:H	1:105:A:LYS:HG3	12	0.33
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	2	0.33
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE3	11	0.33
(1,3271)	1:31:A:MET:HE2	1:34:A:ILE:HD12	16	0.33
(1,3267)	1:31:A:MET:HG2	1:34:A:ILE:HD11	3	0.33
(1,3258)	1:111:A:PHE:HE2	1:34:A:ILE:HD11	15	0.33
(1,3258)	1:111:A:PHE:HE2	1:34:A:ILE:HD12	20	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3231)	1:107:A:ASP:HB2	1:110:A:ALA:HB2	2	0.33
(1,3161)	1:79:A:ALA:H	1:80:A:ALA:HB2	19	0.33
(1,3106)	1:40:A:VAL:HG21	1:35:A:LEU:HD11	15	0.33
(1,3094)	1:56:A:GLN:HB3	1:57:A:THR:HG21	3	0.33
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD11	6	0.33
(1,2930)	1:103:A:ALA:HA	1:105:A:LYS:HG2	6	0.33
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD23	20	0.33
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD13	3	0.33
(1,2832)	1:111:A:PHE:H	1:81:A:LEU:HD11	14	0.33
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD23	5	0.33
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD21	20	0.33
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	8	0.33
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	13	0.33
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	15	0.33
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	16	0.33
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	19	0.33
(1,2631)	1:100:A:VAL:HG21	1:90:A:MET:HB3	11	0.33
(1,2617)	1:95:A:LEU:HD22	1:90:A:MET:HB2	3	0.33
(1,2617)	1:95:A:LEU:HD23	1:90:A:MET:HB2	10	0.33
(1,2530)	1:56:A:GLN:HA	1:56:A:GLN:HG2	3	0.33
(1,2530)	1:56:A:GLN:HA	1:56:A:GLN:HG2	10	0.33
(1,2482)	1:93:A:PHE:HZ	1:40:A:VAL:HB	12	0.33
(1,2252)	1:53:A:SER:HB3	1:54:A:LEU:HB2	17	0.33
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	4	0.33
(1,2081)	1:95:A:LEU:HD11	1:96:A:PRO:HD2	8	0.33
(1,1703)	1:114:A:ALA:HB1	1:98:A:GLU:HA	7	0.33
(1,1572)	1:48:A:LEU:HD12	1:53:A:SER:HB2	4	0.33
(1,1563)	1:112:A:ALA:HB3	1:108:A:VAL:HA	12	0.33
(1,1563)	1:112:A:ALA:HB1	1:108:A:VAL:HA	18	0.33
(1,1562)	1:102:A:ALA:HB3	1:108:A:VAL:HA	8	0.33
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	8	0.33
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	13	0.33
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	15	0.33
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	16	0.33
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	19	0.33
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	17	0.33
(1,1306)	1:49:A:PRO:HD2	1:53:A:SER:H	1	0.33
(1,1299)	1:40:A:VAL:HG22	1:34:A:ILE:H	2	0.33
(1,1299)	1:61:A:ILE:HG21	1:34:A:ILE:H	5	0.33
(1,1299)	1:40:A:VAL:HG23	1:34:A:ILE:H	12	0.33
(1,1287)	1:33:A:PRO:HG2	1:36:A:ALA:H	1	0.33
(1,1287)	1:61:A:ILE:HB	1:36:A:ALA:H	15	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1187)	1:116:A:GLN:HB2	1:118:A:ASN:H	18	0.33
(1,1168)	1:131:A:LYS:HB3	1:134:A:GLU:H	6	0.33
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	5	0.33
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	18	0.33
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	14	0.33
(1,1067)	1:124:A:LYS:HB3	1:126:A:GLY:H	1	0.33
(1,896)	1:72:A:GLN:HG2	1:72:A:GLN:HE22	6	0.33
(1,870)	1:25:A:VAL:HG11	1:24:A:SER:H	16	0.33
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	12	0.33
(1,635)	1:40:A:VAL:HG23	1:36:A:ALA:H	16	0.33
(1,618)	1:37:A:ASN:HA	1:37:A:ASN:HD22	1	0.33
(1,618)	1:37:A:ASN:HA	1:37:A:ASN:HD22	15	0.33
(1,563)	1:54:A:LEU:HD12	1:42:A:GLU:H	4	0.33
(1,562)	1:95:A:LEU:HD22	1:93:A:PHE:H	4	0.33
(1,522)	1:114:A:ALA:HB1	1:113:A:LYS:H	11	0.33
(1,517)	1:42:A:GLU:HB3	1:44:A:LEU:H	11	0.33
(1,506)	1:74:A:LEU:HD23	1:74:A:LEU:H	5	0.33
(1,506)	1:74:A:LEU:HD21	1:74:A:LEU:H	20	0.33
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	3	0.33
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	5	0.33
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	11	0.33
(1,399)	1:117:A:ASN:HB3	1:118:A:ASN:H	17	0.33
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	14	0.33
(1,303)	1:73:A:ALA:HB1	1:72:A:GLN:H	13	0.33
(1,115)	1:80:A:ALA:HB2	1:79:A:ALA:H	19	0.33
(1,60)	1:54:A:LEU:HD13	1:54:A:LEU:H	18	0.33
(1,3642)	1:74:A:LEU:HD21	1:70:A:PHE:HA	18	0.32
(1,3556)	1:77:A:PHE:HB3	1:80:A:ALA:HB3	12	0.32
(1,3547)	1:54:A:LEU:HG	1:76:A:MET:HE3	9	0.32
(1,3541)	1:103:A:ALA:HB3	1:90:A:MET:HE3	14	0.32
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE1	19	0.32
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB3	11	0.32
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB1	13	0.32
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB3	20	0.32
(1,3473)	1:55:A:PRO:HD2	1:65:A:LEU:HD22	1	0.32
(1,3473)	1:55:A:PRO:HD2	1:65:A:LEU:HD21	9	0.32
(1,3464)	1:31:A:MET:HG3	1:26:A:LEU:HD11	19	0.32
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	7	0.32
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	9	0.32
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	2	0.32
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	3	0.32
(1,3332)	1:72:A:GLN:HB3	1:70:A:PHE:HA	18	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3271)	1:31:A:MET:HE2	1:34:A:ILE:HD11	5	0.32
(1,3267)	1:31:A:MET:HG2	1:34:A:ILE:HD11	13	0.32
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD13	5	0.32
(1,3231)	1:107:A:ASP:HB2	1:110:A:ALA:HB1	15	0.32
(1,3194)	1:47:A:TYR:HA	1:79:A:ALA:HB3	7	0.32
(1,3177)	1:27:A:THR:H	1:30:A:ILE:HG23	15	0.32
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB1	8	0.32
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB3	18	0.32
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB3	2	0.32
(1,3117)	1:119:A:ALA:H	1:115:A:MET:HE2	15	0.32
(1,2958)	1:103:A:ALA:HA	1:81:A:LEU:HD11	14	0.32
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD13	5	0.32
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD13	12	0.32
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD11	19	0.32
(1,2921)	1:32:A:ALA:HA	1:35:A:LEU:HD23	12	0.32
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD23	14	0.32
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD23	15	0.32
(1,2803)	1:81:A:LEU:H	1:81:A:LEU:HD22	1	0.32
(1,2769)	1:99:A:ALA:HB2	1:115:A:MET:HB2	3	0.32
(1,2768)	1:64:A:THR:HG23	1:60:A:GLU:HB2	19	0.32
(1,2746)	1:43:A:ARG:HD3	1:88:A:PRO:HG2	20	0.32
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	3	0.32
(1,2694)	1:72:A:GLN:HE21	1:49:A:PRO:HG3	6	0.32
(1,2631)	1:100:A:VAL:HG22	1:90:A:MET:HB3	19	0.32
(1,2617)	1:95:A:LEU:HD21	1:90:A:MET:HB2	16	0.32
(1,2530)	1:56:A:GLN:HA	1:56:A:GLN:HG2	14	0.32
(1,2496)	1:65:A:LEU:H	1:62:A:GLN:HG2	3	0.32
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	7	0.32
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	11	0.32
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	12	0.32
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	12	0.32
(1,2067)	1:99:A:ALA:HB1	1:96:A:PRO:HD2	18	0.32
(1,1707)	1:30:A:ILE:HG13	1:30:A:ILE:HA	12	0.32
(1,1703)	1:114:A:ALA:HB1	1:98:A:GLU:HA	6	0.32
(1,1569)	1:35:A:LEU:HD21	1:28:A:PRO:HA	16	0.32
(1,1563)	1:112:A:ALA:HB2	1:108:A:VAL:HA	7	0.32
(1,1563)	1:112:A:ALA:HB1	1:108:A:VAL:HA	9	0.32
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	3	0.32
(1,1429)	1:116:A:GLN:HB2	1:119:A:ALA:H	9	0.32
(1,1415)	1:72:A:GLN:HA	1:75:A:GLY:H	18	0.32
(1,1398)	1:27:A:THR:HG22	1:24:A:SER:H	1	0.32
(1,1307)	1:51:A:GLY:HA3	1:53:A:SER:H	12	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1287)	1:61:A:ILE:HB	1:36:A:ALA:H	5	0.32
(1,1274)	1:95:A:LEU:HD22	1:91:A:CYS:H	19	0.32
(1,1255)	1:26:A:LEU:HG	1:25:A:VAL:H	4	0.32
(1,1175)	1:113:A:LYS:HG2	1:114:A:ALA:H	9	0.32
(1,1122)	1:114:A:ALA:HB3	1:119:A:ALA:H	12	0.32
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	1	0.32
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	6	0.32
(1,896)	1:72:A:GLN:HG2	1:72:A:GLN:HE22	1	0.32
(1,866)	1:22:A:LEU:HG	1:24:A:SER:H	7	0.32
(1,803)	1:46:A:PRO:HG2	1:85:A:GLN:HE21	15	0.32
(1,786)	1:30:A:ILE:HG23	1:31:A:MET:H	20	0.32
(1,635)	1:40:A:VAL:HG22	1:36:A:ALA:H	8	0.32
(1,618)	1:37:A:ASN:HA	1:37:A:ASN:HD22	6	0.32
(1,618)	1:37:A:ASN:HA	1:37:A:ASN:HD22	12	0.32
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	2	0.32
(1,506)	1:74:A:LEU:HD23	1:74:A:LEU:H	15	0.32
(1,504)	1:22:A:LEU:HD12	1:74:A:LEU:H	14	0.32
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	11	0.32
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	14	0.32
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	19	0.32
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	1	0.32
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	12	0.32
(1,459)	1:37:A:ASN:HB3	1:41:A:GLN:H	11	0.32
(1,424)	1:110:A:ALA:HB1	1:107:A:ASP:H	8	0.32
(1,424)	1:110:A:ALA:HB1	1:107:A:ASP:H	15	0.32
(1,424)	1:110:A:ALA:HB3	1:107:A:ASP:H	18	0.32
(1,377)	1:100:A:VAL:HG21	1:104:A:ASN:H	15	0.32
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	4	0.32
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	13	0.32
(1,305)	1:26:A:LEU:HD22	1:116:A:GLN:H	10	0.32
(1,297)	1:113:A:LYS:HG3	1:114:A:ALA:H	4	0.32
(1,297)	1:113:A:LYS:HG3	1:114:A:ALA:H	19	0.32
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	19	0.32
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	11	0.32
(1,192)	1:108:A:VAL:HG12	1:82:A:ALA:H	4	0.32
(1,105)	1:76:A:MET:HB3	1:48:A:LEU:H	1	0.32
(1,95)	1:119:A:ALA:HB2	1:119:A:ALA:H	14	0.32
(1,3783)	1:26:A:LEU:HD11	1:77:A:PHE:HZ	16	0.31
(1,3663)	1:44:A:LEU:HG	1:47:A:TYR:HD2	3	0.31
(1,3556)	1:77:A:PHE:HB3	1:80:A:ALA:HB1	8	0.31
(1,3547)	1:54:A:LEU:HG	1:76:A:MET:HE1	7	0.31
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE2	20	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE1	10	0.31
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB3	3	0.31
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB1	5	0.31
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB1	3	0.31
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB1	11	0.31
(1,3527)	1:82:A:ALA:HB1	1:108:A:VAL:HG23	4	0.31
(1,3527)	1:82:A:ALA:HB2	1:108:A:VAL:HG23	12	0.31
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD21	7	0.31
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD22	17	0.31
(1,3455)	1:104:A:ASN:H	1:105:A:LYS:HG3	20	0.31
(1,3418)	1:98:A:GLU:HA	1:101:A:GLU:HG3	9	0.31
(1,3380)	1:40:A:VAL:HG11	1:43:A:ARG:HD3	1	0.31
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	11	0.31
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	12	0.31
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	14	0.31
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	6	0.31
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	13	0.31
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE2	18	0.31
(1,3273)	1:96:A:PRO:HD2	1:115:A:MET:HE3	13	0.31
(1,3272)	1:96:A:PRO:HD3	1:115:A:MET:HE2	4	0.31
(1,3258)	1:37:A:ASN:H	1:61:A:ILE:HD11	6	0.31
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD11	11	0.31
(1,3231)	1:107:A:ASP:HB2	1:110:A:ALA:HB1	19	0.31
(1,3231)	1:107:A:ASP:HB2	1:110:A:ALA:HB3	20	0.31
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB1	8	0.31
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB2	8	0.31
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB3	8	0.31
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD11	7	0.31
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD13	3	0.31
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD13	7	0.31
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD12	9	0.31
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD11	20	0.31
(1,2920)	1:43:A:ARG:HA	1:86:A:LEU:HD22	12	0.31
(1,2911)	1:53:A:SER:HA	1:48:A:LEU:HD12	20	0.31
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD12	4	0.31
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD23	1	0.31
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD22	3	0.31
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD21	16	0.31
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD21	19	0.31
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD13	19	0.31
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	1	0.31
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	18	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	18	0.31
(1,2417)	1:114:A:ALA:HB1	1:98:A:GLU:HG3	8	0.31
(1,2417)	1:114:A:ALA:HB2	1:98:A:GLU:HG3	8	0.31
(1,2417)	1:114:A:ALA:HB3	1:98:A:GLU:HG3	8	0.31
(1,2265)	1:37:A:ASN:HB3	1:89:A:LEU:HB3	6	0.31
(1,2081)	1:65:A:LEU:HD13	1:55:A:PRO:HD2	16	0.31
(1,2066)	1:54:A:LEU:HB3	1:55:A:PRO:HD2	2	0.31
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	19	0.31
(1,1859)	1:64:A:THR:HG21	1:60:A:GLU:HA	7	0.31
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	1	0.31
(1,1737)	1:54:A:LEU:HD11	1:41:A:GLN:HA	20	0.31
(1,1707)	1:30:A:ILE:HG13	1:30:A:ILE:HA	9	0.31
(1,1707)	1:30:A:ILE:HG13	1:30:A:ILE:HA	20	0.31
(1,1676)	1:42:A:GLU:HG3	1:42:A:GLU:HA	6	0.31
(1,1563)	1:112:A:ALA:HB1	1:108:A:VAL:HA	20	0.31
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	1	0.31
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	18	0.31
(1,1457)	1:20:A:VAL:HG21	1:109:A:GLU:H	4	0.31
(1,1457)	1:20:A:VAL:HG22	1:109:A:GLU:H	4	0.31
(1,1457)	1:20:A:VAL:HG23	1:109:A:GLU:H	4	0.31
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	2	0.31
(1,1432)	1:119:A:ALA:HB2	1:117:A:ASN:H	13	0.31
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	8	0.31
(1,1320)	1:61:A:ILE:HD11	1:35:A:LEU:H	11	0.31
(1,1232)	1:57:A:THR:HG22	1:59:A:ASP:H	3	0.31
(1,1222)	1:62:A:GLN:HG2	1:59:A:ASP:H	6	0.31
(1,1222)	1:62:A:GLN:HG2	1:59:A:ASP:H	13	0.31
(1,1222)	1:60:A:GLU:HB2	1:59:A:ASP:H	17	0.31
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	7	0.31
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	11	0.31
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	16	0.31
(1,1063)	1:95:A:LEU:HD22	1:94:A:GLY:H	5	0.31
(1,1063)	1:95:A:LEU:HD22	1:94:A:GLY:H	17	0.31
(1,896)	1:72:A:GLN:HG2	1:72:A:GLN:HE22	9	0.31
(1,896)	1:72:A:GLN:HG2	1:72:A:GLN:HE22	14	0.31
(1,896)	1:72:A:GLN:HG2	1:72:A:GLN:HE22	15	0.31
(1,896)	1:72:A:GLN:HG2	1:72:A:GLN:HE22	20	0.31
(1,870)	1:25:A:VAL:HG12	1:24:A:SER:H	12	0.31
(1,786)	1:30:A:ILE:HG21	1:31:A:MET:H	2	0.31
(1,786)	1:30:A:ILE:HG21	1:31:A:MET:H	12	0.31
(1,775)	1:62:A:GLN:HB2	1:63:A:ASN:HD22	19	0.31
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	11	0.31
(1,723)	1:86:A:LEU:HD12	1:86:A:LEU:H	4	0.31
(1,618)	1:37:A:ASN:HA	1:37:A:ASN:HD22	20	0.31
(1,562)	1:95:A:LEU:HD23	1:93:A:PHE:H	11	0.31
(1,506)	1:74:A:LEU:HD23	1:74:A:LEU:H	1	0.31
(1,506)	1:74:A:LEU:HD21	1:74:A:LEU:H	16	0.31
(1,506)	1:74:A:LEU:HD21	1:74:A:LEU:H	19	0.31
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	17	0.31
(1,499)	1:115:A:MET:HB3	1:117:A:ASN:H	7	0.31
(1,499)	1:115:A:MET:HB3	1:117:A:ASN:H	10	0.31
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	6	0.31
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	7	0.31
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	9	0.31
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	20	0.31
(1,452)	1:44:A:LEU:HD11	1:45:A:LEU:H	2	0.31
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	10	0.31
(1,316)	1:47:A:TYR:HE2	1:80:A:ALA:H	15	0.31
(1,192)	1:108:A:VAL:HG11	1:82:A:ALA:H	12	0.31
(1,129)	1:122:A:GLU:HB3	1:122:A:GLU:H	9	0.31
(1,60)	1:48:A:LEU:HD13	1:54:A:LEU:H	19	0.31
(1,3783)	1:26:A:LEU:HD12	1:77:A:PHE:HZ	2	0.3
(1,3782)	1:103:A:ALA:HA	1:111:A:PHE:HZ	5	0.3
(1,3737)	1:89:A:LEU:HG	1:93:A:PHE:HZ	12	0.3
(1,3712)	1:65:A:LEU:HD11	1:70:A:PHE:HD1	16	0.3
(1,3712)	1:65:A:LEU:HD11	1:70:A:PHE:HD1	17	0.3
(1,3698)	1:108:A:VAL:HB	1:111:A:PHE:HD2	8	0.3
(1,3656)	1:80:A:ALA:HA	1:47:A:TYR:HD2	10	0.3
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	3	0.3
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	10	0.3
(1,3615)	1:31:A:MET:HG2	1:30:A:ILE:HD12	12	0.3
(1,3547)	1:54:A:LEU:HG	1:76:A:MET:HE3	6	0.3
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE3	17	0.3
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB2	16	0.3
(1,3470)	1:35:A:LEU:HA	1:44:A:LEU:HD22	13	0.3
(1,3455)	1:104:A:ASN:H	1:105:A:LYS:HG3	8	0.3
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	9	0.3
(1,3418)	1:98:A:GLU:HA	1:101:A:GLU:HG3	8	0.3
(1,3407)	1:32:A:ALA:H	1:29:A:GLU:HG3	6	0.3
(1,3402)	1:22:A:LEU:HD11	1:21:A:ASP:HB2	5	0.3
(1,3379)	1:86:A:LEU:HA	1:43:A:ARG:HD3	9	0.3
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	7	0.3
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	16	0.3
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	17	0.3
(1,3337)	1:14:A:PRO:HD3	1:14:A:PRO:HA	6	0.3
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	9	0.3
(1,3332)	1:72:A:GLN:HB3	1:70:A:PHE:HA	10	0.3
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	12	0.3
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD13	13	0.3
(1,3258)	1:111:A:PHE:HE2	1:34:A:ILE:HD11	11	0.3
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD13	12	0.3
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD11	19	0.3
(1,3239)	1:34:A:ILE:HD12	1:90:A:MET:HE2	9	0.3
(1,3228)	1:61:A:ILE:HB	1:32:A:ALA:HB3	14	0.3
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD13	3	0.3
(1,2994)	1:31:A:MET:HG3	1:35:A:LEU:HD22	15	0.3
(1,2976)	1:111:A:PHE:HB3	1:81:A:LEU:HD23	8	0.3
(1,2940)	1:55:A:PRO:HD3	1:54:A:LEU:HD21	10	0.3
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD13	8	0.3
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD11	17	0.3
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD13	10	0.3
(1,2842)	1:105:A:LYS:H	1:105:A:LYS:HG3	4	0.3
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD22	8	0.3
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD22	11	0.3
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD22	17	0.3
(1,2801)	1:81:A:LEU:H	1:44:A:LEU:HD11	7	0.3
(1,2769)	1:99:A:ALA:HB2	1:115:A:MET:HB2	1	0.3
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	6	0.3
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	10	0.3
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	11	0.3
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	12	0.3
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	14	0.3
(1,2644)	1:89:A:LEU:HD21	1:92:A:GLN:HG3	16	0.3
(1,2644)	1:89:A:LEU:HD22	1:92:A:GLN:HG3	16	0.3
(1,2644)	1:89:A:LEU:HD23	1:92:A:GLN:HG3	16	0.3
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	4	0.3
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	11	0.3
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	14	0.3
(1,2585)	1:77:A:PHE:HB3	1:76:A:MET:HG3	3	0.3
(1,2530)	1:56:A:GLN:HA	1:56:A:GLN:HG2	7	0.3
(1,2265)	1:37:A:ASN:HB3	1:89:A:LEU:HB3	1	0.3
(1,2189)	1:93:A:PHE:HZ	1:89:A:LEU:HB2	6	0.3
(1,2147)	1:74:A:LEU:H	1:65:A:LEU:HB2	17	0.3
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	16	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2066)	1:54:A:LEU:HB3	1:55:A:PRO:HD2	20	0.3
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	6	0.3
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	18	0.3
(1,2030)	1:41:A:GLN:HE22	1:55:A:PRO:HD2	4	0.3
(1,1927)	1:47:A:TYR:HD2	1:80:A:ALA:HA	10	0.3
(1,1883)	1:35:A:LEU:HD22	1:74:A:LEU:HA	3	0.3
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	13	0.3
(1,1734)	1:44:A:LEU:HD11	1:76:A:MET:HA	1	0.3
(1,1563)	1:112:A:ALA:HB3	1:108:A:VAL:HA	2	0.3
(1,1563)	1:112:A:ALA:HB3	1:108:A:VAL:HA	10	0.3
(1,1563)	1:112:A:ALA:HB3	1:108:A:VAL:HA	16	0.3
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	6	0.3
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	10	0.3
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	11	0.3
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	12	0.3
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	14	0.3
(1,1468)	1:44:A:LEU:H	1:40:A:VAL:HA	13	0.3
(1,1320)	1:61:A:ILE:HD13	1:35:A:LEU:H	12	0.3
(1,1320)	1:61:A:ILE:HD11	1:35:A:LEU:H	19	0.3
(1,1310)	1:89:A:LEU:HD21	1:86:A:LEU:H	19	0.3
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	10	0.3
(1,1122)	1:99:A:ALA:HB1	1:119:A:ALA:H	16	0.3
(1,1116)	1:96:A:PRO:HA	1:119:A:ALA:H	13	0.3
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	3	0.3
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	9	0.3
(1,1078)	1:81:A:LEU:HG	1:106:A:GLY:H	6	0.3
(1,1063)	1:95:A:LEU:HD21	1:94:A:GLY:H	13	0.3
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	16	0.3
(1,896)	1:72:A:GLN:HG3	1:72:A:GLN:HE22	4	0.3
(1,896)	1:69:A:GLN:HB3	1:72:A:GLN:HE22	7	0.3
(1,786)	1:30:A:ILE:HG21	1:31:A:MET:H	13	0.3
(1,755)	1:116:A:GLN:HB3	1:115:A:MET:H	17	0.3
(1,618)	1:37:A:ASN:HA	1:37:A:ASN:HD22	4	0.3
(1,563)	1:54:A:LEU:HD13	1:42:A:GLU:H	19	0.3
(1,562)	1:95:A:LEU:HD22	1:93:A:PHE:H	5	0.3
(1,506)	1:35:A:LEU:HD22	1:74:A:LEU:H	3	0.3
(1,506)	1:74:A:LEU:HD22	1:74:A:LEU:H	8	0.3
(1,506)	1:74:A:LEU:HD22	1:74:A:LEU:H	11	0.3
(1,506)	1:74:A:LEU:HD22	1:74:A:LEU:H	17	0.3
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	6	0.3
(1,297)	1:113:A:LYS:HG3	1:114:A:ALA:H	12	0.3
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	14	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:108:A:VAL:HG12	1:82:A:ALA:H	5	0.3
(1,60)	1:54:A:LEU:HD12	1:54:A:LEU:H	9	0.3
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	4	0.29
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	11	0.29
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	14	0.29
(1,3737)	1:89:A:LEU:HG	1:93:A:PHE:HZ	11	0.29
(1,3698)	1:90:A:MET:HE3	1:111:A:PHE:HD1	11	0.29
(1,3558)	1:117:A:ASN:HB2	1:114:A:ALA:HB2	5	0.29
(1,3547)	1:54:A:LEU:HG	1:76:A:MET:HE3	5	0.29
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE1	9	0.29
(1,3536)	1:44:A:LEU:H	1:80:A:ALA:HB2	20	0.29
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB2	7	0.29
(1,3530)	1:35:A:LEU:H	1:36:A:ALA:HB2	9	0.29
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB1	5	0.29
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB2	6	0.29
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB1	12	0.29
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB2	17	0.29
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	14	0.29
(1,3394)	1:33:A:PRO:HG2	1:93:A:PHE:HB3	20	0.29
(1,3375)	1:58:A:ALA:HB3	1:33:A:PRO:HD2	16	0.29
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	10	0.29
(1,3337)	1:14:A:PRO:HD3	1:14:A:PRO:HA	18	0.29
(1,3286)	1:89:A:LEU:HG	1:40:A:VAL:HA	14	0.29
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE3	1	0.29
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE1	5	0.29
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE2	20	0.29
(1,3258)	1:111:A:PHE:HE2	1:34:A:ILE:HD13	13	0.29
(1,3177)	1:27:A:THR:H	1:30:A:ILE:HG21	6	0.29
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD12	9	0.29
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD13	14	0.29
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD11	14	0.29
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD11	16	0.29
(1,2914)	1:45:A:LEU:HA	1:48:A:LEU:HD11	6	0.29
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD12	12	0.29
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD12	20	0.29
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD12	5	0.29
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD11	9	0.29
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD13	16	0.29
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD23	6	0.29
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD22	10	0.29
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD23	14	0.29
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD23	18	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	2	0.29
(1,2721)	1:33:A:PRO:HA	1:33:A:PRO:HG2	20	0.29
(1,2530)	1:56:A:GLN:HA	1:56:A:GLN:HG2	1	0.29
(1,2369)	1:43:A:ARG:H	1:42:A:GLU:HG2	7	0.29
(1,2297)	1:114:A:ALA:HB3	1:111:A:PHE:HB3	8	0.29
(1,2147)	1:32:A:ALA:H	1:65:A:LEU:HB2	1	0.29
(1,2109)	1:49:A:PRO:HD2	1:48:A:LEU:HB3	7	0.29
(1,2109)	1:49:A:PRO:HD3	1:48:A:LEU:HB3	9	0.29
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	2	0.29
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	14	0.29
(1,2030)	1:41:A:GLN:HE22	1:55:A:PRO:HD2	15	0.29
(1,1915)	1:70:A:PHE:HE2	1:26:A:LEU:HA	1	0.29
(1,1883)	1:35:A:LEU:HD21	1:74:A:LEU:HA	6	0.29
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	14	0.29
(1,1707)	1:30:A:ILE:HG13	1:30:A:ILE:HA	1	0.29
(1,1707)	1:114:A:ALA:HB3	1:111:A:PHE:HA	10	0.29
(1,1703)	1:114:A:ALA:HB2	1:98:A:GLU:HA	8	0.29
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	2	0.29
(1,1537)	1:33:A:PRO:HG2	1:33:A:PRO:HA	20	0.29
(1,1307)	1:51:A:GLY:HA3	1:53:A:SER:H	20	0.29
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	15	0.29
(1,1287)	1:33:A:PRO:HG2	1:36:A:ALA:H	3	0.29
(1,1287)	1:33:A:PRO:HG2	1:36:A:ALA:H	6	0.29
(1,1274)	1:95:A:LEU:HD21	1:91:A:CYS:H	8	0.29
(1,1251)	1:92:A:GLN:HE22	1:92:A:GLN:H	18	0.29
(1,1225)	1:72:A:GLN:HG3	1:74:A:LEU:H	4	0.29
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	6	0.29
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	20	0.29
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	20	0.29
(1,1063)	1:95:A:LEU:HD22	1:94:A:GLY:H	20	0.29
(1,896)	1:72:A:GLN:HG2	1:72:A:GLN:HE22	5	0.29
(1,896)	1:72:A:GLN:HG2	1:72:A:GLN:HE22	13	0.29
(1,896)	1:72:A:GLN:HG3	1:72:A:GLN:HE22	19	0.29
(1,786)	1:30:A:ILE:HG22	1:31:A:MET:H	17	0.29
(1,760)	1:96:A:PRO:HB2	1:118:A:ASN:HD22	13	0.29
(1,759)	1:60:A:GLU:HB3	1:63:A:ASN:HD21	8	0.29
(1,723)	1:86:A:LEU:HD13	1:86:A:LEU:H	16	0.29
(1,635)	1:40:A:VAL:HG23	1:36:A:ALA:H	12	0.29
(1,547)	1:40:A:VAL:HB	1:42:A:GLU:H	14	0.29
(1,506)	1:74:A:LEU:HD23	1:74:A:LEU:H	6	0.29
(1,506)	1:74:A:LEU:HD22	1:74:A:LEU:H	10	0.29
(1,506)	1:74:A:LEU:HD23	1:74:A:LEU:H	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,506)	1:74:A:LEU:HD23	1:74:A:LEU:H	18	0.29
(1,504)	1:65:A:LEU:HD13	1:74:A:LEU:H	19	0.29
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	2	0.29
(1,468)	1:57:A:THR:HG23	1:56:A:GLN:H	11	0.29
(1,452)	1:44:A:LEU:HD12	1:45:A:LEU:H	18	0.29
(1,399)	1:118:A:ASN:HB3	1:118:A:ASN:H	16	0.29
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	2	0.29
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	5	0.29
(1,303)	1:73:A:ALA:HB3	1:72:A:GLN:H	20	0.29
(1,297)	1:113:A:LYS:HG3	1:114:A:ALA:H	18	0.29
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	3	0.29
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	20	0.29
(1,192)	1:108:A:VAL:HG12	1:82:A:ALA:H	2	0.29
(1,3766)	1:83:A:SER:H	1:47:A:TYR:HE1	17	0.28
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	1	0.28
(1,3712)	1:26:A:LEU:HD22	1:111:A:PHE:HE2	4	0.28
(1,3712)	1:65:A:LEU:HD13	1:70:A:PHE:HD1	11	0.28
(1,3704)	1:102:A:ALA:HB3	1:111:A:PHE:HD1	9	0.28
(1,3645)	1:55:A:PRO:HD2	1:35:A:LEU:HD13	9	0.28
(1,3601)	1:25:A:VAL:H	1:24:A:SER:HB2	7	0.28
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE3	3	0.28
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE3	8	0.28
(1,3533)	1:111:A:PHE:HD2	1:115:A:MET:HE2	3	0.28
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB3	4	0.28
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD23	6	0.28
(1,3457)	1:105:A:LYS:H	1:81:A:LEU:HD21	16	0.28
(1,3449)	1:94:A:GLY:HA2	1:91:A:CYS:HB2	17	0.28
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	5	0.28
(1,3407)	1:32:A:ALA:H	1:29:A:GLU:HG3	7	0.28
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	13	0.28
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	2	0.28
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	7	0.28
(1,3273)	1:96:A:PRO:HD2	1:115:A:MET:HE2	8	0.28
(1,3271)	1:55:A:PRO:HB2	1:61:A:ILE:HD12	20	0.28
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD11	7	0.28
(1,3242)	1:95:A:LEU:HD11	1:115:A:MET:HE3	1	0.28
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB1	7	0.28
(1,3158)	1:114:A:ALA:H	1:110:A:ALA:HB3	15	0.28
(1,3080)	1:116:A:GLN:HA	1:25:A:VAL:HG23	17	0.28
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD22	18	0.28
(1,2958)	1:103:A:ALA:HA	1:81:A:LEU:HD11	16	0.28
(1,2920)	1:43:A:ARG:HA	1:86:A:LEU:HD21	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2868)	1:79:A:ALA:H	1:86:A:LEU:HD22	1	0.28
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD21	6	0.28
(1,2782)	1:26:A:LEU:HD23	1:115:A:MET:HB3	13	0.28
(1,2638)	1:89:A:LEU:HD23	1:88:A:PRO:HB2	20	0.28
(1,2630)	1:34:A:ILE:HD12	1:90:A:MET:HG3	7	0.28
(1,2542)	1:107:A:ASP:HA	1:108:A:VAL:HB	2	0.28
(1,2450)	1:86:A:LEU:H	1:85:A:GLN:HG3	4	0.28
(1,2297)	1:99:A:ALA:HB3	1:111:A:PHE:HB3	15	0.28
(1,2265)	1:43:A:ARG:HD3	1:89:A:LEU:HB3	11	0.28
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	9	0.28
(1,2109)	1:49:A:PRO:HD3	1:48:A:LEU:HB3	1	0.28
(1,2109)	1:49:A:PRO:HD3	1:48:A:LEU:HB3	5	0.28
(1,2109)	1:49:A:PRO:HD3	1:48:A:LEU:HB3	15	0.28
(1,2109)	1:49:A:PRO:HD3	1:48:A:LEU:HB3	19	0.28
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD2	6	0.28
(1,1997)	1:108:A:VAL:HG11	1:82:A:ALA:HA	2	0.28
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	16	0.28
(1,1565)	1:64:A:THR:HG21	1:61:A:ILE:HA	5	0.28
(1,1562)	1:102:A:ALA:HB3	1:108:A:VAL:HA	1	0.28
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	1	0.28
(1,1320)	1:61:A:ILE:HD11	1:35:A:LEU:H	7	0.28
(1,1306)	1:49:A:PRO:HD2	1:53:A:SER:H	2	0.28
(1,1255)	1:26:A:LEU:HG	1:25:A:VAL:H	3	0.28
(1,1251)	1:92:A:GLN:HE22	1:92:A:GLN:H	19	0.28
(1,1232)	1:57:A:THR:HG21	1:59:A:ASP:H	17	0.28
(1,1222)	1:62:A:GLN:HG2	1:59:A:ASP:H	11	0.28
(1,1187)	1:116:A:GLN:HB2	1:118:A:ASN:H	2	0.28
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	6	0.28
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	17	0.28
(1,1158)	1:119:A:ALA:HB3	1:120:A:LYS:H	1	0.28
(1,1144)	1:44:A:LEU:HG	1:81:A:LEU:H	16	0.28
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	13	0.28
(1,1067)	1:124:A:LYS:HB3	1:126:A:GLY:H	12	0.28
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	9	0.28
(1,896)	1:72:A:GLN:HG2	1:72:A:GLN:HE22	11	0.28
(1,896)	1:72:A:GLN:HG2	1:72:A:GLN:HE22	12	0.28
(1,896)	1:72:A:GLN:HG2	1:72:A:GLN:HE22	16	0.28
(1,896)	1:72:A:GLN:HG3	1:72:A:GLN:HE22	17	0.28
(1,870)	1:25:A:VAL:HG13	1:24:A:SER:H	15	0.28
(1,868)	1:65:A:LEU:HD21	1:69:A:GLN:HE21	14	0.28
(1,786)	1:30:A:ILE:HG22	1:31:A:MET:H	3	0.28
(1,755)	1:116:A:GLN:HB3	1:115:A:MET:H	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	17	0.28
(1,635)	1:40:A:VAL:HG22	1:36:A:ALA:H	3	0.28
(1,618)	1:37:A:ASN:HA	1:37:A:ASN:HD22	14	0.28
(1,562)	1:95:A:LEU:HD22	1:93:A:PHE:H	17	0.28
(1,562)	1:95:A:LEU:HD23	1:93:A:PHE:H	18	0.28
(1,517)	1:42:A:GLU:HB3	1:44:A:LEU:H	17	0.28
(1,499)	1:115:A:MET:HB3	1:117:A:ASN:H	13	0.28
(1,468)	1:57:A:THR:HG22	1:56:A:GLN:H	18	0.28
(1,452)	1:44:A:LEU:HD13	1:45:A:LEU:H	10	0.28
(1,452)	1:44:A:LEU:HD12	1:45:A:LEU:H	13	0.28
(1,424)	1:110:A:ALA:HB1	1:107:A:ASP:H	7	0.28
(1,423)	1:105:A:LYS:HG2	1:107:A:ASP:H	6	0.28
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	3	0.28
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	18	0.28
(1,303)	1:73:A:ALA:HB1	1:72:A:GLN:H	9	0.28
(1,297)	1:113:A:LYS:HG3	1:114:A:ALA:H	2	0.28
(1,263)	1:102:A:ALA:HB3	1:109:A:GLU:H	11	0.28
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	16	0.28
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	19	0.28
(1,192)	1:108:A:VAL:HG12	1:82:A:ALA:H	15	0.28
(1,164)	1:133:A:ASP:HB3	1:133:A:ASP:H	19	0.28
(1,3782)	1:103:A:ALA:HA	1:111:A:PHE:HZ	4	0.27
(1,3756)	1:22:A:LEU:HB3	1:77:A:PHE:HD1	10	0.27
(1,3712)	1:26:A:LEU:HD21	1:111:A:PHE:HE2	14	0.27
(1,3707)	1:95:A:LEU:HD13	1:93:A:PHE:HD2	9	0.27
(1,3634)	1:65:A:LEU:HD12	1:70:A:PHE:HB3	9	0.27
(1,3634)	1:65:A:LEU:HD13	1:70:A:PHE:HB3	19	0.27
(1,3551)	1:57:A:THR:HB	1:36:A:ALA:HB3	18	0.27
(1,3547)	1:54:A:LEU:HG	1:76:A:MET:HE1	1	0.27
(1,3547)	1:54:A:LEU:HG	1:76:A:MET:HE3	2	0.27
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE3	7	0.27
(1,3529)	1:81:A:LEU:H	1:82:A:ALA:HB1	18	0.27
(1,3497)	1:85:A:GLN:HB3	1:86:A:LEU:HD21	9	0.27
(1,3493)	1:76:A:MET:HG2	1:74:A:LEU:HD12	18	0.27
(1,3455)	1:104:A:ASN:H	1:105:A:LYS:HG3	19	0.27
(1,3434)	1:116:A:GLN:HA	1:120:A:LYS:HB2	7	0.27
(1,3403)	1:79:A:ALA:HB2	1:47:A:TYR:HB2	4	0.27
(1,3375)	1:58:A:ALA:HB1	1:33:A:PRO:HD2	4	0.27
(1,3337)	1:11:A:PRO:HD3	1:11:A:PRO:HA	7	0.27
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	11	0.27
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	14	0.27
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	12	0.27
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD12	18	0.27
(1,3196)	1:31:A:MET:HA	1:30:A:ILE:HG23	9	0.27
(1,3188)	1:57:A:THR:HA	1:58:A:ALA:HB2	20	0.27
(1,3187)	1:115:A:MET:HA	1:99:A:ALA:HB2	15	0.27
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB2	12	0.27
(1,3094)	1:56:A:GLN:HB3	1:57:A:THR:HG23	14	0.27
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG11	17	0.27
(1,2958)	1:103:A:ALA:HA	1:81:A:LEU:HD12	4	0.27
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD11	2	0.27
(1,2920)	1:43:A:ARG:HA	1:86:A:LEU:HD23	13	0.27
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD22	4	0.27
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD11	13	0.27
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD11	10	0.27
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD12	11	0.27
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD12	15	0.27
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD22	7	0.27
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD22	9	0.27
(1,2785)	1:74:A:LEU:HD11	1:31:A:MET:HB2	16	0.27
(1,2770)	1:99:A:ALA:HB1	1:96:A:PRO:HG3	3	0.27
(1,2630)	1:34:A:ILE:HD13	1:90:A:MET:HG3	13	0.27
(1,2630)	1:34:A:ILE:HD11	1:90:A:MET:HG3	16	0.27
(1,2542)	1:107:A:ASP:HA	1:108:A:VAL:HB	18	0.27
(1,2530)	1:56:A:GLN:HA	1:56:A:GLN:HG2	8	0.27
(1,2265)	1:37:A:ASN:HB3	1:89:A:LEU:HB3	3	0.27
(1,2265)	1:43:A:ARG:HD3	1:89:A:LEU:HB3	8	0.27
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD2	5	0.27
(1,2067)	1:27:A:THR:HG21	1:28:A:PRO:HD3	8	0.27
(1,2067)	1:99:A:ALA:HB1	1:96:A:PRO:HD2	10	0.27
(1,2066)	1:54:A:LEU:HB3	1:55:A:PRO:HD2	5	0.27
(1,1915)	1:70:A:PHE:HE2	1:26:A:LEU:HA	2	0.27
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	20	0.27
(1,1510)	1:80:A:ALA:H	1:78:A:SER:HB2	7	0.27
(1,1334)	1:60:A:GLU:HB2	1:63:A:ASN:HD21	4	0.27
(1,1309)	1:54:A:LEU:HG	1:53:A:SER:H	2	0.27
(1,1307)	1:51:A:GLY:HA3	1:53:A:SER:H	7	0.27
(1,1307)	1:51:A:GLY:HA3	1:53:A:SER:H	19	0.27
(1,1299)	1:40:A:VAL:HG23	1:34:A:ILE:H	4	0.27
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	5	0.27
(1,1296)	1:26:A:LEU:HD22	1:115:A:MET:H	19	0.27
(1,1287)	1:61:A:ILE:HB	1:36:A:ALA:H	16	0.27
(1,1275)	1:92:A:GLN:HB2	1:91:A:CYS:H	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1274)	1:95:A:LEU:HD22	1:91:A:CYS:H	4	0.27
(1,1255)	1:26:A:LEU:HG	1:25:A:VAL:H	2	0.27
(1,1222)	1:60:A:GLU:HB2	1:59:A:ASP:H	3	0.27
(1,1206)	1:34:A:ILE:HB	1:37:A:ASN:H	5	0.27
(1,1187)	1:116:A:GLN:HB2	1:118:A:ASN:H	13	0.27
(1,1165)	1:70:A:PHE:HE2	1:23:A:ALA:H	4	0.27
(1,1129)	1:44:A:LEU:HA	1:79:A:ALA:H	4	0.27
(1,1116)	1:96:A:PRO:HA	1:119:A:ALA:H	19	0.27
(1,1005)	1:70:A:PHE:HD2	1:70:A:PHE:H	20	0.27
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	11	0.27
(1,896)	1:72:A:GLN:HG2	1:72:A:GLN:HE22	3	0.27
(1,866)	1:22:A:LEU:HG	1:24:A:SER:H	14	0.27
(1,723)	1:86:A:LEU:HD11	1:86:A:LEU:H	10	0.27
(1,723)	1:86:A:LEU:HD12	1:86:A:LEU:H	11	0.27
(1,723)	1:86:A:LEU:HD12	1:86:A:LEU:H	15	0.27
(1,517)	1:42:A:GLU:HB2	1:44:A:LEU:H	8	0.27
(1,506)	1:74:A:LEU:HD22	1:74:A:LEU:H	7	0.27
(1,506)	1:74:A:LEU:HD22	1:74:A:LEU:H	9	0.27
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	6	0.27
(1,468)	1:57:A:THR:HG22	1:56:A:GLN:H	17	0.27
(1,424)	1:110:A:ALA:HB2	1:107:A:ASP:H	12	0.27
(1,402)	1:42:A:GLU:HB2	1:39:A:ASP:H	13	0.27
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	15	0.27
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	17	0.27
(1,303)	1:73:A:ALA:HB3	1:72:A:GLN:H	1	0.27
(1,303)	1:73:A:ALA:HB2	1:72:A:GLN:H	3	0.27
(1,303)	1:73:A:ALA:HB2	1:72:A:GLN:H	8	0.27
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	1	0.27
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	7	0.27
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	20	0.27
(1,209)	1:131:A:LYS:HB2	1:131:A:LYS:H	6	0.27
(1,3758)	1:26:A:LEU:HD11	1:77:A:PHE:HD1	5	0.26
(1,3737)	1:89:A:LEU:HG	1:93:A:PHE:HZ	20	0.26
(1,3704)	1:102:A:ALA:HB3	1:111:A:PHE:HD1	6	0.26
(1,3682)	1:91:A:CYS:HA	1:93:A:PHE:HD2	4	0.26
(1,3663)	1:44:A:LEU:HG	1:47:A:TYR:HD2	13	0.26
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	13	0.26
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	3	0.26
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD12	14	0.26
(1,3565)	1:90:A:MET:HE3	1:31:A:MET:HE2	5	0.26
(1,3556)	1:43:A:ARG:HD3	1:80:A:ALA:HB1	15	0.26
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE1	16	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD21	20	0.26
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG12	5	0.26
(1,3455)	1:104:A:ASN:H	1:105:A:LYS:HG3	2	0.26
(1,3402)	1:22:A:LEU:HD13	1:21:A:ASP:HB2	8	0.26
(1,3383)	1:42:A:GLU:HG3	1:43:A:ARG:HD2	1	0.26
(1,3375)	1:58:A:ALA:HB2	1:33:A:PRO:HD2	20	0.26
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	1	0.26
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	4	0.26
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	8	0.26
(1,3337)	1:11:A:PRO:HD3	1:11:A:PRO:HA	3	0.26
(1,3337)	1:11:A:PRO:HD3	1:11:A:PRO:HA	13	0.26
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	10	0.26
(1,3231)	1:109:A:GLU:HG3	1:110:A:ALA:HB1	10	0.26
(1,3231)	1:107:A:ASP:HB2	1:110:A:ALA:HB3	11	0.26
(1,3230)	1:115:A:MET:HG2	1:99:A:ALA:HB3	18	0.26
(1,3228)	1:61:A:ILE:HB	1:32:A:ALA:HB2	16	0.26
(1,3192)	1:33:A:PRO:HA	1:58:A:ALA:HB1	9	0.26
(1,3191)	1:107:A:ASP:HA	1:82:A:ALA:HB2	18	0.26
(1,3177)	1:27:A:THR:H	1:30:A:ILE:HG21	5	0.26
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB1	6	0.26
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB3	2	0.26
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB2	4	0.26
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB2	13	0.26
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD12	15	0.26
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD11	19	0.26
(1,3054)	1:32:A:ALA:H	1:35:A:LEU:HD12	1	0.26
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD23	8	0.26
(1,2958)	1:103:A:ALA:HA	1:81:A:LEU:HD12	20	0.26
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD22	10	0.26
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD12	13	0.26
(1,2909)	1:86:A:LEU:HA	1:89:A:LEU:HD23	18	0.26
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD11	9	0.26
(1,2842)	1:105:A:LYS:H	1:105:A:LYS:HG3	2	0.26
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD23	2	0.26
(1,2770)	1:99:A:ALA:HB3	1:96:A:PRO:HG3	5	0.26
(1,2638)	1:89:A:LEU:HD21	1:88:A:PRO:HB2	7	0.26
(1,2638)	1:89:A:LEU:HD23	1:88:A:PRO:HB2	13	0.26
(1,2631)	1:100:A:VAL:HG21	1:90:A:MET:HB3	1	0.26
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	2	0.26
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	12	0.26
(1,2585)	1:77:A:PHE:HB3	1:76:A:MET:HG3	1	0.26
(1,2542)	1:107:A:ASP:HA	1:108:A:VAL:HB	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2530)	1:56:A:GLN:HA	1:56:A:GLN:HG2	20	0.26
(1,2456)	1:120:A:LYS:H	1:121:A:PRO:HB3	10	0.26
(1,2252)	1:41:A:GLN:HA	1:54:A:LEU:HB3	14	0.26
(1,1997)	1:108:A:VAL:HG11	1:82:A:ALA:HA	8	0.26
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	13	0.26
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	6	0.26
(1,1707)	1:114:A:ALA:HB3	1:111:A:PHE:HA	7	0.26
(1,1569)	1:74:A:LEU:HD12	1:28:A:PRO:HA	15	0.26
(1,1562)	1:102:A:ALA:HB2	1:108:A:VAL:HA	4	0.26
(1,1556)	1:36:A:ALA:HB2	1:33:A:PRO:HA	10	0.26
(1,1552)	1:89:A:LEU:HB2	1:88:A:PRO:HA	18	0.26
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	6	0.26
(1,1307)	1:51:A:GLY:HA3	1:53:A:SER:H	4	0.26
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	19	0.26
(1,1275)	1:92:A:GLN:HB2	1:91:A:CYS:H	13	0.26
(1,1255)	1:26:A:LEU:HG	1:25:A:VAL:H	17	0.26
(1,1246)	1:44:A:LEU:HD13	1:42:A:GLU:H	14	0.26
(1,1235)	1:93:A:PHE:HZ	1:93:A:PHE:H	4	0.26
(1,1222)	1:60:A:GLU:HB2	1:59:A:ASP:H	20	0.26
(1,1202)	1:40:A:VAL:HA	1:45:A:LEU:H	9	0.26
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	19	0.26
(1,1145)	1:85:A:GLN:HB2	1:81:A:LEU:H	12	0.26
(1,1144)	1:44:A:LEU:HG	1:81:A:LEU:H	4	0.26
(1,1097)	1:74:A:LEU:HG	1:22:A:LEU:H	19	0.26
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	2	0.26
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	19	0.26
(1,1063)	1:95:A:LEU:HD23	1:94:A:GLY:H	11	0.26
(1,522)	1:114:A:ALA:HB2	1:113:A:LYS:H	2	0.26
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	19	0.26
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	10	0.26
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	12	0.26
(1,424)	1:110:A:ALA:HB1	1:107:A:ASP:H	6	0.26
(1,297)	1:113:A:LYS:HG3	1:114:A:ALA:H	14	0.26
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	3	0.26
(1,105)	1:76:A:MET:HB3	1:48:A:LEU:H	8	0.26
(1,105)	1:76:A:MET:HB3	1:48:A:LEU:H	13	0.26
(1,105)	1:76:A:MET:HB3	1:48:A:LEU:H	18	0.26
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	15	0.25
(1,3758)	1:26:A:LEU:HD11	1:77:A:PHE:HD1	12	0.25
(1,3707)	1:26:A:LEU:HD21	1:111:A:PHE:HD2	7	0.25
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	15	0.25
(1,3541)	1:103:A:ALA:HB3	1:90:A:MET:HE3	17	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE3	14	0.25
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE1	6	0.25
(1,3527)	1:82:A:ALA:HB3	1:108:A:VAL:HG22	6	0.25
(1,3527)	1:82:A:ALA:HB1	1:108:A:VAL:HG23	8	0.25
(1,3527)	1:82:A:ALA:HB3	1:108:A:VAL:HG22	15	0.25
(1,3493)	1:76:A:MET:HG2	1:74:A:LEU:HD12	19	0.25
(1,3464)	1:31:A:MET:HG2	1:26:A:LEU:HD11	5	0.25
(1,3434)	1:114:A:ALA:HA	1:113:A:LYS:HB3	1	0.25
(1,3392)	1:87:A:GLY:HA2	1:86:A:LEU:HB2	20	0.25
(1,3375)	1:58:A:ALA:HB1	1:33:A:PRO:HD2	8	0.25
(1,3375)	1:58:A:ALA:HB2	1:33:A:PRO:HD2	13	0.25
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	15	0.25
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	16	0.25
(1,3337)	1:14:A:PRO:HD3	1:14:A:PRO:HA	10	0.25
(1,3314)	1:93:A:PHE:HB2	1:34:A:ILE:HA	17	0.25
(1,3286)	1:89:A:LEU:HG	1:40:A:VAL:HA	4	0.25
(1,3271)	1:55:A:PRO:HB2	1:61:A:ILE:HD13	11	0.25
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD11	15	0.25
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG11	7	0.25
(1,2972)	1:77:A:PHE:HB3	1:44:A:LEU:HD11	3	0.25
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG13	8	0.25
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG11	17	0.25
(1,2949)	1:61:A:ILE:HA	1:65:A:LEU:HD23	18	0.25
(1,2940)	1:55:A:PRO:HD3	1:54:A:LEU:HD21	8	0.25
(1,2930)	1:103:A:ALA:HA	1:105:A:LYS:HG2	2	0.25
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD11	15	0.25
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD22	16	0.25
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD11	3	0.25
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD13	14	0.25
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD23	4	0.25
(1,2694)	1:99:A:ALA:H	1:96:A:PRO:HG3	15	0.25
(1,2638)	1:89:A:LEU:HD13	1:88:A:PRO:HB2	4	0.25
(1,2630)	1:34:A:ILE:HD11	1:90:A:MET:HG3	17	0.25
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	15	0.25
(1,2530)	1:56:A:GLN:HA	1:56:A:GLN:HG2	12	0.25
(1,2482)	1:93:A:PHE:HZ	1:40:A:VAL:HB	2	0.25
(1,2252)	1:53:A:SER:HB3	1:54:A:LEU:HB2	3	0.25
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	13	0.25
(1,2109)	1:49:A:PRO:HD3	1:48:A:LEU:HB3	13	0.25
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD2	18	0.25
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	12	0.25
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	20	0.25
(1,1915)	1:70:A:PHE:HE2	1:26:A:LEU:HA	9	0.25
(1,1859)	1:64:A:THR:HG22	1:60:A:GLU:HA	10	0.25
(1,1859)	1:64:A:THR:HG21	1:60:A:GLU:HA	11	0.25
(1,1849)	1:26:A:LEU:HG	1:112:A:ALA:HA	8	0.25
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	3	0.25
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	7	0.25
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	11	0.25
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	19	0.25
(1,1548)	1:61:A:ILE:HB	1:61:A:ILE:HA	1	0.25
(1,1548)	1:61:A:ILE:HB	1:61:A:ILE:HA	7	0.25
(1,1548)	1:61:A:ILE:HB	1:61:A:ILE:HA	9	0.25
(1,1548)	1:61:A:ILE:HB	1:61:A:ILE:HA	13	0.25
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	5	0.25
(1,1429)	1:116:A:GLN:HB2	1:119:A:ALA:H	2	0.25
(1,1429)	1:116:A:GLN:HB2	1:119:A:ALA:H	13	0.25
(1,1310)	1:89:A:LEU:HD22	1:86:A:LEU:H	13	0.25
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	17	0.25
(1,1287)	1:33:A:PRO:HG2	1:36:A:ALA:H	11	0.25
(1,1287)	1:61:A:ILE:HB	1:36:A:ALA:H	18	0.25
(1,1282)	1:91:A:CYS:HB2	1:89:A:LEU:H	16	0.25
(1,1274)	1:95:A:LEU:HD21	1:91:A:CYS:H	14	0.25
(1,1273)	1:80:A:ALA:HB2	1:85:A:GLN:H	3	0.25
(1,1257)	1:27:A:THR:HG22	1:25:A:VAL:H	16	0.25
(1,1232)	1:57:A:THR:HG21	1:59:A:ASP:H	20	0.25
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	6	0.25
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	19	0.25
(1,965)	1:93:A:PHE:HE1	1:38:A:ALA:H	5	0.25
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	14	0.25
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	4	0.25
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	9	0.25
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	16	0.25
(1,870)	1:25:A:VAL:HG11	1:24:A:SER:H	2	0.25
(1,870)	1:25:A:VAL:HG12	1:24:A:SER:H	7	0.25
(1,775)	1:62:A:GLN:HB2	1:63:A:ASN:HD22	16	0.25
(1,755)	1:116:A:GLN:HB3	1:115:A:MET:H	6	0.25
(1,755)	1:116:A:GLN:HB3	1:115:A:MET:H	13	0.25
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	14	0.25
(1,723)	1:86:A:LEU:HD11	1:86:A:LEU:H	3	0.25
(1,723)	1:86:A:LEU:HD13	1:86:A:LEU:H	14	0.25
(1,699)	1:64:A:THR:HB	1:63:A:ASN:H	3	0.25
(1,635)	1:40:A:VAL:HG23	1:36:A:ALA:H	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,618)	1:37:A:ASN:HA	1:37:A:ASN:HD22	16	0.25
(1,547)	1:40:A:VAL:HB	1:42:A:GLU:H	16	0.25
(1,517)	1:42:A:GLU:HB2	1:44:A:LEU:H	1	0.25
(1,506)	1:74:A:LEU:HD23	1:74:A:LEU:H	4	0.25
(1,468)	1:57:A:THR:HG23	1:56:A:GLN:H	2	0.25
(1,459)	1:37:A:ASN:HB3	1:41:A:GLN:H	12	0.25
(1,425)	1:57:A:THR:HG22	1:60:A:GLU:H	20	0.25
(1,424)	1:110:A:ALA:HB1	1:107:A:ASP:H	19	0.25
(1,399)	1:118:A:ASN:HB3	1:118:A:ASN:H	4	0.25
(1,316)	1:47:A:TYR:HE2	1:80:A:ALA:H	19	0.25
(1,303)	1:73:A:ALA:HB1	1:72:A:GLN:H	11	0.25
(1,297)	1:113:A:LYS:HG3	1:114:A:ALA:H	9	0.25
(1,297)	1:113:A:LYS:HG3	1:114:A:ALA:H	20	0.25
(1,264)	1:110:A:ALA:HB3	1:109:A:GLU:H	18	0.25
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	5	0.25
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	12	0.25
(1,192)	1:108:A:VAL:HG11	1:82:A:ALA:H	11	0.25
(1,165)	1:130:A:ASP:HB3	1:130:A:ASP:H	15	0.25
(1,109)	1:48:A:LEU:HD23	1:48:A:LEU:H	12	0.25
(1,47)	1:20:A:VAL:HG11	1:21:A:ASP:H	17	0.25
(1,47)	1:20:A:VAL:HG12	1:21:A:ASP:H	17	0.25
(1,47)	1:20:A:VAL:HG13	1:21:A:ASP:H	17	0.25
(1,3783)	1:26:A:LEU:HD13	1:77:A:PHE:HZ	12	0.24
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	12	0.24
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	13	0.24
(1,3698)	1:90:A:MET:HE1	1:93:A:PHE:HD2	14	0.24
(1,3698)	1:90:A:MET:HE2	1:111:A:PHE:HD1	18	0.24
(1,3646)	1:62:A:GLN:HB2	1:59:A:ASP:HB2	4	0.24
(1,3642)	1:35:A:LEU:HD21	1:70:A:PHE:HA	3	0.24
(1,3615)	1:29:A:GLU:HG3	1:30:A:ILE:HD12	2	0.24
(1,3551)	1:56:A:GLN:HA	1:36:A:ALA:HB1	10	0.24
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE3	18	0.24
(1,3527)	1:112:A:ALA:HB3	1:108:A:VAL:HG21	2	0.24
(1,3527)	1:82:A:ALA:HB2	1:108:A:VAL:HG22	5	0.24
(1,3416)	1:114:A:ALA:HA	1:117:A:ASN:HB3	7	0.24
(1,3402)	1:25:A:VAL:HG13	1:21:A:ASP:HB2	15	0.24
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	17	0.24
(1,3379)	1:86:A:LEU:HA	1:43:A:ARG:HD3	16	0.24
(1,3375)	1:58:A:ALA:HB3	1:33:A:PRO:HD2	11	0.24
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	3	0.24
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	3	0.24
(1,3337)	1:11:A:PRO:HD3	1:11:A:PRO:HA	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	20	0.24
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE1	15	0.24
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE2	17	0.24
(1,3271)	1:31:A:MET:HE3	1:34:A:ILE:HD13	19	0.24
(1,3258)	1:111:A:PHE:HE2	1:34:A:ILE:HD13	5	0.24
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB1	13	0.24
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB2	13	0.24
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB3	13	0.24
(1,3196)	1:31:A:MET:HA	1:30:A:ILE:HG23	7	0.24
(1,3141)	1:89:A:LEU:H	1:90:A:MET:HE1	10	0.24
(1,3125)	1:62:A:GLN:H	1:32:A:ALA:HB3	20	0.24
(1,3117)	1:116:A:GLN:H	1:115:A:MET:HE2	7	0.24
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG13	3	0.24
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG13	5	0.24
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG13	6	0.24
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG12	10	0.24
(1,2930)	1:103:A:ALA:HA	1:105:A:LYS:HG2	12	0.24
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD12	6	0.24
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD13	10	0.24
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD12	18	0.24
(1,2920)	1:43:A:ARG:HA	1:86:A:LEU:HD22	3	0.24
(1,2894)	1:77:A:PHE:HE1	1:35:A:LEU:HD21	1	0.24
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD21	3	0.24
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD11	5	0.24
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD11	7	0.24
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD11	12	0.24
(1,2768)	1:64:A:THR:HG21	1:60:A:GLU:HB2	7	0.24
(1,2694)	1:99:A:ALA:H	1:96:A:PRO:HG3	1	0.24
(1,2638)	1:89:A:LEU:HD21	1:88:A:PRO:HB2	2	0.24
(1,2638)	1:89:A:LEU:HD23	1:88:A:PRO:HB2	9	0.24
(1,2631)	1:100:A:VAL:HG21	1:90:A:MET:HB3	3	0.24
(1,2631)	1:100:A:VAL:HG23	1:90:A:MET:HB3	17	0.24
(1,2630)	1:34:A:ILE:HD11	1:90:A:MET:HG3	6	0.24
(1,2620)	1:64:A:THR:HG21	1:60:A:GLU:HB2	7	0.24
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	7	0.24
(1,2585)	1:77:A:PHE:HB3	1:76:A:MET:HG3	12	0.24
(1,2417)	1:114:A:ALA:HB1	1:98:A:GLU:HG3	13	0.24
(1,2417)	1:114:A:ALA:HB2	1:98:A:GLU:HG3	13	0.24
(1,2417)	1:114:A:ALA:HB3	1:98:A:GLU:HG3	13	0.24
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	20	0.24
(1,2189)	1:93:A:PHE:HZ	1:89:A:LEU:HB2	2	0.24
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD2	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	11	0.24
(1,1883)	1:35:A:LEU:HD22	1:74:A:LEU:HA	17	0.24
(1,1859)	1:64:A:THR:HG23	1:60:A:GLU:HA	8	0.24
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	9	0.24
(1,1707)	1:30:A:ILE:HG13	1:30:A:ILE:HA	4	0.24
(1,1699)	1:128:A:THR:HG22	1:128:A:THR:HA	15	0.24
(1,1683)	1:29:A:GLU:HG3	1:29:A:GLU:HA	1	0.24
(1,1683)	1:29:A:GLU:HG3	1:29:A:GLU:HA	10	0.24
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	15	0.24
(1,1558)	1:64:A:THR:HG23	1:53:A:SER:HB3	17	0.24
(1,1548)	1:61:A:ILE:HB	1:61:A:ILE:HA	5	0.24
(1,1548)	1:61:A:ILE:HB	1:61:A:ILE:HA	11	0.24
(1,1548)	1:61:A:ILE:HB	1:61:A:ILE:HA	15	0.24
(1,1548)	1:61:A:ILE:HB	1:61:A:ILE:HA	19	0.24
(1,1548)	1:61:A:ILE:HB	1:61:A:ILE:HA	20	0.24
(1,1462)	1:60:A:GLU:HB3	1:57:A:THR:HB	16	0.24
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	3	0.24
(1,1429)	1:116:A:GLN:HB3	1:119:A:ALA:H	1	0.24
(1,1414)	1:87:A:GLY:HA2	1:84:A:GLY:H	14	0.24
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	19	0.24
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	20	0.24
(1,1275)	1:92:A:GLN:HB2	1:91:A:CYS:H	5	0.24
(1,1274)	1:95:A:LEU:HD22	1:91:A:CYS:H	15	0.24
(1,1255)	1:26:A:LEU:HG	1:25:A:VAL:H	6	0.24
(1,1222)	1:62:A:GLN:HG2	1:59:A:ASP:H	18	0.24
(1,1206)	1:34:A:ILE:HB	1:37:A:ASN:H	9	0.24
(1,1202)	1:40:A:VAL:HA	1:45:A:LEU:H	2	0.24
(1,1129)	1:44:A:LEU:HA	1:79:A:ALA:H	17	0.24
(1,1097)	1:74:A:LEU:HG	1:22:A:LEU:H	6	0.24
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	11	0.24
(1,1007)	1:30:A:ILE:HD11	1:119:A:ALA:H	12	0.24
(1,1007)	1:30:A:ILE:HD12	1:119:A:ALA:H	15	0.24
(1,1005)	1:70:A:PHE:HD2	1:70:A:PHE:H	5	0.24
(1,1005)	1:70:A:PHE:HD1	1:70:A:PHE:H	18	0.24
(1,1005)	1:70:A:PHE:HD2	1:70:A:PHE:H	19	0.24
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	12	0.24
(1,900)	1:69:A:GLN:HB2	1:72:A:GLN:HE22	11	0.24
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	11	0.24
(1,870)	1:25:A:VAL:HG11	1:24:A:SER:H	17	0.24
(1,868)	1:65:A:LEU:HD21	1:72:A:GLN:HE21	10	0.24
(1,775)	1:62:A:GLN:HB2	1:63:A:ASN:HD22	5	0.24
(1,767)	1:100:A:VAL:HG23	1:90:A:MET:H	17	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,723)	1:86:A:LEU:HD11	1:86:A:LEU:H	5	0.24
(1,723)	1:86:A:LEU:HD11	1:86:A:LEU:H	7	0.24
(1,723)	1:86:A:LEU:HD11	1:86:A:LEU:H	12	0.24
(1,663)	1:22:A:LEU:HD23	1:78:A:SER:H	13	0.24
(1,635)	1:40:A:VAL:HG22	1:36:A:ALA:H	14	0.24
(1,618)	1:37:A:ASN:HA	1:37:A:ASN:HD22	8	0.24
(1,563)	1:54:A:LEU:HD12	1:42:A:GLU:H	8	0.24
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	7	0.24
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	10	0.24
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	17	0.24
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	18	0.24
(1,468)	1:57:A:THR:HG21	1:56:A:GLN:H	5	0.24
(1,468)	1:57:A:THR:HG22	1:56:A:GLN:H	7	0.24
(1,449)	1:45:A:LEU:HD21	1:45:A:LEU:H	3	0.24
(1,399)	1:118:A:ASN:HB3	1:118:A:ASN:H	15	0.24
(1,264)	1:110:A:ALA:HB3	1:109:A:GLU:H	20	0.24
(1,263)	1:102:A:ALA:HB1	1:109:A:GLU:H	14	0.24
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	13	0.24
(1,221)	1:96:A:PRO:HD2	1:99:A:ALA:H	9	0.24
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	6	0.24
(1,105)	1:76:A:MET:HB3	1:48:A:LEU:H	4	0.24
(1,95)	1:119:A:ALA:HB1	1:119:A:ALA:H	20	0.24
(1,3774)	1:86:A:LEU:HB2	1:47:A:TYR:HE2	10	0.23
(1,3707)	1:95:A:LEU:HD11	1:93:A:PHE:HD2	2	0.23
(1,3698)	1:90:A:MET:HE1	1:111:A:PHE:HD1	12	0.23
(1,3584)	1:10:A:VAL:HG12	1:11:A:PRO:HA	3	0.23
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD13	15	0.23
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE2	12	0.23
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE1	5	0.23
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE3	18	0.23
(1,3519)	1:19:A:GLN:HG2	1:20:A:VAL:HG12	14	0.23
(1,3428)	1:35:A:LEU:H	1:40:A:VAL:HB	13	0.23
(1,3407)	1:32:A:ALA:H	1:29:A:GLU:HG3	11	0.23
(1,3402)	1:22:A:LEU:HD13	1:21:A:ASP:HB2	10	0.23
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	10	0.23
(1,3337)	1:14:A:PRO:HD3	1:14:A:PRO:HA	5	0.23
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	7	0.23
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	13	0.23
(1,3290)	1:55:A:PRO:HB3	1:64:A:THR:HB	1	0.23
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE2	2	0.23
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD11	16	0.23
(1,3192)	1:33:A:PRO:HA	1:58:A:ALA:HB2	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3188)	1:57:A:THR:HA	1:58:A:ALA:HB3	18	0.23
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB2	7	0.23
(1,3141)	1:89:A:LEU:H	1:90:A:MET:HE1	4	0.23
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG12	16	0.23
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD23	6	0.23
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG13	2	0.23
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG12	4	0.23
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG11	7	0.23
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG11	18	0.23
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG12	19	0.23
(1,2856)	1:92:A:GLN:HE22	1:89:A:LEU:HD23	13	0.23
(1,2828)	1:74:A:LEU:H	1:74:A:LEU:HD23	13	0.23
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD13	9	0.23
(1,2769)	1:99:A:ALA:HB1	1:115:A:MET:HB2	19	0.23
(1,2715)	1:123:A:GLN:HA	1:123:A:GLN:HB3	20	0.23
(1,2638)	1:89:A:LEU:HD23	1:88:A:PRO:HB2	6	0.23
(1,2631)	1:100:A:VAL:HG23	1:90:A:MET:HB3	8	0.23
(1,2585)	1:77:A:PHE:HB3	1:76:A:MET:HG3	11	0.23
(1,2585)	1:77:A:PHE:HB3	1:76:A:MET:HG3	15	0.23
(1,2548)	1:131:A:LYS:HA	1:131:A:LYS:HB3	9	0.23
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	2	0.23
(1,2369)	1:43:A:ARG:H	1:42:A:GLU:HG2	5	0.23
(1,2109)	1:49:A:PRO:HD2	1:48:A:LEU:HB3	16	0.23
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD2	12	0.23
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD2	17	0.23
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	9	0.23
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	15	0.23
(1,1997)	1:108:A:VAL:HG12	1:82:A:ALA:HA	3	0.23
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	10	0.23
(1,1707)	1:114:A:ALA:HB2	1:111:A:PHE:HA	3	0.23
(1,1707)	1:114:A:ALA:HB2	1:111:A:PHE:HA	15	0.23
(1,1703)	1:114:A:ALA:HB3	1:98:A:GLU:HA	13	0.23
(1,1683)	1:29:A:GLU:HG3	1:29:A:GLU:HA	16	0.23
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	13	0.23
(1,1432)	1:119:A:ALA:HB2	1:117:A:ASN:H	9	0.23
(1,1429)	1:116:A:GLN:HB2	1:119:A:ALA:H	12	0.23
(1,1398)	1:27:A:THR:HG23	1:24:A:SER:H	4	0.23
(1,1307)	1:51:A:GLY:HA3	1:53:A:SER:H	17	0.23
(1,1296)	1:26:A:LEU:HD23	1:115:A:MET:H	9	0.23
(1,1287)	1:61:A:ILE:HB	1:36:A:ALA:H	14	0.23
(1,1255)	1:26:A:LEU:HG	1:25:A:VAL:H	12	0.23
(1,1251)	1:92:A:GLN:HE22	1:92:A:GLN:H	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:34:A:ILE:HB	1:37:A:ASN:H	3	0.23
(1,1202)	1:40:A:VAL:HA	1:45:A:LEU:H	18	0.23
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	7	0.23
(1,1097)	1:74:A:LEU:HG	1:22:A:LEU:H	11	0.23
(1,1097)	1:74:A:LEU:HG	1:22:A:LEU:H	20	0.23
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	10	0.23
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	9	0.23
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	10	0.23
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	14	0.23
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	8	0.23
(1,1005)	1:70:A:PHE:HD2	1:70:A:PHE:H	10	0.23
(1,997)	1:122:A:GLU:HG2	1:124:A:LYS:H	3	0.23
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	17	0.23
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	1	0.23
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	2	0.23
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	3	0.23
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	6	0.23
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	7	0.23
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	13	0.23
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	20	0.23
(1,868)	1:65:A:LEU:HD22	1:69:A:GLN:HE21	2	0.23
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	8	0.23
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	14	0.23
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	15	0.23
(1,517)	1:42:A:GLU:HB3	1:44:A:LEU:H	20	0.23
(1,506)	1:74:A:LEU:HD23	1:74:A:LEU:H	13	0.23
(1,504)	1:65:A:LEU:HD11	1:74:A:LEU:H	17	0.23
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	5	0.23
(1,468)	1:57:A:THR:HG23	1:56:A:GLN:H	12	0.23
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	9	0.23
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	11	0.23
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	19	0.23
(1,334)	1:81:A:LEU:HB2	1:80:A:ALA:H	19	0.23
(1,264)	1:110:A:ALA:HB2	1:109:A:GLU:H	14	0.23
(1,264)	1:110:A:ALA:HB1	1:109:A:GLU:H	19	0.23
(1,263)	1:102:A:ALA:HB1	1:109:A:GLU:H	10	0.23
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	4	0.23
(1,209)	1:131:A:LYS:HB2	1:131:A:LYS:H	10	0.23
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	17	0.23
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	19	0.23
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	20	0.23
(1,47)	1:20:A:VAL:HG11	1:21:A:ASP:H	16	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:20:A:VAL:HG12	1:21:A:ASP:H	16	0.23
(1,47)	1:20:A:VAL:HG13	1:21:A:ASP:H	16	0.23
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	6	0.22
(1,3737)	1:89:A:LEU:HG	1:93:A:PHE:HZ	14	0.22
(1,3735)	1:89:A:LEU:HB2	1:93:A:PHE:HZ	19	0.22
(1,3698)	1:90:A:MET:HE2	1:111:A:PHE:HD1	3	0.22
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	11	0.22
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	6	0.22
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	11	0.22
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	14	0.22
(1,3584)	1:10:A:VAL:HG11	1:11:A:PRO:HA	16	0.22
(1,3574)	1:57:A:THR:H	1:61:A:ILE:HD13	17	0.22
(1,3554)	1:43:A:ARG:HA	1:80:A:ALA:HB1	16	0.22
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE1	11	0.22
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE2	15	0.22
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE3	8	0.22
(1,3536)	1:44:A:LEU:H	1:80:A:ALA:HB1	18	0.22
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD11	8	0.22
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD11	10	0.22
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD13	11	0.22
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD13	15	0.22
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD11	17	0.22
(1,3497)	1:85:A:GLN:HB3	1:86:A:LEU:HD23	13	0.22
(1,3493)	1:76:A:MET:HG2	1:74:A:LEU:HD13	2	0.22
(1,3493)	1:76:A:MET:HG2	1:74:A:LEU:HD12	16	0.22
(1,3457)	1:105:A:LYS:H	1:81:A:LEU:HD22	10	0.22
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	6	0.22
(1,3434)	1:114:A:ALA:HA	1:113:A:LYS:HB3	9	0.22
(1,3434)	1:114:A:ALA:HA	1:113:A:LYS:HB3	11	0.22
(1,3407)	1:32:A:ALA:H	1:29:A:GLU:HG3	18	0.22
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	7	0.22
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	20	0.22
(1,3314)	1:93:A:PHE:HB2	1:34:A:ILE:HA	12	0.22
(1,3271)	1:31:A:MET:HE3	1:34:A:ILE:HD11	8	0.22
(1,3239)	1:86:A:LEU:HD13	1:90:A:MET:HE1	6	0.22
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB3	20	0.22
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB1	10	0.22
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB2	12	0.22
(1,3117)	1:116:A:GLN:H	1:115:A:MET:HE2	13	0.22
(1,3106)	1:40:A:VAL:HG22	1:35:A:LEU:HD13	11	0.22
(1,3094)	1:56:A:GLN:HB3	1:57:A:THR:HG22	10	0.22
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG12	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3009)	1:74:A:LEU:HB3	1:74:A:LEU:HD13	8	0.22
(1,3009)	1:74:A:LEU:HB3	1:74:A:LEU:HD13	15	0.22
(1,3009)	1:74:A:LEU:HB3	1:74:A:LEU:HD11	16	0.22
(1,3009)	1:74:A:LEU:HB3	1:74:A:LEU:HD11	20	0.22
(1,2994)	1:31:A:MET:HG3	1:35:A:LEU:HD23	6	0.22
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG11	1	0.22
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG13	15	0.22
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG12	20	0.22
(1,2923)	1:43:A:ARG:HA	1:44:A:LEU:HD11	4	0.22
(1,2894)	1:77:A:PHE:HE2	1:35:A:LEU:HD21	10	0.22
(1,2842)	1:105:A:LYS:H	1:105:A:LYS:HG3	7	0.22
(1,2842)	1:105:A:LYS:H	1:105:A:LYS:HG3	16	0.22
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD12	2	0.22
(1,2575)	1:14:A:PRO:HD2	1:14:A:PRO:HB2	13	0.22
(1,2542)	1:9:A:ASN:HA	1:10:A:VAL:HB	11	0.22
(1,2542)	1:107:A:ASP:HA	1:108:A:VAL:HB	12	0.22
(1,2482)	1:93:A:PHE:HZ	1:40:A:VAL:HB	7	0.22
(1,2398)	1:98:A:GLU:HA	1:98:A:GLU:HG2	16	0.22
(1,2347)	1:73:A:ALA:H	1:70:A:PHE:HB2	1	0.22
(1,2274)	1:95:A:LEU:HG	1:93:A:PHE:HB3	8	0.22
(1,2189)	1:93:A:PHE:HZ	1:89:A:LEU:HB2	19	0.22
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	11	0.22
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD2	7	0.22
(1,2066)	1:54:A:LEU:HB3	1:55:A:PRO:HD2	19	0.22
(1,1997)	1:108:A:VAL:HG11	1:82:A:ALA:HA	19	0.22
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	8	0.22
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	19	0.22
(1,1707)	1:114:A:ALA:HB2	1:111:A:PHE:HA	16	0.22
(1,1552)	1:89:A:LEU:HB2	1:88:A:PRO:HA	6	0.22
(1,1548)	1:65:A:LEU:HG	1:61:A:ILE:HA	3	0.22
(1,1548)	1:65:A:LEU:HG	1:61:A:ILE:HA	4	0.22
(1,1548)	1:61:A:ILE:HB	1:61:A:ILE:HA	12	0.22
(1,1543)	1:31:A:MET:HB3	1:28:A:PRO:HA	3	0.22
(1,1525)	1:31:A:MET:HA	1:34:A:ILE:HA	10	0.22
(1,1275)	1:92:A:GLN:HB2	1:91:A:CYS:H	15	0.22
(1,1255)	1:26:A:LEU:HG	1:25:A:VAL:H	15	0.22
(1,1246)	1:44:A:LEU:HD13	1:42:A:GLU:H	16	0.22
(1,1222)	1:62:A:GLN:HG2	1:59:A:ASP:H	7	0.22
(1,1206)	1:35:A:LEU:HG	1:37:A:ASN:H	11	0.22
(1,1202)	1:40:A:VAL:HA	1:45:A:LEU:H	11	0.22
(1,1177)	1:107:A:ASP:H	1:102:A:ALA:H	13	0.22
(1,1145)	1:85:A:GLN:HB2	1:81:A:LEU:H	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	11	0.22
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	15	0.22
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	19	0.22
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	8	0.22
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	13	0.22
(1,1009)	1:116:A:GLN:HG3	1:119:A:ALA:H	7	0.22
(1,1005)	1:70:A:PHE:HD2	1:70:A:PHE:H	1	0.22
(1,1005)	1:70:A:PHE:HD1	1:70:A:PHE:H	6	0.22
(1,1005)	1:70:A:PHE:HD2	1:70:A:PHE:H	13	0.22
(1,1005)	1:70:A:PHE:HD2	1:70:A:PHE:H	14	0.22
(1,996)	1:70:A:PHE:HB2	1:73:A:ALA:H	1	0.22
(1,965)	1:36:A:ALA:H	1:38:A:ALA:H	13	0.22
(1,906)	1:36:A:ALA:HB1	1:41:A:GLN:HE22	10	0.22
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	12	0.22
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	17	0.22
(1,844)	1:36:A:ALA:HA	1:41:A:GLN:HE21	9	0.22
(1,844)	1:36:A:ALA:HA	1:41:A:GLN:HE21	11	0.22
(1,770)	1:59:A:ASP:HA	1:63:A:ASN:HD22	2	0.22
(1,740)	1:111:A:PHE:HA	1:115:A:MET:H	10	0.22
(1,740)	1:111:A:PHE:HA	1:115:A:MET:H	16	0.22
(1,723)	1:86:A:LEU:HD12	1:86:A:LEU:H	2	0.22
(1,699)	1:64:A:THR:HB	1:63:A:ASN:H	14	0.22
(1,683)	1:40:A:VAL:HG12	1:37:A:ASN:HD21	17	0.22
(1,618)	1:37:A:ASN:HA	1:37:A:ASN:HD22	11	0.22
(1,617)	1:92:A:GLN:HE22	1:37:A:ASN:HD22	10	0.22
(1,424)	1:110:A:ALA:HB1	1:107:A:ASP:H	13	0.22
(1,424)	1:110:A:ALA:HB3	1:107:A:ASP:H	20	0.22
(1,299)	1:114:A:ALA:HB3	1:116:A:GLN:H	1	0.22
(1,264)	1:110:A:ALA:HB1	1:109:A:GLU:H	9	0.22
(1,263)	1:102:A:ALA:HB3	1:109:A:GLU:H	2	0.22
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	15	0.22
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	16	0.22
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	9	0.22
(1,221)	1:96:A:PRO:HD2	1:99:A:ALA:H	12	0.22
(1,187)	1:132:A:LYS:HG3	1:133:A:ASP:H	17	0.22
(1,161)	1:39:A:ASP:HB2	1:40:A:VAL:H	1	0.22
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	3	0.22
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	4	0.22
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	8	0.22
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	10	0.22
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	12	0.22
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	16	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	18	0.22
(1,153)	1:79:A:ALA:HA	1:82:A:ALA:H	10	0.22
(1,3782)	1:103:A:ALA:HA	1:111:A:PHE:HZ	9	0.21
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	2	0.21
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	3	0.21
(1,3735)	1:34:A:ILE:HB	1:93:A:PHE:HZ	18	0.21
(1,3704)	1:102:A:ALA:HB1	1:111:A:PHE:HD1	1	0.21
(1,3698)	1:90:A:MET:HE1	1:93:A:PHE:HD2	17	0.21
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	4	0.21
(1,3591)	1:44:A:LEU:HA	1:76:A:MET:HE1	4	0.21
(1,3551)	1:56:A:GLN:HA	1:36:A:ALA:HB1	1	0.21
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE1	5	0.21
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE1	4	0.21
(1,3527)	1:82:A:ALA:HB2	1:108:A:VAL:HG21	3	0.21
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD12	2	0.21
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD11	3	0.21
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD13	5	0.21
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD13	16	0.21
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD11	19	0.21
(1,3493)	1:76:A:MET:HG2	1:74:A:LEU:HD11	14	0.21
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG12	6	0.21
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG12	9	0.21
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG11	11	0.21
(1,3449)	1:94:A:GLY:HA2	1:91:A:CYS:HB2	8	0.21
(1,3434)	1:114:A:ALA:HA	1:113:A:LYS:HB3	8	0.21
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	12	0.21
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	15	0.21
(1,3383)	1:42:A:GLU:HG3	1:43:A:ARG:HD2	14	0.21
(1,3380)	1:40:A:VAL:HG13	1:43:A:ARG:HD3	13	0.21
(1,3379)	1:86:A:LEU:HA	1:43:A:ARG:HD3	4	0.21
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	19	0.21
(1,3332)	1:72:A:GLN:HB2	1:70:A:PHE:HA	5	0.21
(1,3289)	1:60:A:GLU:HB3	1:64:A:THR:HB	8	0.21
(1,3288)	1:65:A:LEU:HB3	1:64:A:THR:HB	1	0.21
(1,3272)	1:96:A:PRO:HD3	1:115:A:MET:HE2	12	0.21
(1,3196)	1:31:A:MET:HA	1:30:A:ILE:HG21	1	0.21
(1,3196)	1:31:A:MET:HA	1:30:A:ILE:HG23	6	0.21
(1,3192)	1:33:A:PRO:HA	1:58:A:ALA:HB2	11	0.21
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB1	1	0.21
(1,3117)	1:116:A:GLN:H	1:115:A:MET:HE2	1	0.21
(1,3009)	1:74:A:LEU:HB3	1:74:A:LEU:HD12	5	0.21
(1,3009)	1:74:A:LEU:HB3	1:74:A:LEU:HD13	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD22	1	0.21
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD21	19	0.21
(1,2958)	1:103:A:ALA:HA	1:81:A:LEU:HD12	17	0.21
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG13	12	0.21
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG11	13	0.21
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD21	7	0.21
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD23	13	0.21
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD21	15	0.21
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD13	17	0.21
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD11	2	0.21
(1,2782)	1:26:A:LEU:HD22	1:115:A:MET:HB3	1	0.21
(1,2638)	1:89:A:LEU:HD21	1:88:A:PRO:HB2	1	0.21
(1,2638)	1:89:A:LEU:HD23	1:88:A:PRO:HB2	17	0.21
(1,2630)	1:34:A:ILE:HD12	1:90:A:MET:HG3	12	0.21
(1,2542)	1:107:A:ASP:HA	1:108:A:VAL:HB	13	0.21
(1,2482)	1:93:A:PHE:HZ	1:40:A:VAL:HB	13	0.21
(1,2482)	1:93:A:PHE:HZ	1:40:A:VAL:HB	14	0.21
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	1	0.21
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	18	0.21
(1,2398)	1:98:A:GLU:HA	1:98:A:GLU:HG2	18	0.21
(1,2109)	1:49:A:PRO:HD2	1:48:A:LEU:HB3	8	0.21
(1,2109)	1:49:A:PRO:HD3	1:48:A:LEU:HB3	18	0.21
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD2	10	0.21
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD2	14	0.21
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	16	0.21
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	17	0.21
(1,1997)	1:108:A:VAL:HG13	1:82:A:ALA:HA	14	0.21
(1,1915)	1:70:A:PHE:HE2	1:26:A:LEU:HA	17	0.21
(1,1915)	1:70:A:PHE:HE2	1:26:A:LEU:HA	18	0.21
(1,1887)	1:26:A:LEU:HD22	1:112:A:ALA:HA	4	0.21
(1,1857)	1:36:A:ALA:HB1	1:56:A:GLN:HA	1	0.21
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	17	0.21
(1,1569)	1:35:A:LEU:HD21	1:28:A:PRO:HA	8	0.21
(1,1562)	1:102:A:ALA:HB3	1:108:A:VAL:HA	13	0.21
(1,1525)	1:31:A:MET:HA	1:34:A:ILE:HA	2	0.21
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	6	0.21
(1,1282)	1:91:A:CYS:HB3	1:89:A:LEU:H	13	0.21
(1,1275)	1:92:A:GLN:HB2	1:91:A:CYS:H	17	0.21
(1,1273)	1:80:A:ALA:HB2	1:85:A:GLN:H	5	0.21
(1,1273)	1:80:A:ALA:HB3	1:85:A:GLN:H	10	0.21
(1,1222)	1:60:A:GLU:HB2	1:59:A:ASP:H	16	0.21
(1,1213)	1:35:A:LEU:HD11	1:41:A:GLN:H	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:34:A:ILE:HB	1:37:A:ASN:H	16	0.21
(1,1202)	1:40:A:VAL:HA	1:45:A:LEU:H	5	0.21
(1,1181)	1:111:A:PHE:HA	1:102:A:ALA:H	15	0.21
(1,1168)	1:132:A:LYS:HB3	1:134:A:GLU:H	13	0.21
(1,1138)	1:108:A:VAL:HA	1:81:A:LEU:H	3	0.21
(1,1129)	1:44:A:LEU:HA	1:79:A:ALA:H	16	0.21
(1,1129)	1:44:A:LEU:HA	1:79:A:ALA:H	18	0.21
(1,1122)	1:99:A:ALA:HB2	1:119:A:ALA:H	6	0.21
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	6	0.21
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	4	0.21
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	12	0.21
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	13	0.21
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	16	0.21
(1,1005)	1:70:A:PHE:HD2	1:70:A:PHE:H	2	0.21
(1,1005)	1:70:A:PHE:HD1	1:70:A:PHE:H	3	0.21
(1,1005)	1:70:A:PHE:HD1	1:70:A:PHE:H	15	0.21
(1,1005)	1:70:A:PHE:HD2	1:70:A:PHE:H	17	0.21
(1,972)	1:96:A:PRO:HD2	1:97:A:ALA:H	18	0.21
(1,929)	1:105:A:LYS:HE3	1:106:A:GLY:H	10	0.21
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	13	0.21
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	5	0.21
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	10	0.21
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	15	0.21
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	19	0.21
(1,866)	1:22:A:LEU:HG	1:24:A:SER:H	11	0.21
(1,765)	1:114:A:ALA:HB1	1:115:A:MET:H	13	0.21
(1,765)	1:114:A:ALA:HB2	1:115:A:MET:H	15	0.21
(1,723)	1:86:A:LEU:HD13	1:86:A:LEU:H	17	0.21
(1,618)	1:37:A:ASN:HA	1:37:A:ASN:HD22	5	0.21
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	8	0.21
(1,499)	1:115:A:MET:HB2	1:117:A:ASN:H	5	0.21
(1,499)	1:115:A:MET:HB2	1:117:A:ASN:H	17	0.21
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	13	0.21
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	14	0.21
(1,399)	1:118:A:ASN:HB3	1:118:A:ASN:H	5	0.21
(1,334)	1:81:A:LEU:HB2	1:80:A:ALA:H	8	0.21
(1,334)	1:81:A:LEU:HB2	1:80:A:ALA:H	12	0.21
(1,303)	1:73:A:ALA:HB1	1:72:A:GLN:H	7	0.21
(1,303)	1:73:A:ALA:HB1	1:72:A:GLN:H	12	0.21
(1,299)	1:114:A:ALA:HB1	1:116:A:GLN:H	13	0.21
(1,297)	1:113:A:LYS:HG3	1:114:A:ALA:H	3	0.21
(1,261)	1:22:A:LEU:HG	1:23:A:ALA:H	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:134:A:GLU:HG3	1:134:A:GLU:H	13	0.21
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	5	0.21
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	10	0.21
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	12	0.21
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	15	0.21
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	17	0.21
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	2	0.21
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	7	0.21
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	9	0.21
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	11	0.21
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	13	0.21
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	14	0.21
(1,109)	1:48:A:LEU:HD11	1:48:A:LEU:H	9	0.21
(1,109)	1:48:A:LEU:HD11	1:48:A:LEU:H	10	0.21
(1,75)	1:132:A:LYS:HB2	1:132:A:LYS:H	20	0.21
(1,3782)	1:103:A:ALA:HA	1:111:A:PHE:HZ	7	0.2
(1,3766)	1:83:A:SER:H	1:47:A:TYR:HE2	20	0.2
(1,3758)	1:26:A:LEU:HD13	1:77:A:PHE:HD1	3	0.2
(1,3758)	1:26:A:LEU:HD11	1:77:A:PHE:HD1	15	0.2
(1,3735)	1:34:A:ILE:HB	1:93:A:PHE:HZ	2	0.2
(1,3707)	1:95:A:LEU:HD13	1:93:A:PHE:HD2	17	0.2
(1,3704)	1:102:A:ALA:HB2	1:111:A:PHE:HD1	14	0.2
(1,3663)	1:44:A:LEU:HG	1:47:A:TYR:HD2	5	0.2
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	7	0.2
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	8	0.2
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	16	0.2
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	20	0.2
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE1	10	0.2
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE1	16	0.2
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE1	11	0.2
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE2	20	0.2
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD13	4	0.2
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD13	6	0.2
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD12	7	0.2
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD13	12	0.2
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD11	13	0.2
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD13	20	0.2
(1,3519)	1:109:A:GLU:HG3	1:20:A:VAL:HG13	11	0.2
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG12	8	0.2
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG11	12	0.2
(1,3473)	1:55:A:PRO:HD2	1:65:A:LEU:HD21	17	0.2
(1,3470)	1:80:A:ALA:HA	1:44:A:LEU:HD21	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3457)	1:105:A:LYS:H	1:81:A:LEU:HD23	5	0.2
(1,3457)	1:105:A:LYS:H	1:81:A:LEU:HD22	17	0.2
(1,3446)	1:93:A:PHE:H	1:91:A:CYS:HB2	13	0.2
(1,3422)	1:28:A:PRO:HD3	1:29:A:GLU:HG2	8	0.2
(1,3369)	1:88:A:PRO:HB2	1:87:A:GLY:HA3	5	0.2
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	11	0.2
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	5	0.2
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE2	12	0.2
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD13	4	0.2
(1,3231)	1:107:A:ASP:HB2	1:110:A:ALA:HB3	3	0.2
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB1	11	0.2
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB2	11	0.2
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB3	11	0.2
(1,3177)	1:27:A:THR:H	1:30:A:ILE:HG21	14	0.2
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB3	11	0.2
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB1	14	0.2
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB1	19	0.2
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD11	8	0.2
(1,3052)	1:20:A:VAL:H	1:20:A:VAL:HG13	18	0.2
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG11	20	0.2
(1,3009)	1:74:A:LEU:HB3	1:74:A:LEU:HD11	3	0.2
(1,3009)	1:74:A:LEU:HB3	1:74:A:LEU:HD11	6	0.2
(1,3009)	1:74:A:LEU:HB3	1:74:A:LEU:HD13	12	0.2
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG13	9	0.2
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG12	14	0.2
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG13	16	0.2
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD12	2	0.2
(1,2875)	1:47:A:TYR:HD2	1:44:A:LEU:HD13	10	0.2
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD13	12	0.2
(1,2857)	1:52:A:GLU:H	1:48:A:LEU:HD22	12	0.2
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD12	8	0.2
(1,2785)	1:74:A:LEU:HD12	1:31:A:MET:HB2	17	0.2
(1,2770)	1:99:A:ALA:HB1	1:96:A:PRO:HG3	7	0.2
(1,2715)	1:123:A:GLN:HA	1:123:A:GLN:HB3	14	0.2
(1,2638)	1:89:A:LEU:HD12	1:88:A:PRO:HB2	5	0.2
(1,2638)	1:89:A:LEU:HD12	1:88:A:PRO:HB2	8	0.2
(1,2638)	1:89:A:LEU:HD22	1:88:A:PRO:HB2	19	0.2
(1,2631)	1:100:A:VAL:HG22	1:90:A:MET:HB3	14	0.2
(1,2542)	1:107:A:ASP:HA	1:108:A:VAL:HB	17	0.2
(1,2518)	1:116:A:GLN:HE22	1:116:A:GLN:HG2	15	0.2
(1,2417)	1:114:A:ALA:HB1	1:98:A:GLU:HG3	11	0.2
(1,2417)	1:114:A:ALA:HB2	1:98:A:GLU:HG3	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2417)	1:114:A:ALA:HB3	1:98:A:GLU:HG3	11	0.2
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	4	0.2
(1,2297)	1:99:A:ALA:HB1	1:111:A:PHE:HB3	5	0.2
(1,2252)	1:53:A:SER:HB3	1:54:A:LEU:HB2	11	0.2
(1,2109)	1:49:A:PRO:HD3	1:48:A:LEU:HB3	12	0.2
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	7	0.2
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	8	0.2
(1,1915)	1:70:A:PHE:HE2	1:26:A:LEU:HA	19	0.2
(1,1887)	1:25:A:VAL:HG22	1:112:A:ALA:HA	17	0.2
(1,1849)	1:115:A:MET:HB2	1:112:A:ALA:HA	4	0.2
(1,1849)	1:115:A:MET:HB2	1:112:A:ALA:HA	12	0.2
(1,1838)	1:18:A:GLN:HG2	1:18:A:GLN:HA	8	0.2
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	11	0.2
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	17	0.2
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	15	0.2
(1,1707)	1:114:A:ALA:HB3	1:111:A:PHE:HA	5	0.2
(1,1707)	1:114:A:ALA:HB3	1:111:A:PHE:HA	8	0.2
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	6	0.2
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	8	0.2
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	10	0.2
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	13	0.2
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	14	0.2
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	14	0.2
(1,1676)	1:42:A:GLU:HG3	1:42:A:GLU:HA	20	0.2
(1,1552)	1:89:A:LEU:HB2	1:88:A:PRO:HA	11	0.2
(1,1320)	1:61:A:ILE:HD13	1:35:A:LEU:H	4	0.2
(1,1307)	1:51:A:GLY:HA3	1:53:A:SER:H	3	0.2
(1,1307)	1:51:A:GLY:HA3	1:53:A:SER:H	18	0.2
(1,1299)	1:61:A:ILE:HG23	1:34:A:ILE:H	16	0.2
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	8	0.2
(1,1274)	1:95:A:LEU:HD21	1:91:A:CYS:H	6	0.2
(1,1202)	1:40:A:VAL:HA	1:45:A:LEU:H	6	0.2
(1,1181)	1:111:A:PHE:HA	1:102:A:ALA:H	7	0.2
(1,1181)	1:111:A:PHE:HA	1:102:A:ALA:H	12	0.2
(1,1181)	1:111:A:PHE:HA	1:102:A:ALA:H	13	0.2
(1,1153)	1:19:A:GLN:HB2	1:19:A:GLN:H	11	0.2
(1,1145)	1:85:A:GLN:HB2	1:81:A:LEU:H	5	0.2
(1,1144)	1:44:A:LEU:HG	1:81:A:LEU:H	18	0.2
(1,1131)	1:47:A:TYR:HB2	1:79:A:ALA:H	4	0.2
(1,1097)	1:74:A:LEU:HG	1:22:A:LEU:H	16	0.2
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	15	0.2
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1007)	1:30:A:ILE:HD13	1:119:A:ALA:H	2	0.2
(1,1005)	1:70:A:PHE:HD1	1:70:A:PHE:H	9	0.2
(1,1005)	1:70:A:PHE:HD2	1:70:A:PHE:H	12	0.2
(1,972)	1:96:A:PRO:HD2	1:97:A:ALA:H	1	0.2
(1,972)	1:96:A:PRO:HD2	1:97:A:ALA:H	4	0.2
(1,965)	1:36:A:ALA:H	1:38:A:ALA:H	17	0.2
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	15	0.2
(1,905)	1:58:A:ALA:HB2	1:62:A:GLN:HE22	15	0.2
(1,897)	1:116:A:GLN:HG2	1:116:A:GLN:HE22	15	0.2
(1,866)	1:22:A:LEU:HG	1:24:A:SER:H	10	0.2
(1,765)	1:114:A:ALA:HB3	1:115:A:MET:H	1	0.2
(1,723)	1:86:A:LEU:HD12	1:86:A:LEU:H	8	0.2
(1,699)	1:59:A:ASP:HA	1:63:A:ASN:H	12	0.2
(1,699)	1:59:A:ASP:HA	1:63:A:ASN:H	17	0.2
(1,547)	1:40:A:VAL:HB	1:42:A:GLU:H	12	0.2
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	5	0.2
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	12	0.2
(1,517)	1:42:A:GLU:HB3	1:44:A:LEU:H	6	0.2
(1,459)	1:37:A:ASN:HB3	1:41:A:GLN:H	5	0.2
(1,425)	1:57:A:THR:HG23	1:60:A:GLU:H	8	0.2
(1,411)	1:40:A:VAL:HG21	1:39:A:ASP:H	14	0.2
(1,399)	1:118:A:ASN:HB3	1:118:A:ASN:H	6	0.2
(1,399)	1:118:A:ASN:HB3	1:118:A:ASN:H	10	0.2
(1,305)	1:25:A:VAL:HG23	1:116:A:GLN:H	17	0.2
(1,264)	1:110:A:ALA:HB3	1:109:A:GLU:H	10	0.2
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	18	0.2
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	5	0.2
(1,161)	1:40:A:VAL:HB	1:40:A:VAL:H	15	0.2
(1,109)	1:48:A:LEU:HD13	1:48:A:LEU:H	7	0.2
(1,47)	1:20:A:VAL:HG11	1:21:A:ASP:H	20	0.2
(1,47)	1:20:A:VAL:HG12	1:21:A:ASP:H	20	0.2
(1,47)	1:20:A:VAL:HG13	1:21:A:ASP:H	20	0.2
(1,3783)	1:26:A:LEU:HD11	1:77:A:PHE:HZ	11	0.19
(1,3704)	1:102:A:ALA:HB1	1:111:A:PHE:HD1	13	0.19
(1,3668)	1:46:A:PRO:HB2	1:47:A:TYR:HD2	2	0.19
(1,3646)	1:136:A:GLU:HB2	1:137:A:ASP:HB3	8	0.19
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD11	9	0.19
(1,3493)	1:76:A:MET:HG2	1:74:A:LEU:HD12	3	0.19
(1,3434)	1:114:A:ALA:HA	1:113:A:LYS:HB3	2	0.19
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	6	0.19
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	13	0.19
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3375)	1:35:A:LEU:HB2	1:33:A:PRO:HD2	10	0.19
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	8	0.19
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	11	0.19
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	12	0.19
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	16	0.19
(1,3286)	1:89:A:LEU:HG	1:40:A:VAL:HA	12	0.19
(1,3196)	1:31:A:MET:HA	1:30:A:ILE:HG23	10	0.19
(1,3177)	1:27:A:THR:H	1:30:A:ILE:HG23	11	0.19
(1,3167)	1:70:A:PHE:HE1	1:61:A:ILE:HG22	16	0.19
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB1	9	0.19
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB2	18	0.19
(1,3052)	1:20:A:VAL:H	1:20:A:VAL:HG12	14	0.19
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG12	2	0.19
(1,2994)	1:31:A:MET:HG3	1:35:A:LEU:HD21	16	0.19
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD23	13	0.19
(1,2950)	1:100:A:VAL:HA	1:100:A:VAL:HG12	11	0.19
(1,2921)	1:32:A:ALA:HA	1:35:A:LEU:HD21	4	0.19
(1,2920)	1:43:A:ARG:HA	1:86:A:LEU:HD23	2	0.19
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD12	19	0.19
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD22	12	0.19
(1,2859)	1:70:A:PHE:HE1	1:74:A:LEU:HD11	18	0.19
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD12	9	0.19
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD12	10	0.19
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD13	16	0.19
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD11	17	0.19
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD11	19	0.19
(1,2769)	1:99:A:ALA:HB3	1:115:A:MET:HB2	20	0.19
(1,2768)	1:64:A:THR:HG21	1:60:A:GLU:HB2	11	0.19
(1,2644)	1:89:A:LEU:HD21	1:92:A:GLN:HG3	10	0.19
(1,2644)	1:89:A:LEU:HD22	1:92:A:GLN:HG3	10	0.19
(1,2644)	1:89:A:LEU:HD23	1:92:A:GLN:HG3	10	0.19
(1,2638)	1:89:A:LEU:HD11	1:88:A:PRO:HB2	10	0.19
(1,2638)	1:89:A:LEU:HD13	1:88:A:PRO:HB2	12	0.19
(1,2620)	1:64:A:THR:HG21	1:60:A:GLU:HB2	11	0.19
(1,2610)	1:35:A:LEU:HB2	1:41:A:GLN:HG2	9	0.19
(1,2585)	1:77:A:PHE:HB3	1:76:A:MET:HG3	5	0.19
(1,2585)	1:77:A:PHE:HB3	1:76:A:MET:HG3	6	0.19
(1,2582)	1:28:A:PRO:HA	1:28:A:PRO:HB2	10	0.19
(1,2575)	1:11:A:PRO:HD2	1:11:A:PRO:HB2	14	0.19
(1,2482)	1:93:A:PHE:HZ	1:40:A:VAL:HB	3	0.19
(1,2456)	1:120:A:LYS:H	1:121:A:PRO:HB3	8	0.19
(1,2456)	1:63:A:ASN:H	1:55:A:PRO:HB3	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	7	0.19
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	8	0.19
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	10	0.19
(1,2398)	1:98:A:GLU:HA	1:98:A:GLU:HG2	12	0.19
(1,2347)	1:73:A:ALA:H	1:70:A:PHE:HB2	6	0.19
(1,2309)	1:22:A:LEU:HB2	1:26:A:LEU:HB3	9	0.19
(1,2252)	1:41:A:GLN:HA	1:54:A:LEU:HB3	1	0.19
(1,2252)	1:53:A:SER:HB3	1:54:A:LEU:HB2	13	0.19
(1,2109)	1:49:A:PRO:HD3	1:48:A:LEU:HB3	4	0.19
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD2	9	0.19
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	10	0.19
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	3	0.19
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	5	0.19
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	18	0.19
(1,1737)	1:44:A:LEU:HD22	1:41:A:GLN:HA	11	0.19
(1,1737)	1:54:A:LEU:HD21	1:41:A:GLN:HA	12	0.19
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	3	0.19
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	5	0.19
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	7	0.19
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	9	0.19
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	11	0.19
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	12	0.19
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	7	0.19
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	9	0.19
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	20	0.19
(1,1562)	1:102:A:ALA:HB2	1:108:A:VAL:HA	19	0.19
(1,1548)	1:65:A:LEU:HG	1:61:A:ILE:HA	17	0.19
(1,1462)	1:56:A:GLN:HB2	1:57:A:THR:HB	14	0.19
(1,1405)	1:56:A:GLN:HG2	1:41:A:GLN:HE22	18	0.19
(1,1307)	1:51:A:GLY:HA3	1:53:A:SER:H	10	0.19
(1,1307)	1:51:A:GLY:HA3	1:53:A:SER:H	15	0.19
(1,1307)	1:51:A:GLY:HA3	1:53:A:SER:H	16	0.19
(1,1299)	1:40:A:VAL:HG22	1:34:A:ILE:H	1	0.19
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	16	0.19
(1,1296)	1:26:A:LEU:HD23	1:115:A:MET:H	16	0.19
(1,1274)	1:95:A:LEU:HD23	1:91:A:CYS:H	18	0.19
(1,1251)	1:92:A:GLN:HE22	1:92:A:GLN:H	2	0.19
(1,1251)	1:92:A:GLN:HE22	1:92:A:GLN:H	7	0.19
(1,1232)	1:57:A:THR:HG22	1:59:A:ASP:H	8	0.19
(1,1206)	1:34:A:ILE:HB	1:37:A:ASN:H	12	0.19
(1,1206)	1:34:A:ILE:HB	1:37:A:ASN:H	15	0.19
(1,1202)	1:40:A:VAL:HA	1:45:A:LEU:H	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1181)	1:111:A:PHE:HA	1:102:A:ALA:H	4	0.19
(1,1158)	1:119:A:ALA:HB3	1:120:A:LYS:H	18	0.19
(1,1129)	1:44:A:LEU:HA	1:79:A:ALA:H	20	0.19
(1,1097)	1:74:A:LEU:HG	1:22:A:LEU:H	17	0.19
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	1	0.19
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	2	0.19
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	18	0.19
(1,1061)	1:73:A:ALA:HB3	1:72:A:GLN:HE21	3	0.19
(1,1005)	1:70:A:PHE:HD1	1:70:A:PHE:H	11	0.19
(1,1005)	1:70:A:PHE:HD1	1:70:A:PHE:H	16	0.19
(1,996)	1:70:A:PHE:HB2	1:73:A:ALA:H	6	0.19
(1,898)	1:41:A:GLN:HG2	1:41:A:GLN:HE22	18	0.19
(1,723)	1:86:A:LEU:HD12	1:86:A:LEU:H	9	0.19
(1,699)	1:59:A:ASP:HA	1:63:A:ASN:H	6	0.19
(1,635)	1:40:A:VAL:HG23	1:36:A:ALA:H	7	0.19
(1,633)	1:34:A:ILE:HB	1:36:A:ALA:H	15	0.19
(1,588)	1:114:A:ALA:HB2	1:98:A:GLU:H	18	0.19
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	2	0.19
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	3	0.19
(1,499)	1:115:A:MET:HB2	1:117:A:ASN:H	12	0.19
(1,499)	1:120:A:LYS:HB2	1:117:A:ASN:H	19	0.19
(1,494)	1:72:A:GLN:HB2	1:74:A:LEU:H	8	0.19
(1,468)	1:57:A:THR:HG22	1:56:A:GLN:H	10	0.19
(1,468)	1:57:A:THR:HG21	1:56:A:GLN:H	19	0.19
(1,459)	1:37:A:ASN:HB3	1:41:A:GLN:H	4	0.19
(1,424)	1:110:A:ALA:HB1	1:107:A:ASP:H	9	0.19
(1,404)	1:96:A:PRO:HG2	1:118:A:ASN:H	7	0.19
(1,399)	1:118:A:ASN:HB3	1:118:A:ASN:H	3	0.19
(1,334)	1:81:A:LEU:HB2	1:80:A:ALA:H	18	0.19
(1,297)	1:113:A:LYS:HG3	1:114:A:ALA:H	7	0.19
(1,297)	1:113:A:LYS:HG3	1:114:A:ALA:H	16	0.19
(1,291)	1:116:A:GLN:HB3	1:116:A:GLN:H	1	0.19
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	9	0.19
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	10	0.19
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	18	0.19
(1,248)	1:108:A:VAL:HA	1:112:A:ALA:H	2	0.19
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	6	0.19
(1,97)	1:35:A:LEU:HD22	1:73:A:ALA:H	4	0.19
(1,47)	1:20:A:VAL:HG11	1:21:A:ASP:H	3	0.19
(1,47)	1:20:A:VAL:HG12	1:21:A:ASP:H	3	0.19
(1,47)	1:20:A:VAL:HG13	1:21:A:ASP:H	3	0.19
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3783)	1:26:A:LEU:HD11	1:77:A:PHE:HZ	19	0.18
(1,3775)	1:46:A:PRO:HG2	1:47:A:TYR:HE2	13	0.18
(1,3698)	1:90:A:MET:HE1	1:93:A:PHE:HD2	13	0.18
(1,3698)	1:90:A:MET:HE3	1:111:A:PHE:HD1	16	0.18
(1,3682)	1:89:A:LEU:HA	1:93:A:PHE:HD2	5	0.18
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	16	0.18
(1,3646)	1:62:A:GLN:HB2	1:59:A:ASP:HB3	14	0.18
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	2	0.18
(1,3591)	1:44:A:LEU:HA	1:76:A:MET:HE3	14	0.18
(1,3591)	1:44:A:LEU:HA	1:76:A:MET:HE1	19	0.18
(1,3565)	1:90:A:MET:HE1	1:31:A:MET:HE1	18	0.18
(1,3556)	1:43:A:ARG:HD3	1:80:A:ALA:HB2	13	0.18
(1,3547)	1:54:A:LEU:HG	1:76:A:MET:HE3	15	0.18
(1,3540)	1:86:A:LEU:HB3	1:90:A:MET:HE1	4	0.18
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE1	13	0.18
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD13	14	0.18
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD11	18	0.18
(1,3517)	1:77:A:PHE:HA	1:35:A:LEU:HD13	3	0.18
(1,3500)	1:86:A:LEU:HB3	1:81:A:LEU:HD22	10	0.18
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG13	3	0.18
(1,3449)	1:94:A:GLY:HA2	1:91:A:CYS:HB2	6	0.18
(1,3442)	1:99:A:ALA:HB2	1:96:A:PRO:HB2	18	0.18
(1,3434)	1:114:A:ALA:HA	1:113:A:LYS:HB3	12	0.18
(1,3392)	1:40:A:VAL:HA	1:86:A:LEU:HB2	6	0.18
(1,3388)	1:20:A:VAL:HA	1:21:A:ASP:HB2	12	0.18
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	10	0.18
(1,3337)	1:11:A:PRO:HD3	1:11:A:PRO:HA	8	0.18
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	19	0.18
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	18	0.18
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD12	16	0.18
(1,3196)	1:31:A:MET:HA	1:30:A:ILE:HG23	5	0.18
(1,3196)	1:31:A:MET:HA	1:30:A:ILE:HG22	17	0.18
(1,3196)	1:31:A:MET:HA	1:30:A:ILE:HG21	19	0.18
(1,3188)	1:57:A:THR:HA	1:58:A:ALA:HB3	8	0.18
(1,3187)	1:115:A:MET:HA	1:99:A:ALA:HB1	7	0.18
(1,3187)	1:115:A:MET:HA	1:99:A:ALA:HB2	17	0.18
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB1	15	0.18
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB1	16	0.18
(1,3094)	1:56:A:GLN:HB3	1:57:A:THR:HG21	6	0.18
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD12	17	0.18
(1,2997)	1:43:A:ARG:HB2	1:86:A:LEU:HD11	11	0.18
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD21	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2934)	1:71:A:GLN:HA	1:74:A:LEU:HG	8	0.18
(1,2875)	1:47:A:TYR:HD2	1:44:A:LEU:HD13	5	0.18
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD23	3	0.18
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD12	6	0.18
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD11	13	0.18
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD13	18	0.18
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD12	19	0.18
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD12	3	0.18
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD11	12	0.18
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD12	18	0.18
(1,2638)	1:89:A:LEU:HD12	1:88:A:PRO:HB2	3	0.18
(1,2582)	1:28:A:PRO:HA	1:28:A:PRO:HB2	5	0.18
(1,2582)	1:28:A:PRO:HA	1:28:A:PRO:HB2	14	0.18
(1,2582)	1:28:A:PRO:HA	1:28:A:PRO:HB2	16	0.18
(1,2482)	1:93:A:PHE:HZ	1:40:A:VAL:HB	11	0.18
(1,2456)	1:63:A:ASN:H	1:55:A:PRO:HB3	3	0.18
(1,2354)	1:109:A:GLU:H	1:109:A:GLU:HG2	17	0.18
(1,2324)	1:25:A:VAL:HG13	1:26:A:LEU:HB2	1	0.18
(1,2313)	1:81:A:LEU:HG	1:111:A:PHE:HB2	8	0.18
(1,2109)	1:49:A:PRO:HD2	1:48:A:LEU:HB3	6	0.18
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD2	8	0.18
(1,2081)	1:65:A:LEU:HD11	1:55:A:PRO:HD2	4	0.18
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	1	0.18
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	4	0.18
(1,2042)	1:104:A:ASN:HB3	1:87:A:GLY:HA2	19	0.18
(1,1874)	1:34:A:ILE:HD12	1:90:A:MET:HA	19	0.18
(1,1849)	1:115:A:MET:HB3	1:112:A:ALA:HA	6	0.18
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	1	0.18
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	2	0.18
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	11	0.18
(1,1737)	1:44:A:LEU:HD21	1:41:A:GLN:HA	10	0.18
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	2	0.18
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	16	0.18
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	17	0.18
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	19	0.18
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	20	0.18
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	3	0.18
(1,1569)	1:35:A:LEU:HD21	1:28:A:PRO:HA	4	0.18
(1,1565)	1:64:A:THR:HG23	1:61:A:ILE:HA	3	0.18
(1,1565)	1:64:A:THR:HG23	1:61:A:ILE:HA	16	0.18
(1,1565)	1:64:A:THR:HG21	1:61:A:ILE:HA	20	0.18
(1,1562)	1:102:A:ALA:HB3	1:108:A:VAL:HA	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1562)	1:102:A:ALA:HB2	1:108:A:VAL:HA	6	0.18
(1,1552)	1:89:A:LEU:HB2	1:88:A:PRO:HA	16	0.18
(1,1552)	1:89:A:LEU:HB2	1:88:A:PRO:HA	19	0.18
(1,1548)	1:61:A:ILE:HB	1:61:A:ILE:HA	8	0.18
(1,1320)	1:61:A:ILE:HD12	1:35:A:LEU:H	16	0.18
(1,1307)	1:51:A:GLY:HA3	1:53:A:SER:H	6	0.18
(1,1299)	1:61:A:ILE:HG22	1:34:A:ILE:H	15	0.18
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	9	0.18
(1,1296)	1:26:A:LEU:HD22	1:115:A:MET:H	12	0.18
(1,1273)	1:80:A:ALA:HB1	1:85:A:GLN:H	15	0.18
(1,1255)	1:26:A:LEU:HG	1:25:A:VAL:H	9	0.18
(1,1222)	1:62:A:GLN:HG2	1:59:A:ASP:H	10	0.18
(1,1202)	1:40:A:VAL:HA	1:45:A:LEU:H	8	0.18
(1,1181)	1:111:A:PHE:HA	1:102:A:ALA:H	18	0.18
(1,1144)	1:44:A:LEU:HG	1:81:A:LEU:H	6	0.18
(1,1122)	1:114:A:ALA:HB1	1:119:A:ALA:H	2	0.18
(1,1067)	1:124:A:LYS:HB2	1:126:A:GLY:H	2	0.18
(1,1005)	1:70:A:PHE:HD2	1:70:A:PHE:H	7	0.18
(1,965)	1:36:A:ALA:H	1:38:A:ALA:H	19	0.18
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	7	0.18
(1,870)	1:25:A:VAL:HG11	1:24:A:SER:H	18	0.18
(1,844)	1:36:A:ALA:HA	1:41:A:GLN:HE21	13	0.18
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	1	0.18
(1,723)	1:86:A:LEU:HD12	1:86:A:LEU:H	6	0.18
(1,723)	1:86:A:LEU:HD11	1:86:A:LEU:H	13	0.18
(1,723)	1:86:A:LEU:HD13	1:86:A:LEU:H	18	0.18
(1,723)	1:86:A:LEU:HD12	1:86:A:LEU:H	19	0.18
(1,684)	1:48:A:LEU:HD11	1:53:A:SER:H	2	0.18
(1,635)	1:40:A:VAL:HG22	1:36:A:ALA:H	19	0.18
(1,547)	1:40:A:VAL:HB	1:42:A:GLU:H	5	0.18
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	6	0.18
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	19	0.18
(1,468)	1:57:A:THR:HG23	1:56:A:GLN:H	9	0.18
(1,411)	1:40:A:VAL:HG21	1:39:A:ASP:H	8	0.18
(1,377)	1:100:A:VAL:HG21	1:104:A:ASN:H	9	0.18
(1,368)	1:101:A:GLU:HB3	1:103:A:ALA:H	20	0.18
(1,334)	1:81:A:LEU:HB2	1:80:A:ALA:H	20	0.18
(1,303)	1:73:A:ALA:HB2	1:72:A:GLN:H	17	0.18
(1,297)	1:113:A:LYS:HG3	1:114:A:ALA:H	10	0.18
(1,264)	1:110:A:ALA:HB1	1:109:A:GLU:H	7	0.18
(1,264)	1:110:A:ALA:HB2	1:109:A:GLU:H	12	0.18
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,248)	1:111:A:PHE:HB2	1:112:A:ALA:H	8	0.18
(1,221)	1:96:A:PRO:HD2	1:99:A:ALA:H	6	0.18
(1,192)	1:108:A:VAL:HG13	1:82:A:ALA:H	1	0.18
(1,129)	1:122:A:GLU:HB3	1:122:A:GLU:H	16	0.18
(1,109)	1:48:A:LEU:HD12	1:48:A:LEU:H	1	0.18
(1,109)	1:48:A:LEU:HD11	1:48:A:LEU:H	11	0.18
(1,109)	1:48:A:LEU:HD11	1:48:A:LEU:H	18	0.18
(1,75)	1:132:A:LYS:HB2	1:132:A:LYS:H	11	0.18
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	9	0.18
(1,3792)	1:40:A:VAL:HG22	1:93:A:PHE:HE2	8	0.17
(1,3775)	1:46:A:PRO:HG2	1:47:A:TYR:HE2	4	0.17
(1,3707)	1:95:A:LEU:HD13	1:93:A:PHE:HD2	18	0.17
(1,3698)	1:90:A:MET:HE3	1:111:A:PHE:HD1	10	0.17
(1,3682)	1:89:A:LEU:HA	1:93:A:PHE:HD2	12	0.17
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	19	0.17
(1,3565)	1:90:A:MET:HE1	1:31:A:MET:HE3	14	0.17
(1,3557)	1:47:A:TYR:HB3	1:80:A:ALA:HB1	13	0.17
(1,3554)	1:43:A:ARG:HA	1:80:A:ALA:HB2	17	0.17
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE3	7	0.17
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE3	14	0.17
(1,3530)	1:41:A:GLN:HE21	1:36:A:ALA:HB1	10	0.17
(1,3493)	1:76:A:MET:HG2	1:74:A:LEU:HD12	6	0.17
(1,3434)	1:114:A:ALA:HA	1:113:A:LYS:HB3	20	0.17
(1,3416)	1:114:A:ALA:HA	1:117:A:ASN:HB3	3	0.17
(1,3407)	1:32:A:ALA:H	1:29:A:GLU:HG3	14	0.17
(1,3388)	1:20:A:VAL:HA	1:21:A:ASP:HB2	14	0.17
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	5	0.17
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	11	0.17
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	14	0.17
(1,3379)	1:86:A:LEU:HA	1:43:A:ARG:HD3	11	0.17
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	11	0.17
(1,3314)	1:93:A:PHE:HB2	1:34:A:ILE:HA	1	0.17
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	17	0.17
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	4	0.17
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	9	0.17
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	20	0.17
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD11	17	0.17
(1,3228)	1:61:A:ILE:HB	1:32:A:ALA:HB2	9	0.17
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB3	3	0.17
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB3	5	0.17
(1,3158)	1:114:A:ALA:H	1:110:A:ALA:HB3	19	0.17
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB1	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB3	20	0.17
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD11	5	0.17
(1,3088)	1:109:A:GLU:HA	1:108:A:VAL:HG22	18	0.17
(1,3009)	1:26:A:LEU:HB3	1:74:A:LEU:HD11	1	0.17
(1,3009)	1:74:A:LEU:HB3	1:74:A:LEU:HD12	13	0.17
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD22	16	0.17
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD22	17	0.17
(1,2972)	1:43:A:ARG:HD3	1:86:A:LEU:HD11	11	0.17
(1,2940)	1:55:A:PRO:HD3	1:65:A:LEU:HD13	20	0.17
(1,2906)	1:114:A:ALA:HA	1:113:A:LYS:HG2	1	0.17
(1,2906)	1:114:A:ALA:HA	1:113:A:LYS:HG2	13	0.17
(1,2900)	1:27:A:THR:HB	1:28:A:PRO:HG2	7	0.17
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD22	3	0.17
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD22	5	0.17
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD22	2	0.17
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD23	11	0.17
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD22	19	0.17
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD21	13	0.17
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD11	20	0.17
(1,2770)	1:99:A:ALA:HB2	1:96:A:PRO:HG3	11	0.17
(1,2770)	1:99:A:ALA:HB1	1:96:A:PRO:HG3	20	0.17
(1,2638)	1:89:A:LEU:HD11	1:88:A:PRO:HB2	15	0.17
(1,2630)	1:34:A:ILE:HD12	1:90:A:MET:HG3	1	0.17
(1,2585)	1:77:A:PHE:HB3	1:76:A:MET:HG3	9	0.17
(1,2582)	1:28:A:PRO:HD2	1:28:A:PRO:HB2	12	0.17
(1,2582)	1:28:A:PRO:HA	1:28:A:PRO:HB2	20	0.17
(1,2476)	1:120:A:LYS:H	1:120:A:LYS:HB3	6	0.17
(1,2265)	1:37:A:ASN:HB3	1:89:A:LEU:HB3	19	0.17
(1,2252)	1:41:A:GLN:HA	1:54:A:LEU:HB3	7	0.17
(1,2116)	1:86:A:LEU:HD11	1:43:A:ARG:HD3	11	0.17
(1,2042)	1:104:A:ASN:HB3	1:87:A:GLY:HA2	20	0.17
(1,1883)	1:35:A:LEU:HD22	1:74:A:LEU:HA	20	0.17
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	2	0.17
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	6	0.17
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	7	0.17
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	12	0.17
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	4	0.17
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	10	0.17
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	14	0.17
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	5	0.17
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	6	0.17
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1676)	1:98:A:GLU:HG2	1:98:A:GLU:HA	13	0.17
(1,1571)	1:61:A:ILE:HG23	1:28:A:PRO:HA	5	0.17
(1,1565)	1:64:A:THR:HG21	1:61:A:ILE:HA	10	0.17
(1,1552)	1:89:A:LEU:HB2	1:88:A:PRO:HA	2	0.17
(1,1552)	1:103:A:ALA:HB1	1:88:A:PRO:HA	10	0.17
(1,1552)	1:89:A:LEU:HB2	1:88:A:PRO:HA	12	0.17
(1,1552)	1:89:A:LEU:HB2	1:88:A:PRO:HA	20	0.17
(1,1447)	1:89:A:LEU:HD21	1:37:A:ASN:HD22	10	0.17
(1,1447)	1:89:A:LEU:HD22	1:37:A:ASN:HD22	10	0.17
(1,1447)	1:89:A:LEU:HD23	1:37:A:ASN:HD22	10	0.17
(1,1433)	1:111:A:PHE:HB2	1:113:A:LYS:H	15	0.17
(1,1429)	1:116:A:GLN:HB3	1:119:A:ALA:H	5	0.17
(1,1365)	1:88:A:PRO:HG3	1:104:A:ASN:HD22	18	0.17
(1,1320)	1:61:A:ILE:HD11	1:35:A:LEU:H	8	0.17
(1,1320)	1:61:A:ILE:HD13	1:35:A:LEU:H	14	0.17
(1,1320)	1:61:A:ILE:HD11	1:35:A:LEU:H	17	0.17
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	11	0.17
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	18	0.17
(1,1274)	1:95:A:LEU:HD22	1:91:A:CYS:H	20	0.17
(1,1255)	1:26:A:LEU:HG	1:25:A:VAL:H	10	0.17
(1,1255)	1:26:A:LEU:HG	1:25:A:VAL:H	11	0.17
(1,1206)	1:34:A:ILE:HB	1:37:A:ASN:H	7	0.17
(1,1202)	1:40:A:VAL:HA	1:45:A:LEU:H	10	0.17
(1,1181)	1:111:A:PHE:HA	1:102:A:ALA:H	1	0.17
(1,1181)	1:111:A:PHE:HA	1:102:A:ALA:H	16	0.17
(1,1175)	1:110:A:ALA:HB2	1:114:A:ALA:H	1	0.17
(1,1168)	1:132:A:LYS:HB3	1:134:A:GLU:H	9	0.17
(1,1168)	1:132:A:LYS:HB3	1:134:A:GLU:H	14	0.17
(1,1158)	1:119:A:ALA:HB2	1:120:A:LYS:H	8	0.17
(1,1144)	1:44:A:LEU:HG	1:81:A:LEU:H	2	0.17
(1,1116)	1:96:A:PRO:HA	1:119:A:ALA:H	20	0.17
(1,1094)	1:26:A:LEU:H	1:22:A:LEU:H	14	0.17
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	7	0.17
(1,1072)	1:80:A:ALA:HB3	1:84:A:GLY:H	10	0.17
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	10	0.17
(1,972)	1:96:A:PRO:HD2	1:97:A:ALA:H	8	0.17
(1,972)	1:96:A:PRO:HD2	1:97:A:ALA:H	9	0.17
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	1	0.17
(1,906)	1:58:A:ALA:HB1	1:62:A:GLN:HE22	4	0.17
(1,870)	1:25:A:VAL:HG12	1:24:A:SER:H	4	0.17
(1,866)	1:22:A:LEU:HG	1:24:A:SER:H	3	0.17
(1,849)	1:36:A:ALA:HB1	1:41:A:GLN:HE21	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:36:A:ALA:HA	1:41:A:GLN:HE21	2	0.17
(1,784)	1:32:A:ALA:HB1	1:31:A:MET:H	13	0.17
(1,784)	1:32:A:ALA:HB2	1:31:A:MET:H	14	0.17
(1,755)	1:116:A:GLN:HB3	1:115:A:MET:H	12	0.17
(1,734)	1:118:A:ASN:HA	1:118:A:ASN:HD22	8	0.17
(1,633)	1:34:A:ILE:HB	1:36:A:ALA:H	1	0.17
(1,633)	1:34:A:ILE:HB	1:36:A:ALA:H	17	0.17
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	20	0.17
(1,522)	1:114:A:ALA:HB1	1:113:A:LYS:H	19	0.17
(1,504)	1:22:A:LEU:HD13	1:74:A:LEU:H	15	0.17
(1,494)	1:72:A:GLN:HB3	1:74:A:LEU:H	10	0.17
(1,468)	1:57:A:THR:HG22	1:56:A:GLN:H	1	0.17
(1,449)	1:45:A:LEU:HD21	1:45:A:LEU:H	13	0.17
(1,424)	1:110:A:ALA:HB3	1:107:A:ASP:H	3	0.17
(1,424)	1:110:A:ALA:HB3	1:107:A:ASP:H	5	0.17
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	15	0.17
(1,377)	1:100:A:VAL:HG22	1:104:A:ASN:H	7	0.17
(1,334)	1:81:A:LEU:HB2	1:80:A:ALA:H	2	0.17
(1,334)	1:81:A:LEU:HB2	1:80:A:ALA:H	9	0.17
(1,334)	1:81:A:LEU:HB2	1:80:A:ALA:H	16	0.17
(1,305)	1:26:A:LEU:HD21	1:116:A:GLN:H	6	0.17
(1,291)	1:116:A:GLN:HB3	1:116:A:GLN:H	15	0.17
(1,291)	1:116:A:GLN:HB3	1:116:A:GLN:H	17	0.17
(1,272)	1:115:A:MET:H	1:116:A:GLN:H	1	0.17
(1,264)	1:110:A:ALA:HB2	1:109:A:GLU:H	4	0.17
(1,261)	1:22:A:LEU:HG	1:23:A:ALA:H	11	0.17
(1,183)	1:120:A:LYS:HB3	1:120:A:LYS:H	6	0.17
(1,129)	1:122:A:GLU:HB3	1:122:A:GLU:H	4	0.17
(1,129)	1:122:A:GLU:HB3	1:122:A:GLU:H	12	0.17
(1,60)	1:54:A:LEU:HD13	1:54:A:LEU:H	8	0.17
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	15	0.17
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	19	0.17
(2,13)	1:43:A:ARG:H	1:39:A:ASP:O	18	0.16
(2,13)	1:43:A:ARG:H	1:39:A:ASP:O	20	0.16
(1,3766)	1:45:A:LEU:H	1:47:A:TYR:HE2	7	0.16
(1,3766)	1:83:A:SER:H	1:47:A:TYR:HE2	13	0.16
(1,3758)	1:26:A:LEU:HD11	1:77:A:PHE:HD1	16	0.16
(1,3758)	1:26:A:LEU:HD12	1:77:A:PHE:HD1	20	0.16
(1,3735)	1:89:A:LEU:HB2	1:93:A:PHE:HZ	3	0.16
(1,3730)	1:37:A:ASN:HA	1:93:A:PHE:HZ	1	0.16
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	10	0.16
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	13	0.16
(1,3554)	1:43:A:ARG:HA	1:80:A:ALA:HB3	10	0.16
(1,3551)	1:57:A:THR:HB	1:36:A:ALA:HB1	12	0.16
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE2	12	0.16
(1,3523)	1:95:A:LEU:HB3	1:95:A:LEU:HD13	1	0.16
(1,3497)	1:85:A:GLN:HB3	1:86:A:LEU:HD21	18	0.16
(1,3493)	1:76:A:MET:HG2	1:74:A:LEU:HD13	4	0.16
(1,3473)	1:55:A:PRO:HD2	1:65:A:LEU:HD23	15	0.16
(1,3455)	1:104:A:ASN:H	1:105:A:LYS:HG3	3	0.16
(1,3455)	1:104:A:ASN:H	1:105:A:LYS:HG3	6	0.16
(1,3446)	1:93:A:PHE:H	1:91:A:CYS:HB2	4	0.16
(1,3446)	1:93:A:PHE:H	1:91:A:CYS:HB2	9	0.16
(1,3446)	1:89:A:LEU:H	1:91:A:CYS:HB2	19	0.16
(1,3422)	1:28:A:PRO:HD3	1:29:A:GLU:HG2	4	0.16
(1,3403)	1:79:A:ALA:HB3	1:47:A:TYR:HB2	17	0.16
(1,3402)	1:22:A:LEU:HD13	1:21:A:ASP:HB2	13	0.16
(1,3392)	1:87:A:GLY:HA2	1:86:A:LEU:HB2	1	0.16
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	3	0.16
(1,3375)	1:58:A:ALA:HB1	1:33:A:PRO:HD2	18	0.16
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	15	0.16
(1,3314)	1:93:A:PHE:HB2	1:34:A:ILE:HA	14	0.16
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	13	0.16
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	2	0.16
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	3	0.16
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	7	0.16
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	14	0.16
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	15	0.16
(1,3273)	1:96:A:PRO:HD2	1:115:A:MET:HE2	19	0.16
(1,3271)	1:31:A:MET:HE1	1:34:A:ILE:HD12	6	0.16
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD12	9	0.16
(1,3258)	1:111:A:PHE:HE2	1:34:A:ILE:HD13	3	0.16
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD12	6	0.16
(1,3255)	1:41:A:GLN:HE21	1:61:A:ILE:HD12	14	0.16
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD11	18	0.16
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD13	20	0.16
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB1	17	0.16
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB2	17	0.16
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB3	17	0.16
(1,3191)	1:107:A:ASP:HA	1:82:A:ALA:HB1	4	0.16
(1,3188)	1:57:A:THR:HA	1:58:A:ALA:HB2	6	0.16
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB2	4	0.16
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB1	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3117)	1:116:A:GLN:H	1:115:A:MET:HE1	11	0.16
(1,3094)	1:56:A:GLN:HB3	1:57:A:THR:HG23	2	0.16
(1,3094)	1:56:A:GLN:HB3	1:57:A:THR:HG23	9	0.16
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD23	7	0.16
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD21	12	0.16
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD23	14	0.16
(1,2958)	1:103:A:ALA:HA	1:81:A:LEU:HD11	9	0.16
(1,2940)	1:55:A:PRO:HD3	1:54:A:LEU:HD21	18	0.16
(1,2934)	1:71:A:GLN:HA	1:74:A:LEU:HG	20	0.16
(1,2930)	1:103:A:ALA:HA	1:105:A:LYS:HG2	17	0.16
(1,2914)	1:45:A:LEU:HA	1:48:A:LEU:HD22	15	0.16
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD23	7	0.16
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD21	14	0.16
(1,2842)	1:105:A:LYS:H	1:105:A:LYS:HG3	12	0.16
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD11	20	0.16
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD11	4	0.16
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD12	5	0.16
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD13	6	0.16
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD13	14	0.16
(1,2785)	1:74:A:LEU:HD12	1:31:A:MET:HB2	15	0.16
(1,2699)	1:93:A:PHE:HD1	1:34:A:ILE:HG13	15	0.16
(1,2638)	1:89:A:LEU:HD12	1:88:A:PRO:HB2	14	0.16
(1,2638)	1:89:A:LEU:HD13	1:88:A:PRO:HB2	16	0.16
(1,2629)	1:100:A:VAL:HG23	1:90:A:MET:HG3	8	0.16
(1,2585)	1:77:A:PHE:HB3	1:76:A:MET:HG3	8	0.16
(1,2582)	1:28:A:PRO:HD2	1:28:A:PRO:HB2	6	0.16
(1,2582)	1:28:A:PRO:HD2	1:28:A:PRO:HB2	9	0.16
(1,2582)	1:28:A:PRO:HD2	1:28:A:PRO:HB2	11	0.16
(1,2582)	1:28:A:PRO:HA	1:28:A:PRO:HB2	13	0.16
(1,2582)	1:28:A:PRO:HD2	1:28:A:PRO:HB2	15	0.16
(1,2551)	1:49:A:PRO:HA	1:49:A:PRO:HB2	17	0.16
(1,2551)	1:49:A:PRO:HA	1:49:A:PRO:HB2	20	0.16
(1,2417)	1:114:A:ALA:HB1	1:98:A:GLU:HG3	17	0.16
(1,2417)	1:114:A:ALA:HB2	1:98:A:GLU:HG3	17	0.16
(1,2417)	1:114:A:ALA:HB3	1:98:A:GLU:HG3	17	0.16
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	13	0.16
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	15	0.16
(1,2324)	1:25:A:VAL:HG13	1:26:A:LEU:HB2	13	0.16
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD2	13	0.16
(1,2073)	1:54:A:LEU:HD21	1:55:A:PRO:HD3	18	0.16
(1,2063)	1:32:A:ALA:HB2	1:33:A:PRO:HD2	10	0.16
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	4	0.16
(1,1569)	1:35:A:LEU:HD23	1:28:A:PRO:HA	14	0.16
(1,1556)	1:36:A:ALA:HB1	1:33:A:PRO:HA	9	0.16
(1,1552)	1:89:A:LEU:HB2	1:88:A:PRO:HA	4	0.16
(1,1552)	1:103:A:ALA:HB3	1:88:A:PRO:HA	8	0.16
(1,1548)	1:65:A:LEU:HG	1:61:A:ILE:HA	6	0.16
(1,1429)	1:116:A:GLN:HB3	1:119:A:ALA:H	17	0.16
(1,1320)	1:61:A:ILE:HD12	1:35:A:LEU:H	6	0.16
(1,1320)	1:61:A:ILE:HD11	1:35:A:LEU:H	18	0.16
(1,1320)	1:61:A:ILE:HD13	1:35:A:LEU:H	20	0.16
(1,1309)	1:48:A:LEU:HG	1:53:A:SER:H	5	0.16
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	4	0.16
(1,1275)	1:92:A:GLN:HB2	1:91:A:CYS:H	7	0.16
(1,1274)	1:95:A:LEU:HD22	1:91:A:CYS:H	5	0.16
(1,1274)	1:95:A:LEU:HD23	1:91:A:CYS:H	10	0.16
(1,1255)	1:26:A:LEU:HG	1:25:A:VAL:H	13	0.16
(1,1225)	1:72:A:GLN:HG2	1:74:A:LEU:H	10	0.16
(1,1206)	1:34:A:ILE:HB	1:37:A:ASN:H	6	0.16
(1,1206)	1:34:A:ILE:HB	1:37:A:ASN:H	17	0.16
(1,1145)	1:85:A:GLN:HB2	1:81:A:LEU:H	1	0.16
(1,1144)	1:44:A:LEU:HG	1:81:A:LEU:H	3	0.16
(1,1097)	1:74:A:LEU:HG	1:22:A:LEU:H	9	0.16
(1,1097)	1:74:A:LEU:HG	1:22:A:LEU:H	15	0.16
(1,1078)	1:81:A:LEU:HG	1:106:A:GLY:H	10	0.16
(1,844)	1:36:A:ALA:HA	1:41:A:GLN:HE21	6	0.16
(1,786)	1:30:A:ILE:HG23	1:31:A:MET:H	4	0.16
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	18	0.16
(1,723)	1:86:A:LEU:HD11	1:86:A:LEU:H	20	0.16
(1,683)	1:40:A:VAL:HG11	1:37:A:ASN:HD21	2	0.16
(1,637)	1:89:A:LEU:HD22	1:43:A:ARG:H	4	0.16
(1,633)	1:34:A:ILE:HB	1:36:A:ALA:H	9	0.16
(1,562)	1:95:A:LEU:HD21	1:93:A:PHE:H	2	0.16
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	1	0.16
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	11	0.16
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	13	0.16
(1,500)	1:61:A:ILE:HB	1:59:A:ASP:H	2	0.16
(1,499)	1:115:A:MET:HB2	1:117:A:ASN:H	9	0.16
(1,468)	1:57:A:THR:HG22	1:56:A:GLN:H	20	0.16
(1,459)	1:37:A:ASN:HB3	1:41:A:GLN:H	20	0.16
(1,424)	1:110:A:ALA:HB2	1:107:A:ASP:H	4	0.16
(1,423)	1:105:A:LYS:HG2	1:107:A:ASP:H	17	0.16
(1,402)	1:42:A:GLU:HB2	1:39:A:ASP:H	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:118:A:ASN:HB3	1:118:A:ASN:H	7	0.16
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	16	0.16
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	17	0.16
(1,306)	1:4:A:ILE:HG23	1:4:A:ILE:H	7	0.16
(1,264)	1:110:A:ALA:HB3	1:109:A:GLU:H	1	0.16
(1,264)	1:110:A:ALA:HB1	1:109:A:GLU:H	13	0.16
(1,109)	1:48:A:LEU:HD13	1:48:A:LEU:H	8	0.16
(1,56)	1:53:A:SER:HB3	1:54:A:LEU:H	15	0.16
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	1	0.16
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	10	0.16
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	11	0.16
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	16	0.16
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	18	0.16
(1,26)	1:5:A:LEU:HD21	1:5:A:LEU:H	18	0.16
(1,26)	1:5:A:LEU:HD22	1:5:A:LEU:H	18	0.16
(1,26)	1:5:A:LEU:HD23	1:5:A:LEU:H	18	0.16
(2,13)	1:43:A:ARG:H	1:39:A:ASP:O	13	0.15
(1,3792)	1:89:A:LEU:HD22	1:93:A:PHE:HE2	12	0.15
(1,3773)	1:46:A:PRO:HB3	1:47:A:TYR:HE2	3	0.15
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	10	0.15
(1,3756)	1:22:A:LEU:HB3	1:77:A:PHE:HD1	9	0.15
(1,3707)	1:95:A:LEU:HD12	1:93:A:PHE:HD2	6	0.15
(1,3642)	1:35:A:LEU:HD23	1:70:A:PHE:HA	12	0.15
(1,3592)	1:85:A:GLN:HB3	1:80:A:ALA:HB1	7	0.15
(1,3584)	1:10:A:VAL:HG13	1:11:A:PRO:HA	19	0.15
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD11	1	0.15
(1,3565)	1:90:A:MET:HE2	1:31:A:MET:HE3	8	0.15
(1,3565)	1:90:A:MET:HE3	1:31:A:MET:HE3	20	0.15
(1,3541)	1:89:A:LEU:HB2	1:90:A:MET:HE2	20	0.15
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG12	10	0.15
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG11	20	0.15
(1,3470)	1:35:A:LEU:HA	1:44:A:LEU:HD23	9	0.15
(1,3457)	1:105:A:LYS:H	1:81:A:LEU:HD23	6	0.15
(1,3457)	1:105:A:LYS:H	1:81:A:LEU:HD22	19	0.15
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	20	0.15
(1,3434)	1:114:A:ALA:HA	1:113:A:LYS:HB3	16	0.15
(1,3407)	1:32:A:ALA:H	1:29:A:GLU:HG3	9	0.15
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	1	0.15
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	8	0.15
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	18	0.15
(1,3375)	1:58:A:ALA:HB2	1:33:A:PRO:HD2	17	0.15
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3352)	1:111:A:PHE:HB2	1:112:A:ALA:HA	13	0.15
(1,3337)	1:14:A:PRO:HD3	1:14:A:PRO:HA	1	0.15
(1,3311)	1:55:A:PRO:HA	1:61:A:ILE:HA	16	0.15
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	10	0.15
(1,3286)	1:89:A:LEU:HG	1:40:A:VAL:HA	18	0.15
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB1	15	0.15
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB2	15	0.15
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB3	15	0.15
(1,3228)	1:61:A:ILE:HB	1:32:A:ALA:HB1	6	0.15
(1,3187)	1:115:A:MET:HA	1:99:A:ALA:HB3	8	0.15
(1,3117)	1:116:A:GLN:H	1:115:A:MET:HE3	2	0.15
(1,2997)	1:43:A:ARG:HB2	1:86:A:LEU:HD11	15	0.15
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD23	9	0.15
(1,2954)	1:28:A:PRO:HA	1:35:A:LEU:HD21	3	0.15
(1,2934)	1:93:A:PHE:HB3	1:95:A:LEU:HD21	16	0.15
(1,2927)	1:45:A:LEU:HA	1:45:A:LEU:HG	3	0.15
(1,2870)	1:70:A:PHE:HE1	1:35:A:LEU:HD21	4	0.15
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD23	16	0.15
(1,2861)	1:45:A:LEU:H	1:54:A:LEU:HD12	19	0.15
(1,2842)	1:105:A:LYS:H	1:105:A:LYS:HG3	3	0.15
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD13	1	0.15
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD11	13	0.15
(1,2629)	1:100:A:VAL:HG22	1:90:A:MET:HG3	6	0.15
(1,2585)	1:77:A:PHE:HB3	1:76:A:MET:HG3	7	0.15
(1,2582)	1:28:A:PRO:HD2	1:28:A:PRO:HB2	1	0.15
(1,2582)	1:28:A:PRO:HD2	1:28:A:PRO:HB2	3	0.15
(1,2582)	1:28:A:PRO:HD2	1:28:A:PRO:HB2	4	0.15
(1,2552)	1:27:A:THR:HA	1:28:A:PRO:HB3	14	0.15
(1,2543)	1:11:A:PRO:HA	1:11:A:PRO:HB2	6	0.15
(1,2496)	1:65:A:LEU:H	1:62:A:GLN:HG2	8	0.15
(1,2482)	1:93:A:PHE:HZ	1:40:A:VAL:HB	5	0.15
(1,2456)	1:63:A:ASN:H	1:55:A:PRO:HB3	9	0.15
(1,2450)	1:86:A:LEU:H	1:85:A:GLN:HG3	3	0.15
(1,2417)	1:114:A:ALA:HB1	1:98:A:GLU:HG3	15	0.15
(1,2417)	1:114:A:ALA:HB2	1:98:A:GLU:HG3	15	0.15
(1,2417)	1:114:A:ALA:HB3	1:98:A:GLU:HG3	15	0.15
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	19	0.15
(1,2189)	1:93:A:PHE:HZ	1:89:A:LEU:HB2	7	0.15
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	8	0.15
(1,2109)	1:49:A:PRO:HD2	1:48:A:LEU:HB3	11	0.15
(1,1849)	1:115:A:MET:HB2	1:112:A:ALA:HA	20	0.15
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	5	0.15
(1,1760)	1:136:A:GLU:H	1:136:A:GLU:HA	11	0.15
(1,1703)	1:114:A:ALA:HB1	1:98:A:GLU:HA	2	0.15
(1,1703)	1:114:A:ALA:HB1	1:98:A:GLU:HA	3	0.15
(1,1703)	1:114:A:ALA:HB2	1:98:A:GLU:HA	9	0.15
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	12	0.15
(1,1569)	1:35:A:LEU:HD21	1:28:A:PRO:HA	3	0.15
(1,1556)	1:36:A:ALA:HB1	1:33:A:PRO:HA	18	0.15
(1,1548)	1:65:A:LEU:HG	1:61:A:ILE:HA	16	0.15
(1,1541)	1:11:A:PRO:HB2	1:11:A:PRO:HA	6	0.15
(1,1462)	1:56:A:GLN:HB2	1:57:A:THR:HB	8	0.15
(1,1457)	1:20:A:VAL:HG21	1:109:A:GLU:H	11	0.15
(1,1457)	1:20:A:VAL:HG22	1:109:A:GLU:H	11	0.15
(1,1457)	1:20:A:VAL:HG23	1:109:A:GLU:H	11	0.15
(1,1309)	1:54:A:LEU:HG	1:53:A:SER:H	14	0.15
(1,1306)	1:49:A:PRO:HD2	1:53:A:SER:H	9	0.15
(1,1296)	1:26:A:LEU:HD21	1:115:A:MET:H	6	0.15
(1,1282)	1:91:A:CYS:HB3	1:89:A:LEU:H	3	0.15
(1,1274)	1:95:A:LEU:HD21	1:91:A:CYS:H	13	0.15
(1,1187)	1:116:A:GLN:HB2	1:118:A:ASN:H	11	0.15
(1,1181)	1:111:A:PHE:HA	1:102:A:ALA:H	14	0.15
(1,1181)	1:111:A:PHE:HA	1:102:A:ALA:H	19	0.15
(1,1176)	1:111:A:PHE:HD1	1:102:A:ALA:H	1	0.15
(1,1144)	1:44:A:LEU:HG	1:81:A:LEU:H	12	0.15
(1,1079)	1:107:A:ASP:HB2	1:106:A:GLY:H	12	0.15
(1,941)	1:27:A:THR:HG21	1:27:A:THR:H	7	0.15
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	6	0.15
(1,870)	1:25:A:VAL:HG11	1:24:A:SER:H	10	0.15
(1,870)	1:25:A:VAL:HG11	1:24:A:SER:H	19	0.15
(1,868)	1:65:A:LEU:HD23	1:69:A:GLN:HE21	20	0.15
(1,803)	1:46:A:PRO:HG2	1:85:A:GLN:HE21	7	0.15
(1,755)	1:116:A:GLN:HB3	1:115:A:MET:H	16	0.15
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	9	0.15
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	15	0.15
(1,699)	1:59:A:ASP:HA	1:63:A:ASN:H	9	0.15
(1,633)	1:34:A:ILE:HB	1:36:A:ALA:H	11	0.15
(1,633)	1:34:A:ILE:HB	1:36:A:ALA:H	12	0.15
(1,633)	1:34:A:ILE:HB	1:36:A:ALA:H	20	0.15
(1,562)	1:95:A:LEU:HD21	1:93:A:PHE:H	12	0.15
(1,547)	1:40:A:VAL:HB	1:42:A:GLU:H	8	0.15
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	4	0.15
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,543)	1:93:A:PHE:HB3	1:93:A:PHE:H	16	0.15
(1,504)	1:22:A:LEU:HD12	1:74:A:LEU:H	16	0.15
(1,499)	1:115:A:MET:HB3	1:117:A:ASN:H	20	0.15
(1,459)	1:37:A:ASN:HB3	1:41:A:GLN:H	14	0.15
(1,449)	1:54:A:LEU:HD12	1:45:A:LEU:H	19	0.15
(1,399)	1:118:A:ASN:HB3	1:118:A:ASN:H	19	0.15
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	4	0.15
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	5	0.15
(1,334)	1:81:A:LEU:HB2	1:80:A:ALA:H	3	0.15
(1,334)	1:81:A:LEU:HB2	1:80:A:ALA:H	14	0.15
(1,293)	1:4:A:ILE:HB	1:4:A:ILE:H	8	0.15
(1,263)	1:102:A:ALA:HB2	1:109:A:GLU:H	9	0.15
(1,164)	1:133:A:ASP:HB3	1:133:A:ASP:H	9	0.15
(1,129)	1:122:A:GLU:HB3	1:122:A:GLU:H	10	0.15
(1,129)	1:121:A:PRO:HB2	1:122:A:GLU:H	15	0.15
(1,109)	1:48:A:LEU:HD11	1:48:A:LEU:H	5	0.15
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	4	0.15
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	6	0.15
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	12	0.15
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	13	0.15
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	17	0.15
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	20	0.15
(2,13)	1:43:A:ARG:H	1:39:A:ASP:O	11	0.14
(2,13)	1:43:A:ARG:H	1:39:A:ASP:O	16	0.14
(1,3769)	1:44:A:LEU:HA	1:47:A:TYR:HE2	18	0.14
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	7	0.14
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	19	0.14
(1,3759)	1:40:A:VAL:HG22	1:77:A:PHE:HE2	13	0.14
(1,3737)	1:92:A:GLN:HB3	1:93:A:PHE:HZ	5	0.14
(1,3737)	1:89:A:LEU:HG	1:93:A:PHE:HZ	9	0.14
(1,3682)	1:89:A:LEU:HA	1:93:A:PHE:HD2	15	0.14
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	2	0.14
(1,3651)	1:45:A:LEU:H	1:47:A:TYR:HD2	6	0.14
(1,3634)	1:65:A:LEU:HD13	1:70:A:PHE:HB3	12	0.14
(1,3584)	1:10:A:VAL:HG11	1:11:A:PRO:HA	5	0.14
(1,3541)	1:103:A:ALA:HB2	1:90:A:MET:HE2	15	0.14
(1,3536)	1:44:A:LEU:H	1:80:A:ALA:HB2	2	0.14
(1,3536)	1:85:A:GLN:H	1:80:A:ALA:HB1	14	0.14
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG12	15	0.14
(1,3474)	1:111:A:PHE:HB3	1:108:A:VAL:HG12	16	0.14
(1,3457)	1:105:A:LYS:H	1:81:A:LEU:HD23	9	0.14
(1,3446)	1:89:A:LEU:H	1:91:A:CYS:HB2	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3407)	1:32:A:ALA:H	1:29:A:GLU:HG3	10	0.14
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	4	0.14
(1,3337)	1:11:A:PRO:HD3	1:11:A:PRO:HA	17	0.14
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	1	0.14
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	8	0.14
(1,3286)	1:89:A:LEU:HG	1:40:A:VAL:HA	16	0.14
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB1	2	0.14
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB2	2	0.14
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB3	2	0.14
(1,3192)	1:33:A:PRO:HA	1:58:A:ALA:HB3	8	0.14
(1,3188)	1:57:A:THR:HA	1:58:A:ALA:HB1	7	0.14
(1,3177)	1:27:A:THR:H	1:30:A:ILE:HG22	19	0.14
(1,3167)	1:70:A:PHE:HD1	1:61:A:ILE:HG23	1	0.14
(1,3167)	1:70:A:PHE:HD1	1:61:A:ILE:HG21	18	0.14
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB3	11	0.14
(1,3052)	1:20:A:VAL:H	1:20:A:VAL:HG11	11	0.14
(1,2994)	1:31:A:MET:HG3	1:35:A:LEU:HD21	9	0.14
(1,2994)	1:31:A:MET:HG3	1:35:A:LEU:HD23	11	0.14
(1,2986)	1:31:A:MET:HG2	1:74:A:LEU:HD11	13	0.14
(1,2986)	1:31:A:MET:HG2	1:74:A:LEU:HD12	13	0.14
(1,2986)	1:31:A:MET:HG2	1:74:A:LEU:HD13	13	0.14
(1,2986)	1:31:A:MET:HG3	1:74:A:LEU:HD11	13	0.14
(1,2986)	1:31:A:MET:HG3	1:74:A:LEU:HD12	13	0.14
(1,2986)	1:31:A:MET:HG3	1:74:A:LEU:HD13	13	0.14
(1,2976)	1:111:A:PHE:HB3	1:81:A:LEU:HD21	19	0.14
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD21	4	0.14
(1,2921)	1:32:A:ALA:HA	1:35:A:LEU:HD23	7	0.14
(1,2914)	1:45:A:LEU:HA	1:48:A:LEU:HD22	8	0.14
(1,2900)	1:27:A:THR:HB	1:28:A:PRO:HG2	4	0.14
(1,2900)	1:27:A:THR:HB	1:28:A:PRO:HG2	14	0.14
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD23	5	0.14
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD12	11	0.14
(1,2796)	1:54:A:LEU:H	1:48:A:LEU:HD12	20	0.14
(1,2785)	1:74:A:LEU:HD11	1:31:A:MET:HB2	19	0.14
(1,2694)	1:99:A:ALA:H	1:96:A:PRO:HG3	18	0.14
(1,2638)	1:89:A:LEU:HD12	1:88:A:PRO:HB2	11	0.14
(1,2591)	1:70:A:PHE:HB2	1:28:A:PRO:HB2	5	0.14
(1,2582)	1:28:A:PRO:HD2	1:28:A:PRO:HB2	2	0.14
(1,2582)	1:28:A:PRO:HD2	1:28:A:PRO:HB2	7	0.14
(1,2552)	1:27:A:THR:HA	1:28:A:PRO:HB3	1	0.14
(1,2552)	1:27:A:THR:HA	1:28:A:PRO:HB3	2	0.14
(1,2552)	1:27:A:THR:HA	1:28:A:PRO:HB3	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2551)	1:55:A:PRO:HA	1:55:A:PRO:HB2	2	0.14
(1,2551)	1:55:A:PRO:HA	1:55:A:PRO:HB2	8	0.14
(1,2506)	1:60:A:GLU:H	1:60:A:GLU:HB2	19	0.14
(1,2450)	1:86:A:LEU:H	1:85:A:GLN:HG3	7	0.14
(1,2417)	1:114:A:ALA:HB1	1:98:A:GLU:HG3	2	0.14
(1,2417)	1:114:A:ALA:HB2	1:98:A:GLU:HG3	2	0.14
(1,2417)	1:114:A:ALA:HB3	1:98:A:GLU:HG3	2	0.14
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	5	0.14
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	16	0.14
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	17	0.14
(1,2347)	1:73:A:ALA:H	1:70:A:PHE:HB2	19	0.14
(1,2313)	1:81:A:LEU:HG	1:111:A:PHE:HB2	18	0.14
(1,2297)	1:99:A:ALA:HB2	1:111:A:PHE:HB3	2	0.14
(1,2238)	1:70:A:PHE:HA	1:74:A:LEU:HB2	4	0.14
(1,2238)	1:70:A:PHE:HA	1:74:A:LEU:HB2	8	0.14
(1,2139)	1:133:A:ASP:H	1:133:A:ASP:HB2	16	0.14
(1,2109)	1:49:A:PRO:HD3	1:48:A:LEU:HB3	3	0.14
(1,1997)	1:108:A:VAL:HG11	1:82:A:ALA:HA	15	0.14
(1,1956)	1:96:A:PRO:HB3	1:95:A:LEU:HA	20	0.14
(1,1859)	1:64:A:THR:HG23	1:60:A:GLU:HA	16	0.14
(1,1714)	1:74:A:LEU:HB2	1:71:A:GLN:HA	17	0.14
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	15	0.14
(1,1654)	1:100:A:VAL:HA	1:91:A:CYS:HA	5	0.14
(1,1654)	1:100:A:VAL:HA	1:91:A:CYS:HA	15	0.14
(1,1654)	1:100:A:VAL:HA	1:91:A:CYS:HA	20	0.14
(1,1571)	1:61:A:ILE:HG22	1:28:A:PRO:HA	11	0.14
(1,1565)	1:64:A:THR:HG22	1:61:A:ILE:HA	4	0.14
(1,1556)	1:36:A:ALA:HB1	1:33:A:PRO:HA	7	0.14
(1,1398)	1:27:A:THR:HG21	1:24:A:SER:H	18	0.14
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	20	0.14
(1,1275)	1:92:A:GLN:HB2	1:91:A:CYS:H	3	0.14
(1,1273)	1:80:A:ALA:HB1	1:85:A:GLN:H	14	0.14
(1,1181)	1:111:A:PHE:HA	1:102:A:ALA:H	8	0.14
(1,1181)	1:111:A:PHE:HA	1:102:A:ALA:H	11	0.14
(1,1181)	1:111:A:PHE:HA	1:102:A:ALA:H	17	0.14
(1,1144)	1:44:A:LEU:HG	1:81:A:LEU:H	9	0.14
(1,1129)	1:44:A:LEU:HA	1:79:A:ALA:H	14	0.14
(1,1116)	1:96:A:PRO:HA	1:119:A:ALA:H	14	0.14
(1,1097)	1:74:A:LEU:HG	1:22:A:LEU:H	5	0.14
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	3	0.14
(1,1079)	1:107:A:ASP:HB2	1:106:A:GLY:H	16	0.14
(1,1078)	1:81:A:LEU:HG	1:106:A:GLY:H	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1072)	1:81:A:LEU:HG	1:84:A:GLY:H	7	0.14
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	18	0.14
(1,1061)	1:73:A:ALA:HB2	1:72:A:GLN:HE21	11	0.14
(1,1009)	1:116:A:GLN:HG3	1:119:A:ALA:H	19	0.14
(1,1005)	1:70:A:PHE:HD1	1:70:A:PHE:H	8	0.14
(1,996)	1:70:A:PHE:HB2	1:73:A:ALA:H	8	0.14
(1,996)	1:70:A:PHE:HB2	1:73:A:ALA:H	19	0.14
(1,972)	1:96:A:PRO:HD2	1:97:A:ALA:H	10	0.14
(1,972)	1:96:A:PRO:HD2	1:97:A:ALA:H	12	0.14
(1,972)	1:96:A:PRO:HD2	1:97:A:ALA:H	15	0.14
(1,965)	1:93:A:PHE:HE1	1:38:A:ALA:H	7	0.14
(1,941)	1:27:A:THR:HG21	1:27:A:THR:H	18	0.14
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	2	0.14
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	4	0.14
(1,929)	1:105:A:LYS:HE2	1:106:A:GLY:H	20	0.14
(1,916)	1:84:A:GLY:HA3	1:84:A:GLY:H	20	0.14
(1,905)	1:58:A:ALA:HB3	1:62:A:GLN:HE22	14	0.14
(1,884)	1:82:A:ALA:HB2	1:83:A:SER:H	7	0.14
(1,870)	1:25:A:VAL:HG11	1:24:A:SER:H	11	0.14
(1,790)	1:7:A:THR:HA	1:7:A:THR:H	11	0.14
(1,755)	1:116:A:GLN:HB3	1:115:A:MET:H	3	0.14
(1,588)	1:99:A:ALA:HB2	1:98:A:GLU:H	12	0.14
(1,571)	1:25:A:VAL:HA	1:25:A:VAL:H	1	0.14
(1,571)	1:25:A:VAL:HA	1:25:A:VAL:H	18	0.14
(1,506)	1:35:A:LEU:HD21	1:74:A:LEU:H	2	0.14
(1,459)	1:37:A:ASN:HB3	1:41:A:GLN:H	6	0.14
(1,424)	1:110:A:ALA:HB3	1:107:A:ASP:H	11	0.14
(1,419)	1:49:A:PRO:HB3	1:52:A:GLU:H	12	0.14
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	7	0.14
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	10	0.14
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	13	0.14
(1,334)	1:81:A:LEU:HB2	1:80:A:ALA:H	4	0.14
(1,334)	1:81:A:LEU:HB2	1:80:A:ALA:H	5	0.14
(1,291)	1:116:A:GLN:HB3	1:116:A:GLN:H	5	0.14
(1,291)	1:116:A:GLN:HB3	1:116:A:GLN:H	6	0.14
(1,263)	1:102:A:ALA:HB1	1:109:A:GLU:H	3	0.14
(1,261)	1:22:A:LEU:HG	1:23:A:ALA:H	7	0.14
(1,129)	1:122:A:GLU:HB3	1:122:A:GLU:H	17	0.14
(1,109)	1:48:A:LEU:HD12	1:48:A:LEU:H	13	0.14
(1,109)	1:48:A:LEU:HD12	1:48:A:LEU:H	19	0.14
(1,105)	1:76:A:MET:HB3	1:48:A:LEU:H	17	0.14
(1,97)	1:35:A:LEU:HD22	1:73:A:ALA:H	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:20:A:VAL:HG11	1:21:A:ASP:H	2	0.14
(1,47)	1:20:A:VAL:HG12	1:21:A:ASP:H	2	0.14
(1,47)	1:20:A:VAL:HG13	1:21:A:ASP:H	2	0.14
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	5	0.14
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	8	0.14
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	14	0.14
(2,13)	1:43:A:ARG:H	1:39:A:ASP:O	5	0.13
(2,13)	1:43:A:ARG:H	1:39:A:ASP:O	6	0.13
(2,13)	1:43:A:ARG:H	1:39:A:ASP:O	10	0.13
(2,13)	1:43:A:ARG:H	1:39:A:ASP:O	14	0.13
(1,3783)	1:26:A:LEU:HD12	1:77:A:PHE:HZ	6	0.13
(1,3783)	1:26:A:LEU:HD13	1:77:A:PHE:HZ	8	0.13
(1,3775)	1:46:A:PRO:HG2	1:47:A:TYR:HE2	20	0.13
(1,3766)	1:83:A:SER:H	1:47:A:TYR:HE2	11	0.13
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	17	0.13
(1,3704)	1:102:A:ALA:HB1	1:111:A:PHE:HD1	2	0.13
(1,3704)	1:102:A:ALA:HB2	1:111:A:PHE:HD1	7	0.13
(1,3698)	1:90:A:MET:HE3	1:111:A:PHE:HD1	5	0.13
(1,3698)	1:108:A:VAL:HB	1:111:A:PHE:HD2	9	0.13
(1,3668)	1:46:A:PRO:HB2	1:47:A:TYR:HD2	11	0.13
(1,3663)	1:44:A:LEU:HG	1:47:A:TYR:HD2	19	0.13
(1,3603)	1:25:A:VAL:HB	1:24:A:SER:HA	5	0.13
(1,3591)	1:44:A:LEU:HA	1:76:A:MET:HE1	18	0.13
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE2	15	0.13
(1,3536)	1:44:A:LEU:H	1:80:A:ALA:HB3	7	0.13
(1,3536)	1:85:A:GLN:H	1:80:A:ALA:HB2	17	0.13
(1,3464)	1:31:A:MET:HG3	1:26:A:LEU:HD12	20	0.13
(1,3457)	1:105:A:LYS:H	1:81:A:LEU:HD22	1	0.13
(1,3457)	1:105:A:LYS:H	1:81:A:LEU:HD21	7	0.13
(1,3447)	1:93:A:PHE:HZ	1:34:A:ILE:HG13	1	0.13
(1,3434)	1:114:A:ALA:HA	1:113:A:LYS:HB3	3	0.13
(1,3422)	1:28:A:PRO:HD3	1:29:A:GLU:HG2	17	0.13
(1,3416)	1:114:A:ALA:HA	1:117:A:ASN:HB3	2	0.13
(1,3403)	1:79:A:ALA:HB1	1:47:A:TYR:HB2	13	0.13
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	20	0.13
(1,3383)	1:42:A:GLU:HG3	1:43:A:ARG:HD2	9	0.13
(1,3375)	1:58:A:ALA:HB2	1:33:A:PRO:HD2	9	0.13
(1,3365)	1:70:A:PHE:HE2	1:28:A:PRO:HD2	5	0.13
(1,3333)	1:69:A:GLN:HB2	1:70:A:PHE:HA	6	0.13
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	5	0.13
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	6	0.13
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	17	0.13
(1,3307)	1:99:A:ALA:HA	1:100:A:VAL:HA	19	0.13
(1,3286)	1:89:A:LEU:HG	1:40:A:VAL:HA	15	0.13
(1,3271)	1:31:A:MET:HE3	1:34:A:ILE:HD12	15	0.13
(1,3259)	1:77:A:PHE:HE2	1:34:A:ILE:HD13	14	0.13
(1,3258)	1:111:A:PHE:HE2	1:34:A:ILE:HD11	16	0.13
(1,3221)	1:93:A:PHE:HB3	1:34:A:ILE:HG23	20	0.13
(1,3196)	1:31:A:MET:HA	1:30:A:ILE:HG23	8	0.13
(1,3196)	1:31:A:MET:HA	1:30:A:ILE:HG23	14	0.13
(1,3177)	1:27:A:THR:H	1:30:A:ILE:HG22	13	0.13
(1,3167)	1:70:A:PHE:HD1	1:61:A:ILE:HG21	4	0.13
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB2	14	0.13
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB2	17	0.13
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB3	5	0.13
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB3	13	0.13
(1,3141)	1:89:A:LEU:H	1:90:A:MET:HE1	16	0.13
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG12	6	0.13
(1,3041)	1:81:A:LEU:H	1:108:A:VAL:HG13	13	0.13
(1,2994)	1:31:A:MET:HG3	1:35:A:LEU:HD21	4	0.13
(1,2976)	1:111:A:PHE:HB3	1:81:A:LEU:HD22	18	0.13
(1,2954)	1:61:A:ILE:HA	1:35:A:LEU:HD21	16	0.13
(1,2930)	1:103:A:ALA:HA	1:105:A:LYS:HG2	5	0.13
(1,2911)	1:53:A:SER:HA	1:48:A:LEU:HD12	11	0.13
(1,2900)	1:27:A:THR:HA	1:28:A:PRO:HG2	13	0.13
(1,2894)	1:77:A:PHE:HE2	1:35:A:LEU:HD21	2	0.13
(1,2871)	1:80:A:ALA:H	1:44:A:LEU:HD11	14	0.13
(1,2822)	1:91:A:CYS:H	1:100:A:VAL:HG12	17	0.13
(1,2768)	1:57:A:THR:HG22	1:60:A:GLU:HB2	17	0.13
(1,2694)	1:72:A:GLN:HE21	1:49:A:PRO:HG3	9	0.13
(1,2693)	1:93:A:PHE:HD1	1:33:A:PRO:HG2	15	0.13
(1,2686)	1:70:A:PHE:HE1	1:31:A:MET:HB3	13	0.13
(1,2686)	1:70:A:PHE:HE2	1:31:A:MET:HB3	13	0.13
(1,2669)	1:86:A:LEU:H	1:43:A:ARG:HG3	20	0.13
(1,2631)	1:100:A:VAL:HG23	1:90:A:MET:HB3	15	0.13
(1,2622)	1:95:A:LEU:HD22	1:115:A:MET:HG3	14	0.13
(1,2552)	1:27:A:THR:HB	1:28:A:PRO:HB3	3	0.13
(1,2552)	1:27:A:THR:HA	1:28:A:PRO:HB3	6	0.13
(1,2552)	1:27:A:THR:HB	1:28:A:PRO:HB3	9	0.13
(1,2551)	1:55:A:PRO:HA	1:55:A:PRO:HB2	4	0.13
(1,2551)	1:49:A:PRO:HA	1:49:A:PRO:HB2	12	0.13
(1,2551)	1:55:A:PRO:HA	1:55:A:PRO:HB2	15	0.13
(1,2551)	1:55:A:PRO:HA	1:55:A:PRO:HB2	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2450)	1:86:A:LEU:H	1:85:A:GLN:HG3	16	0.13
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	6	0.13
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	11	0.13
(1,2347)	1:73:A:ALA:H	1:70:A:PHE:HB2	15	0.13
(1,2347)	1:73:A:ALA:H	1:70:A:PHE:HB2	18	0.13
(1,2347)	1:73:A:ALA:H	1:70:A:PHE:HB2	20	0.13
(1,2081)	1:65:A:LEU:HD13	1:55:A:PRO:HD2	7	0.13
(1,2063)	1:32:A:ALA:HB1	1:33:A:PRO:HD2	2	0.13
(1,2063)	1:32:A:ALA:HB3	1:33:A:PRO:HD2	17	0.13
(1,2063)	1:32:A:ALA:HB1	1:33:A:PRO:HD2	20	0.13
(1,2045)	1:88:A:PRO:HG2	1:87:A:GLY:HA3	5	0.13
(1,2042)	1:104:A:ASN:HB3	1:87:A:GLY:HA2	4	0.13
(1,1997)	1:108:A:VAL:HG11	1:82:A:ALA:HA	4	0.13
(1,1915)	1:70:A:PHE:HE2	1:26:A:LEU:HA	20	0.13
(1,1879)	1:44:A:LEU:HD11	1:44:A:LEU:HA	1	0.13
(1,1879)	1:44:A:LEU:HD12	1:44:A:LEU:HA	1	0.13
(1,1879)	1:44:A:LEU:HD13	1:44:A:LEU:HA	1	0.13
(1,1866)	1:28:A:PRO:HB3	1:62:A:GLN:HA	13	0.13
(1,1809)	1:91:A:CYS:HB3	1:90:A:MET:HA	15	0.13
(1,1760)	1:136:A:GLU:H	1:136:A:GLU:HA	15	0.13
(1,1703)	1:114:A:ALA:HB3	1:98:A:GLU:HA	4	0.13
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	17	0.13
(1,1654)	1:100:A:VAL:HA	1:91:A:CYS:HA	18	0.13
(1,1550)	1:33:A:PRO:HB3	1:34:A:ILE:HA	10	0.13
(1,1548)	1:65:A:LEU:HG	1:61:A:ILE:HA	14	0.13
(1,1545)	1:29:A:GLU:HB2	1:30:A:ILE:HA	19	0.13
(1,1543)	1:31:A:MET:HB3	1:28:A:PRO:HA	10	0.13
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	13	0.13
(1,1282)	1:91:A:CYS:HB3	1:89:A:LEU:H	10	0.13
(1,1282)	1:91:A:CYS:HB3	1:89:A:LEU:H	12	0.13
(1,1282)	1:91:A:CYS:HB3	1:89:A:LEU:H	18	0.13
(1,1274)	1:95:A:LEU:HD23	1:91:A:CYS:H	11	0.13
(1,1273)	1:80:A:ALA:HB2	1:85:A:GLN:H	17	0.13
(1,1257)	1:27:A:THR:HG22	1:25:A:VAL:H	5	0.13
(1,1255)	1:26:A:LEU:HG	1:25:A:VAL:H	16	0.13
(1,1222)	1:60:A:GLU:HB2	1:59:A:ASP:H	4	0.13
(1,1222)	1:62:A:GLN:HG2	1:59:A:ASP:H	8	0.13
(1,1207)	1:42:A:GLU:HB3	1:45:A:LEU:H	4	0.13
(1,1206)	1:34:A:ILE:HB	1:37:A:ASN:H	4	0.13
(1,1079)	1:107:A:ASP:HB2	1:106:A:GLY:H	3	0.13
(1,1079)	1:107:A:ASP:HB2	1:106:A:GLY:H	17	0.13
(1,1078)	1:81:A:LEU:HG	1:106:A:GLY:H	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1064)	1:92:A:GLN:HB3	1:94:A:GLY:H	10	0.13
(1,1064)	1:92:A:GLN:HB3	1:94:A:GLY:H	12	0.13
(1,996)	1:70:A:PHE:HB2	1:73:A:ALA:H	15	0.13
(1,996)	1:70:A:PHE:HB2	1:73:A:ALA:H	18	0.13
(1,996)	1:70:A:PHE:HB2	1:73:A:ALA:H	20	0.13
(1,965)	1:93:A:PHE:HE1	1:38:A:ALA:H	12	0.13
(1,941)	1:27:A:THR:HG23	1:27:A:THR:H	4	0.13
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	5	0.13
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	19	0.13
(1,884)	1:92:A:GLN:HG3	1:92:A:GLN:HE21	17	0.13
(1,879)	1:92:A:GLN:HG2	1:92:A:GLN:HE21	7	0.13
(1,866)	1:22:A:LEU:HG	1:24:A:SER:H	12	0.13
(1,844)	1:36:A:ALA:HA	1:41:A:GLN:HE21	3	0.13
(1,844)	1:36:A:ALA:HA	1:41:A:GLN:HE21	5	0.13
(1,784)	1:32:A:ALA:HB2	1:31:A:MET:H	7	0.13
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	7	0.13
(1,739)	1:59:A:ASP:HA	1:63:A:ASN:HD21	19	0.13
(1,699)	1:59:A:ASP:HA	1:63:A:ASN:H	15	0.13
(1,699)	1:59:A:ASP:HA	1:63:A:ASN:H	19	0.13
(1,635)	1:40:A:VAL:HG22	1:36:A:ALA:H	17	0.13
(1,633)	1:34:A:ILE:HB	1:36:A:ALA:H	3	0.13
(1,633)	1:34:A:ILE:HB	1:36:A:ALA:H	13	0.13
(1,547)	1:40:A:VAL:HB	1:42:A:GLU:H	11	0.13
(1,504)	1:65:A:LEU:HD11	1:74:A:LEU:H	20	0.13
(1,468)	1:57:A:THR:HG21	1:56:A:GLN:H	6	0.13
(1,459)	1:37:A:ASN:HB3	1:41:A:GLN:H	16	0.13
(1,424)	1:110:A:ALA:HB2	1:107:A:ASP:H	14	0.13
(1,424)	1:110:A:ALA:HB2	1:107:A:ASP:H	17	0.13
(1,399)	1:118:A:ASN:HB3	1:118:A:ASN:H	2	0.13
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	1	0.13
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	18	0.13
(1,341)	1:44:A:LEU:HD11	1:80:A:ALA:H	14	0.13
(1,291)	1:116:A:GLN:HB3	1:116:A:GLN:H	13	0.13
(1,173)	1:19:A:GLN:HB3	1:19:A:GLN:H	13	0.13
(1,173)	1:19:A:GLN:HB3	1:19:A:GLN:H	18	0.13
(1,146)	1:136:A:GLU:HA	1:136:A:GLU:H	15	0.13
(1,105)	1:76:A:MET:HB3	1:48:A:LEU:H	6	0.13
(1,105)	1:76:A:MET:HB3	1:48:A:LEU:H	15	0.13
(1,105)	1:76:A:MET:HB3	1:48:A:LEU:H	19	0.13
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	3	0.13
(1,3775)	1:46:A:PRO:HG2	1:47:A:TYR:HE2	5	0.12
(1,3769)	1:44:A:LEU:HA	1:47:A:TYR:HE2	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3707)	1:95:A:LEU:HD12	1:93:A:PHE:HD2	15	0.12
(1,3682)	1:89:A:LEU:HA	1:93:A:PHE:HD2	16	0.12
(1,3668)	1:46:A:PRO:HB2	1:47:A:TYR:HD2	6	0.12
(1,3663)	1:44:A:LEU:HG	1:47:A:TYR:HD2	15	0.12
(1,3645)	1:55:A:PRO:HD2	1:35:A:LEU:HD12	4	0.12
(1,3580)	1:93:A:PHE:HB2	1:34:A:ILE:HD13	17	0.12
(1,3574)	1:57:A:THR:H	1:61:A:ILE:HD11	10	0.12
(1,3565)	1:90:A:MET:HE3	1:31:A:MET:HE1	2	0.12
(1,3558)	1:117:A:ASN:HB2	1:114:A:ALA:HB1	16	0.12
(1,3554)	1:83:A:SER:HB2	1:80:A:ALA:HB3	8	0.12
(1,3537)	1:86:A:LEU:HA	1:90:A:MET:HE3	1	0.12
(1,3536)	1:44:A:LEU:H	1:80:A:ALA:HB1	13	0.12
(1,3473)	1:55:A:PRO:HD2	1:65:A:LEU:HD21	4	0.12
(1,3449)	1:94:A:GLY:HA2	1:91:A:CYS:HB2	10	0.12
(1,3442)	1:99:A:ALA:HB2	1:96:A:PRO:HB2	15	0.12
(1,3428)	1:35:A:LEU:H	1:40:A:VAL:HB	18	0.12
(1,3416)	1:114:A:ALA:HA	1:117:A:ASN:HB3	4	0.12
(1,3403)	1:79:A:ALA:HB2	1:47:A:TYR:HB2	16	0.12
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	2	0.12
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	9	0.12
(1,3385)	1:23:A:ALA:H	1:22:A:LEU:HB2	19	0.12
(1,3255)	1:41:A:GLN:HE21	1:61:A:ILE:HD13	8	0.12
(1,3231)	1:109:A:GLU:HG3	1:110:A:ALA:HB1	18	0.12
(1,3228)	1:61:A:ILE:HB	1:32:A:ALA:HB1	10	0.12
(1,3228)	1:61:A:ILE:HB	1:32:A:ALA:HB2	13	0.12
(1,3196)	1:31:A:MET:HA	1:30:A:ILE:HG22	18	0.12
(1,3188)	1:57:A:THR:HA	1:58:A:ALA:HB1	13	0.12
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB3	1	0.12
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB2	16	0.12
(1,3148)	1:24:A:SER:H	1:23:A:ALA:HB3	9	0.12
(1,3145)	1:115:A:MET:H	1:115:A:MET:HE1	6	0.12
(1,3145)	1:115:A:MET:H	1:115:A:MET:HE2	6	0.12
(1,3145)	1:115:A:MET:H	1:115:A:MET:HE3	6	0.12
(1,3142)	1:93:A:PHE:HE2	1:90:A:MET:HE1	6	0.12
(1,3117)	1:116:A:GLN:H	1:115:A:MET:HE1	19	0.12
(1,3094)	1:56:A:GLN:HB3	1:57:A:THR:HG22	1	0.12
(1,3094)	1:56:A:GLN:HB3	1:57:A:THR:HG23	8	0.12
(1,3092)	1:77:A:PHE:HB3	1:35:A:LEU:HD12	20	0.12
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD22	20	0.12
(1,2934)	1:93:A:PHE:HB3	1:95:A:LEU:HD23	10	0.12
(1,2914)	1:45:A:LEU:HA	1:48:A:LEU:HD22	5	0.12
(1,2900)	1:27:A:THR:HB	1:28:A:PRO:HG2	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2900)	1:27:A:THR:HA	1:28:A:PRO:HG2	16	0.12
(1,2871)	1:80:A:ALA:H	1:44:A:LEU:HD12	13	0.12
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD22	14	0.12
(1,2861)	1:45:A:LEU:H	1:45:A:LEU:HD22	16	0.12
(1,2857)	1:52:A:GLU:H	1:48:A:LEU:HD21	17	0.12
(1,2856)	1:92:A:GLN:HE22	1:89:A:LEU:HD21	2	0.12
(1,2842)	1:105:A:LYS:H	1:105:A:LYS:HG3	1	0.12
(1,2829)	1:86:A:LEU:H	1:86:A:LEU:HD12	1	0.12
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD13	15	0.12
(1,2785)	1:74:A:LEU:HD11	1:31:A:MET:HB2	11	0.12
(1,2768)	1:64:A:THR:HG22	1:60:A:GLU:HB2	6	0.12
(1,2694)	1:72:A:GLN:HE21	1:49:A:PRO:HG3	20	0.12
(1,2630)	1:34:A:ILE:HD12	1:90:A:MET:HG3	18	0.12
(1,2620)	1:64:A:THR:HG22	1:60:A:GLU:HB2	6	0.12
(1,2552)	1:27:A:THR:HB	1:28:A:PRO:HB3	10	0.12
(1,2552)	1:27:A:THR:HA	1:28:A:PRO:HB3	12	0.12
(1,2551)	1:49:A:PRO:HA	1:49:A:PRO:HB2	3	0.12
(1,2551)	1:55:A:PRO:HA	1:55:A:PRO:HB2	7	0.12
(1,2551)	1:55:A:PRO:HA	1:55:A:PRO:HB2	11	0.12
(1,2551)	1:55:A:PRO:HA	1:55:A:PRO:HB2	16	0.12
(1,2515)	1:65:A:LEU:H	1:28:A:PRO:HB3	10	0.12
(1,2506)	1:52:A:GLU:H	1:52:A:GLU:HB3	5	0.12
(1,2414)	1:74:A:LEU:HB3	1:77:A:PHE:HB3	9	0.12
(1,2347)	1:73:A:ALA:H	1:70:A:PHE:HB2	16	0.12
(1,2313)	1:81:A:LEU:HG	1:111:A:PHE:HB2	17	0.12
(1,2309)	1:22:A:LEU:HB2	1:26:A:LEU:HB3	2	0.12
(1,2189)	1:93:A:PHE:HZ	1:89:A:LEU:HB2	17	0.12
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD2	1	0.12
(1,2066)	1:54:A:LEU:HB3	1:55:A:PRO:HD2	18	0.12
(1,2063)	1:32:A:ALA:HB3	1:33:A:PRO:HD2	12	0.12
(1,2042)	1:104:A:ASN:HB3	1:87:A:GLY:HA2	5	0.12
(1,1961)	1:56:A:GLN:HB3	1:36:A:ALA:HA	13	0.12
(1,1915)	1:70:A:PHE:HE2	1:26:A:LEU:HA	15	0.12
(1,1849)	1:115:A:MET:HB2	1:112:A:ALA:HA	17	0.12
(1,1849)	1:115:A:MET:HB2	1:112:A:ALA:HA	18	0.12
(1,1808)	1:46:A:PRO:HD3	1:44:A:LEU:HA	12	0.12
(1,1703)	1:114:A:ALA:HB2	1:98:A:GLU:HA	17	0.12
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	2	0.12
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	4	0.12
(1,1683)	1:29:A:GLU:HG2	1:29:A:GLU:HA	13	0.12
(1,1672)	1:96:A:PRO:HG3	1:96:A:PRO:HA	1	0.12
(1,1654)	1:100:A:VAL:HA	1:91:A:CYS:HA	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1654)	1:100:A:VAL:HA	1:91:A:CYS:HA	12	0.12
(1,1556)	1:36:A:ALA:HB2	1:33:A:PRO:HA	1	0.12
(1,1550)	1:33:A:PRO:HB3	1:34:A:ILE:HA	20	0.12
(1,1391)	1:113:A:LYS:HB3	1:116:A:GLN:HE21	12	0.12
(1,1310)	1:89:A:LEU:HD22	1:86:A:LEU:H	9	0.12
(1,1309)	1:54:A:LEU:HG	1:53:A:SER:H	17	0.12
(1,1282)	1:91:A:CYS:HB3	1:89:A:LEU:H	2	0.12
(1,1273)	1:80:A:ALA:HB2	1:85:A:GLN:H	13	0.12
(1,1222)	1:62:A:GLN:HG2	1:59:A:ASP:H	9	0.12
(1,1202)	1:40:A:VAL:HA	1:45:A:LEU:H	12	0.12
(1,1144)	1:44:A:LEU:HG	1:81:A:LEU:H	13	0.12
(1,1144)	1:44:A:LEU:HG	1:81:A:LEU:H	14	0.12
(1,1142)	1:120:A:LYS:HG3	1:122:A:GLU:H	6	0.12
(1,1122)	1:99:A:ALA:HB2	1:119:A:ALA:H	9	0.12
(1,1102)	1:60:A:GLU:HG2	1:58:A:ALA:H	8	0.12
(1,1097)	1:74:A:LEU:HG	1:22:A:LEU:H	14	0.12
(1,1079)	1:107:A:ASP:HB2	1:106:A:GLY:H	14	0.12
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	9	0.12
(1,1009)	1:116:A:GLN:HG3	1:119:A:ALA:H	5	0.12
(1,1009)	1:116:A:GLN:HG3	1:119:A:ALA:H	9	0.12
(1,1009)	1:116:A:GLN:HG3	1:119:A:ALA:H	17	0.12
(1,996)	1:70:A:PHE:HB2	1:73:A:ALA:H	16	0.12
(1,965)	1:36:A:ALA:H	1:38:A:ALA:H	2	0.12
(1,941)	1:27:A:THR:HG23	1:27:A:THR:H	2	0.12
(1,929)	1:107:A:ASP:HB3	1:106:A:GLY:H	8	0.12
(1,916)	1:84:A:GLY:HA3	1:84:A:GLY:H	9	0.12
(1,916)	1:84:A:GLY:HA3	1:84:A:GLY:H	10	0.12
(1,907)	1:65:A:LEU:HD21	1:72:A:GLN:HE22	8	0.12
(1,907)	1:65:A:LEU:HD22	1:72:A:GLN:HE22	8	0.12
(1,907)	1:65:A:LEU:HD23	1:72:A:GLN:HE22	8	0.12
(1,879)	1:62:A:GLN:HB3	1:62:A:GLN:HE21	1	0.12
(1,866)	1:22:A:LEU:HG	1:24:A:SER:H	15	0.12
(1,866)	1:22:A:LEU:HG	1:24:A:SER:H	20	0.12
(1,844)	1:36:A:ALA:HA	1:41:A:GLN:HE21	7	0.12
(1,790)	1:7:A:THR:HA	1:7:A:THR:H	7	0.12
(1,784)	1:32:A:ALA:HB1	1:31:A:MET:H	11	0.12
(1,767)	1:100:A:VAL:HG22	1:90:A:MET:H	19	0.12
(1,760)	1:96:A:PRO:HB2	1:118:A:ASN:HD22	8	0.12
(1,755)	1:116:A:GLN:HB3	1:115:A:MET:H	2	0.12
(1,723)	1:86:A:LEU:HD12	1:86:A:LEU:H	1	0.12
(1,633)	1:34:A:ILE:HB	1:36:A:ALA:H	14	0.12
(1,633)	1:34:A:ILE:HB	1:36:A:ALA:H	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,588)	1:114:A:ALA:HB3	1:98:A:GLU:H	14	0.12
(1,571)	1:25:A:VAL:HA	1:25:A:VAL:H	4	0.12
(1,571)	1:25:A:VAL:HA	1:25:A:VAL:H	9	0.12
(1,547)	1:40:A:VAL:HB	1:42:A:GLU:H	3	0.12
(1,547)	1:40:A:VAL:HB	1:42:A:GLU:H	4	0.12
(1,547)	1:40:A:VAL:HB	1:42:A:GLU:H	20	0.12
(1,518)	1:43:A:ARG:HB2	1:44:A:LEU:H	3	0.12
(1,499)	1:115:A:MET:HB3	1:117:A:ASN:H	6	0.12
(1,468)	1:57:A:THR:HG22	1:56:A:GLN:H	16	0.12
(1,459)	1:37:A:ASN:HB3	1:41:A:GLN:H	1	0.12
(1,449)	1:45:A:LEU:HD22	1:45:A:LEU:H	14	0.12
(1,449)	1:45:A:LEU:HD22	1:45:A:LEU:H	16	0.12
(1,424)	1:110:A:ALA:HB3	1:107:A:ASP:H	1	0.12
(1,424)	1:110:A:ALA:HB2	1:107:A:ASP:H	16	0.12
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	3	0.12
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	6	0.12
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	11	0.12
(1,341)	1:44:A:LEU:HD12	1:80:A:ALA:H	13	0.12
(1,316)	1:47:A:TYR:HE2	1:80:A:ALA:H	20	0.12
(1,297)	1:113:A:LYS:HG3	1:114:A:ALA:H	11	0.12
(1,291)	1:116:A:GLN:HB3	1:116:A:GLN:H	3	0.12
(1,291)	1:116:A:GLN:HB3	1:116:A:GLN:H	19	0.12
(1,272)	1:115:A:MET:H	1:116:A:GLN:H	5	0.12
(1,221)	1:96:A:PRO:HD2	1:99:A:ALA:H	16	0.12
(1,174)	1:8:A:MET:HB2	1:8:A:MET:H	6	0.12
(1,173)	1:19:A:GLN:HB3	1:19:A:GLN:H	19	0.12
(1,171)	1:123:A:GLN:HB3	1:123:A:GLN:H	17	0.12
(1,165)	1:130:A:ASP:HB3	1:130:A:ASP:H	14	0.12
(1,109)	1:48:A:LEU:HD13	1:48:A:LEU:H	3	0.12
(1,109)	1:48:A:LEU:HD11	1:48:A:LEU:H	14	0.12
(1,109)	1:48:A:LEU:HD12	1:48:A:LEU:H	16	0.12
(1,62)	1:12:A:ALA:HA	1:12:A:ALA:H	4	0.12
(1,43)	1:108:A:VAL:HB	1:108:A:VAL:H	7	0.12
(2,13)	1:43:A:ARG:H	1:39:A:ASP:O	15	0.11
(1,3792)	1:40:A:VAL:HG21	1:93:A:PHE:HE2	15	0.11
(1,3783)	1:26:A:LEU:HD11	1:77:A:PHE:HZ	7	0.11
(1,3783)	1:26:A:LEU:HD12	1:77:A:PHE:HZ	18	0.11
(1,3782)	1:103:A:ALA:HA	1:111:A:PHE:HZ	16	0.11
(1,3775)	1:46:A:PRO:HG2	1:47:A:TYR:HE2	11	0.11
(1,3758)	1:26:A:LEU:HD13	1:77:A:PHE:HD1	2	0.11
(1,3698)	1:108:A:VAL:HB	1:111:A:PHE:HD2	15	0.11
(1,3682)	1:89:A:LEU:HA	1:93:A:PHE:HD2	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3591)	1:44:A:LEU:HA	1:76:A:MET:HE2	7	0.11
(1,3556)	1:43:A:ARG:HD3	1:80:A:ALA:HB3	6	0.11
(1,3554)	1:43:A:ARG:HA	1:80:A:ALA:HB1	14	0.11
(1,3517)	1:77:A:PHE:HA	1:35:A:LEU:HD11	6	0.11
(1,3473)	1:55:A:PRO:HD2	1:65:A:LEU:HD22	20	0.11
(1,3446)	1:93:A:PHE:H	1:91:A:CYS:HB2	1	0.11
(1,3407)	1:32:A:ALA:H	1:29:A:GLU:HG3	19	0.11
(1,3403)	1:79:A:ALA:HB1	1:47:A:TYR:HB2	10	0.11
(1,3352)	1:111:A:PHE:HB2	1:112:A:ALA:HA	11	0.11
(1,3352)	1:111:A:PHE:HB2	1:112:A:ALA:HA	14	0.11
(1,3309)	1:86:A:LEU:HA	1:40:A:VAL:HA	3	0.11
(1,3274)	1:93:A:PHE:HB2	1:115:A:MET:HE2	9	0.11
(1,3255)	1:35:A:LEU:H	1:61:A:ILE:HD11	9	0.11
(1,3188)	1:57:A:THR:HA	1:58:A:ALA:HB2	2	0.11
(1,3188)	1:57:A:THR:HA	1:58:A:ALA:HB2	11	0.11
(1,3158)	1:107:A:ASP:H	1:110:A:ALA:HB2	2	0.11
(1,3158)	1:114:A:ALA:H	1:110:A:ALA:HB3	13	0.11
(1,3145)	1:115:A:MET:H	1:115:A:MET:HE1	10	0.11
(1,3145)	1:115:A:MET:H	1:115:A:MET:HE2	10	0.11
(1,3145)	1:115:A:MET:H	1:115:A:MET:HE3	10	0.11
(1,3141)	1:89:A:LEU:H	1:90:A:MET:HE1	9	0.11
(1,3117)	1:116:A:GLN:H	1:115:A:MET:HE1	14	0.11
(1,3009)	1:26:A:LEU:HB3	1:74:A:LEU:HD11	2	0.11
(1,3009)	1:26:A:LEU:HB3	1:74:A:LEU:HD13	9	0.11
(1,2997)	1:43:A:ARG:HB2	1:86:A:LEU:HD11	8	0.11
(1,2973)	1:77:A:PHE:HB3	1:74:A:LEU:HD22	11	0.11
(1,2966)	1:105:A:LYS:HE3	1:105:A:LYS:HG3	16	0.11
(1,2958)	1:103:A:ALA:HA	1:81:A:LEU:HD12	13	0.11
(1,2876)	1:107:A:ASP:H	1:81:A:LEU:HD12	8	0.11
(1,2871)	1:80:A:ALA:H	1:44:A:LEU:HD11	16	0.11
(1,2866)	1:44:A:LEU:H	1:86:A:LEU:HD23	13	0.11
(1,2862)	1:65:A:LEU:H	1:65:A:LEU:HD23	12	0.11
(1,2822)	1:95:A:LEU:H	1:100:A:VAL:HG13	20	0.11
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD11	7	0.11
(1,2802)	1:81:A:LEU:H	1:81:A:LEU:HD11	8	0.11
(1,2694)	1:72:A:GLN:HE21	1:49:A:PRO:HG3	8	0.11
(1,2669)	1:86:A:LEU:H	1:43:A:ARG:HG3	9	0.11
(1,2631)	1:100:A:VAL:HG21	1:90:A:MET:HB3	12	0.11
(1,2585)	1:77:A:PHE:HB3	1:76:A:MET:HG3	16	0.11
(1,2582)	1:28:A:PRO:HD2	1:28:A:PRO:HB2	19	0.11
(1,2552)	1:27:A:THR:HA	1:28:A:PRO:HB3	4	0.11
(1,2552)	1:27:A:THR:HA	1:28:A:PRO:HB3	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2552)	1:27:A:THR:HA	1:28:A:PRO:HB3	15	0.11
(1,2552)	1:27:A:THR:HA	1:28:A:PRO:HB3	19	0.11
(1,2543)	1:121:A:PRO:HA	1:121:A:PRO:HB2	17	0.11
(1,2506)	1:60:A:GLU:H	1:60:A:GLU:HB2	2	0.11
(1,2496)	1:65:A:LEU:H	1:62:A:GLN:HG2	4	0.11
(1,2440)	1:56:A:GLN:H	1:55:A:PRO:HB3	5	0.11
(1,2347)	1:72:A:GLN:H	1:70:A:PHE:HB2	8	0.11
(1,2347)	1:73:A:ALA:H	1:70:A:PHE:HB2	17	0.11
(1,2324)	1:25:A:VAL:HG13	1:26:A:LEU:HB2	19	0.11
(1,2309)	1:22:A:LEU:HB2	1:26:A:LEU:HB3	13	0.11
(1,2297)	1:99:A:ALA:HB2	1:111:A:PHE:HB3	14	0.11
(1,2265)	1:43:A:ARG:HD3	1:89:A:LEU:HB3	18	0.11
(1,2242)	1:38:A:ALA:HA	1:37:A:ASN:HB3	14	0.11
(1,2110)	1:46:A:PRO:HD3	1:43:A:ARG:HD2	18	0.11
(1,2092)	1:44:A:LEU:H	1:43:A:ARG:HD2	20	0.11
(1,2066)	1:119:A:ALA:HB1	1:96:A:PRO:HD2	1	0.11
(1,2063)	1:32:A:ALA:HB1	1:33:A:PRO:HD2	7	0.11
(1,2063)	1:32:A:ALA:HB2	1:33:A:PRO:HD2	18	0.11
(1,1956)	1:96:A:PRO:HB3	1:95:A:LEU:HA	6	0.11
(1,1883)	1:35:A:LEU:HD22	1:74:A:LEU:HA	8	0.11
(1,1866)	1:28:A:PRO:HB3	1:62:A:GLN:HA	14	0.11
(1,1866)	1:28:A:PRO:HB3	1:62:A:GLN:HA	18	0.11
(1,1737)	1:44:A:LEU:HD21	1:41:A:GLN:HA	6	0.11
(1,1723)	1:25:A:VAL:HG11	1:24:A:SER:HA	6	0.11
(1,1708)	1:112:A:ALA:HB1	1:20:A:VAL:HA	4	0.11
(1,1708)	1:112:A:ALA:HB2	1:20:A:VAL:HA	4	0.11
(1,1708)	1:112:A:ALA:HB3	1:20:A:VAL:HA	4	0.11
(1,1692)	1:96:A:PRO:HB2	1:96:A:PRO:HA	4	0.11
(1,1654)	1:100:A:VAL:HA	1:91:A:CYS:HA	11	0.11
(1,1654)	1:100:A:VAL:HA	1:91:A:CYS:HA	16	0.11
(1,1594)	1:129:A:LYS:H	1:128:A:THR:HA	10	0.11
(1,1565)	1:64:A:THR:HG21	1:61:A:ILE:HA	7	0.11
(1,1550)	1:33:A:PRO:HB3	1:34:A:ILE:HA	2	0.11
(1,1541)	1:121:A:PRO:HB2	1:121:A:PRO:HA	17	0.11
(1,1468)	1:44:A:LEU:H	1:40:A:VAL:HA	9	0.11
(1,1462)	1:56:A:GLN:HB2	1:57:A:THR:HB	3	0.11
(1,1335)	1:86:A:LEU:HG	1:90:A:MET:H	9	0.11
(1,1320)	1:61:A:ILE:HD11	1:35:A:LEU:H	9	0.11
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	12	0.11
(1,1273)	1:80:A:ALA:HB1	1:85:A:GLN:H	19	0.11
(1,1251)	1:92:A:GLN:HE22	1:92:A:GLN:H	14	0.11
(1,1240)	1:102:A:ALA:HA	1:105:A:LYS:H	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:62:A:GLN:HG2	1:59:A:ASP:H	19	0.11
(1,1206)	1:34:A:ILE:HB	1:37:A:ASN:H	8	0.11
(1,1206)	1:34:A:ILE:HB	1:37:A:ASN:H	18	0.11
(1,1187)	1:116:A:GLN:HB2	1:118:A:ASN:H	3	0.11
(1,1181)	1:111:A:PHE:HA	1:102:A:ALA:H	5	0.11
(1,1131)	1:47:A:TYR:HB2	1:79:A:ALA:H	18	0.11
(1,1097)	1:74:A:LEU:HG	1:22:A:LEU:H	7	0.11
(1,1097)	1:74:A:LEU:HG	1:22:A:LEU:H	12	0.11
(1,1091)	1:104:A:ASN:H	1:87:A:GLY:H	5	0.11
(1,1079)	1:107:A:ASP:HB2	1:106:A:GLY:H	1	0.11
(1,1079)	1:107:A:ASP:HB2	1:106:A:GLY:H	8	0.11
(1,1063)	1:95:A:LEU:HD23	1:94:A:GLY:H	18	0.11
(1,996)	1:70:A:PHE:HB2	1:73:A:ALA:H	17	0.11
(1,972)	1:96:A:PRO:HD2	1:97:A:ALA:H	5	0.11
(1,972)	1:96:A:PRO:HD2	1:97:A:ALA:H	11	0.11
(1,916)	1:84:A:GLY:HA3	1:84:A:GLY:H	3	0.11
(1,916)	1:84:A:GLY:HA3	1:84:A:GLY:H	14	0.11
(1,916)	1:84:A:GLY:HA3	1:84:A:GLY:H	17	0.11
(1,916)	1:84:A:GLY:HA3	1:84:A:GLY:H	18	0.11
(1,844)	1:36:A:ALA:HA	1:41:A:GLN:HE21	4	0.11
(1,844)	1:36:A:ALA:HA	1:41:A:GLN:HE21	18	0.11
(1,755)	1:116:A:GLN:HB3	1:115:A:MET:H	14	0.11
(1,740)	1:112:A:ALA:HA	1:115:A:MET:H	5	0.11
(1,633)	1:34:A:ILE:HB	1:36:A:ALA:H	5	0.11
(1,633)	1:34:A:ILE:HB	1:36:A:ALA:H	6	0.11
(1,571)	1:25:A:VAL:HA	1:25:A:VAL:H	3	0.11
(1,571)	1:25:A:VAL:HA	1:25:A:VAL:H	12	0.11
(1,571)	1:25:A:VAL:HA	1:25:A:VAL:H	19	0.11
(1,571)	1:25:A:VAL:HA	1:25:A:VAL:H	20	0.11
(1,547)	1:40:A:VAL:HB	1:42:A:GLU:H	1	0.11
(1,504)	1:65:A:LEU:HD12	1:74:A:LEU:H	9	0.11
(1,468)	1:57:A:THR:HG23	1:56:A:GLN:H	8	0.11
(1,463)	1:55:A:PRO:HB3	1:56:A:GLN:H	5	0.11
(1,459)	1:37:A:ASN:HB3	1:41:A:GLN:H	9	0.11
(1,459)	1:37:A:ASN:HB3	1:41:A:GLN:H	15	0.11
(1,424)	1:110:A:ALA:HB2	1:107:A:ASP:H	2	0.11
(1,411)	1:40:A:VAL:HG22	1:39:A:ASP:H	12	0.11
(1,411)	1:40:A:VAL:HG22	1:39:A:ASP:H	16	0.11
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	14	0.11
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	19	0.11
(1,341)	1:44:A:LEU:HD11	1:80:A:ALA:H	16	0.11
(1,338)	1:65:A:LEU:HD13	1:65:A:LEU:H	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,334)	1:81:A:LEU:HB2	1:80:A:ALA:H	13	0.11
(1,316)	1:47:A:TYR:HE2	1:80:A:ALA:H	5	0.11
(1,291)	1:116:A:GLN:HB3	1:116:A:GLN:H	2	0.11
(1,291)	1:116:A:GLN:HB3	1:116:A:GLN:H	4	0.11
(1,291)	1:116:A:GLN:HB3	1:116:A:GLN:H	12	0.11
(1,291)	1:116:A:GLN:HB3	1:116:A:GLN:H	18	0.11
(1,261)	1:22:A:LEU:HG	1:23:A:ALA:H	13	0.11
(1,146)	1:136:A:GLU:HA	1:136:A:GLU:H	17	0.11
(1,145)	1:19:A:GLN:HA	1:19:A:GLN:H	1	0.11
(1,145)	1:19:A:GLN:HA	1:19:A:GLN:H	4	0.11
(1,145)	1:19:A:GLN:HA	1:19:A:GLN:H	5	0.11
(1,145)	1:19:A:GLN:HA	1:19:A:GLN:H	13	0.11
(1,129)	1:122:A:GLU:HB3	1:122:A:GLU:H	6	0.11
(1,129)	1:122:A:GLU:HB3	1:122:A:GLU:H	14	0.11
(1,109)	1:48:A:LEU:HD11	1:48:A:LEU:H	20	0.11
(1,85)	1:70:A:PHE:HD1	1:73:A:ALA:H	6	0.11
(1,84)	1:120:A:LYS:H	1:119:A:ALA:H	7	0.11
(1,47)	1:20:A:VAL:HG11	1:21:A:ASP:H	19	0.11
(1,47)	1:20:A:VAL:HG12	1:21:A:ASP:H	19	0.11
(1,47)	1:20:A:VAL:HG13	1:21:A:ASP:H	19	0.11
(2,13)	1:43:A:ARG:H	1:39:A:ASP:O	3	0.1
(1,3783)	1:26:A:LEU:HD12	1:77:A:PHE:HZ	3	0.1
(1,3765)	1:47:A:TYR:H	1:47:A:TYR:HE2	16	0.1
(1,3738)	1:89:A:LEU:HB3	1:93:A:PHE:HZ	5	0.1
(1,3735)	1:34:A:ILE:HB	1:93:A:PHE:HZ	10	0.1
(1,3735)	1:34:A:ILE:HB	1:93:A:PHE:HZ	12	0.1
(1,3592)	1:85:A:GLN:HB3	1:80:A:ALA:HB2	17	0.1
(1,3554)	1:43:A:ARG:HA	1:80:A:ALA:HB1	15	0.1
(1,3547)	1:48:A:LEU:HG	1:76:A:MET:HE3	10	0.1
(1,3547)	1:54:A:LEU:HG	1:76:A:MET:HE3	18	0.1
(1,3446)	1:93:A:PHE:H	1:91:A:CYS:HB2	11	0.1
(1,3407)	1:32:A:ALA:H	1:29:A:GLU:HG3	3	0.1
(1,3272)	1:96:A:PRO:HD3	1:115:A:MET:HE1	10	0.1
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB1	6	0.1
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB2	6	0.1
(1,3229)	1:98:A:GLU:HG3	1:114:A:ALA:HB3	6	0.1
(1,3221)	1:93:A:PHE:HB3	1:34:A:ILE:HG23	1	0.1
(1,3188)	1:57:A:THR:HA	1:58:A:ALA:HB2	10	0.1
(1,3141)	1:89:A:LEU:H	1:90:A:MET:HE3	8	0.1
(1,2997)	1:43:A:ARG:HB2	1:86:A:LEU:HD13	10	0.1
(1,2994)	1:31:A:MET:HG3	1:35:A:LEU:HD23	19	0.1
(1,2900)	1:27:A:THR:HB	1:28:A:PRO:HG2	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2817)	1:77:A:PHE:H	1:74:A:LEU:HD13	2	0.1
(1,2769)	1:99:A:ALA:HB1	1:115:A:MET:HB2	14	0.1
(1,2582)	1:28:A:PRO:HD2	1:28:A:PRO:HB2	17	0.1
(1,2552)	1:27:A:THR:HA	1:28:A:PRO:HB3	17	0.1
(1,2552)	1:27:A:THR:HA	1:28:A:PRO:HB3	20	0.1
(1,2506)	1:52:A:GLU:H	1:52:A:GLU:HB3	9	0.1
(1,2482)	1:93:A:PHE:HZ	1:40:A:VAL:HB	10	0.1
(1,2417)	1:114:A:ALA:HB1	1:98:A:GLU:HG3	6	0.1
(1,2417)	1:114:A:ALA:HB2	1:98:A:GLU:HG3	6	0.1
(1,2417)	1:114:A:ALA:HB3	1:98:A:GLU:HG3	6	0.1
(1,2347)	1:73:A:ALA:H	1:70:A:PHE:HB2	9	0.1
(1,1997)	1:108:A:VAL:HG13	1:82:A:ALA:HA	11	0.1
(1,1956)	1:96:A:PRO:HB3	1:95:A:LEU:HA	11	0.1
(1,1883)	1:35:A:LEU:HD22	1:74:A:LEU:HA	18	0.1
(1,1737)	1:44:A:LEU:HD23	1:41:A:GLN:HA	18	0.1
(1,1657)	1:11:A:PRO:HD2	1:10:A:VAL:HA	1	0.1
(1,1657)	1:11:A:PRO:HD3	1:10:A:VAL:HA	1	0.1
(1,1562)	1:102:A:ALA:HB1	1:108:A:VAL:HA	17	0.1
(1,1525)	1:31:A:MET:HA	1:34:A:ILE:HA	1	0.1
(1,1525)	1:31:A:MET:HA	1:34:A:ILE:HA	18	0.1
(1,1298)	1:35:A:LEU:HB2	1:34:A:ILE:H	1	0.1
(1,1282)	1:91:A:CYS:HB3	1:89:A:LEU:H	9	0.1
(1,1274)	1:95:A:LEU:HD22	1:91:A:CYS:H	17	0.1
(1,1273)	1:80:A:ALA:HB3	1:85:A:GLN:H	6	0.1
(1,1255)	1:26:A:LEU:HG	1:25:A:VAL:H	8	0.1
(1,1246)	1:44:A:LEU:HD13	1:42:A:GLU:H	4	0.1
(1,1206)	1:34:A:ILE:HB	1:37:A:ASN:H	14	0.1
(1,1206)	1:34:A:ILE:HB	1:37:A:ASN:H	19	0.1
(1,1206)	1:34:A:ILE:HB	1:37:A:ASN:H	20	0.1
(1,1097)	1:74:A:LEU:HG	1:22:A:LEU:H	18	0.1
(1,1079)	1:107:A:ASP:HB2	1:106:A:GLY:H	20	0.1
(1,1078)	1:81:A:LEU:HG	1:106:A:GLY:H	7	0.1
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	1	0.1
(1,1070)	1:30:A:ILE:HA	1:27:A:THR:H	12	0.1
(1,1029)	1:114:A:ALA:HB2	1:117:A:ASN:H	7	0.1
(1,1005)	1:70:A:PHE:HD2	1:70:A:PHE:H	4	0.1
(1,996)	1:70:A:PHE:HB2	1:73:A:ALA:H	9	0.1
(1,916)	1:84:A:GLY:HA3	1:84:A:GLY:H	13	0.1
(1,866)	1:22:A:LEU:HG	1:24:A:SER:H	1	0.1
(1,866)	1:22:A:LEU:HG	1:24:A:SER:H	16	0.1
(1,765)	1:114:A:ALA:HB3	1:115:A:MET:H	10	0.1
(1,765)	1:114:A:ALA:HB2	1:115:A:MET:H	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,684)	1:48:A:LEU:HD23	1:53:A:SER:H	20	0.1
(1,633)	1:34:A:ILE:HB	1:36:A:ALA:H	7	0.1
(1,571)	1:25:A:VAL:HA	1:25:A:VAL:H	5	0.1
(1,547)	1:39:A:ASP:HB2	1:42:A:GLU:H	13	0.1
(1,389)	1:118:A:ASN:HA	1:118:A:ASN:H	2	0.1
(1,380)	1:74:A:LEU:HD13	1:77:A:PHE:H	2	0.1
(1,360)	1:104:A:ASN:HB3	1:104:A:ASN:H	10	0.1
(1,334)	1:81:A:LEU:HB2	1:80:A:ALA:H	11	0.1
(1,272)	1:115:A:MET:H	1:116:A:GLN:H	6	0.1
(1,261)	1:22:A:LEU:HG	1:23:A:ALA:H	17	0.1
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	4	0.1
(1,257)	1:108:A:VAL:HB	1:112:A:ALA:H	17	0.1
(1,192)	1:108:A:VAL:HG13	1:82:A:ALA:H	13	0.1
(1,164)	1:133:A:ASP:HB3	1:133:A:ASP:H	13	0.1
(1,145)	1:19:A:GLN:HA	1:19:A:GLN:H	10	0.1
(1,109)	1:48:A:LEU:HD11	1:48:A:LEU:H	17	0.1
(1,86)	1:118:A:ASN:HA	1:119:A:ALA:H	14	0.1

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

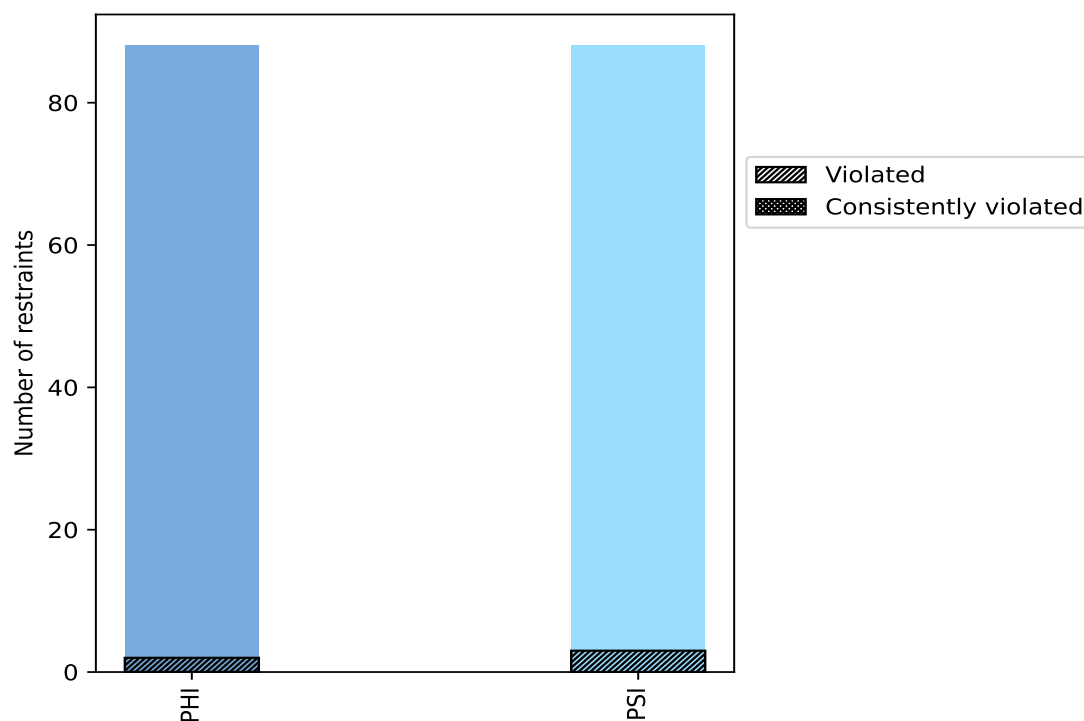
10.1 Summary of dihedral-angle violations [i](#)

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	88	50.0	2	2.3	1.1	0	0.0	0.0
PSI	88	50.0	3	3.4	1.7	0	0.0	0.0
Total	176	100.0	5	2.8	2.8	0	0.0	0.0

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

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



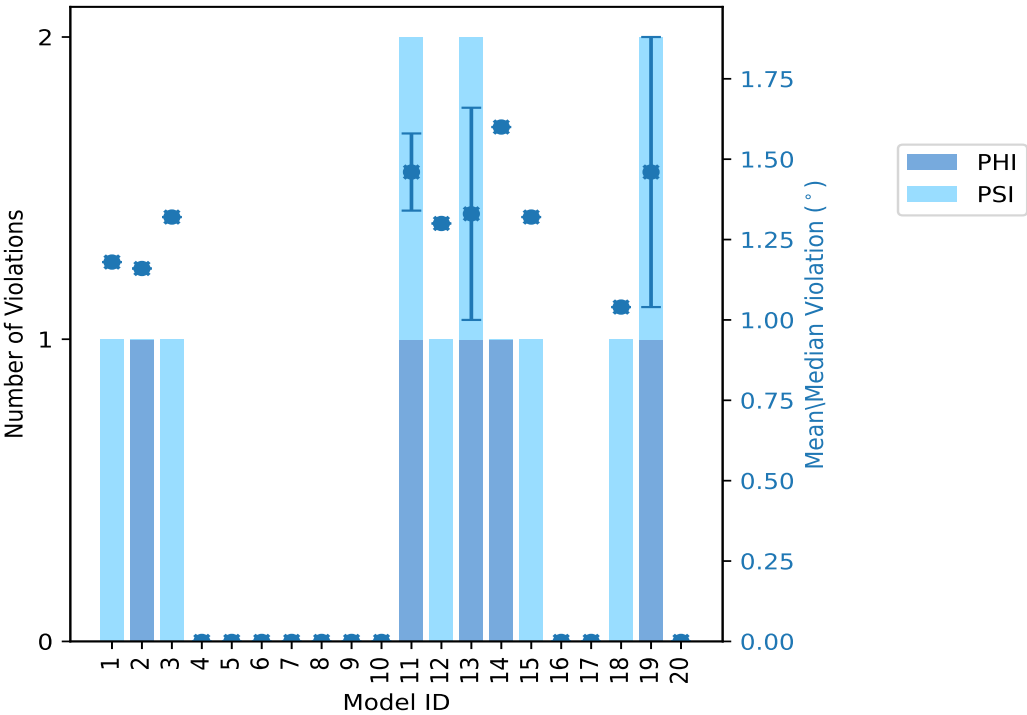
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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	0	1	1	1.18	1.18	0.0	1.18
2	1	0	1	1.16	1.16	0.0	1.16
3	0	1	1	1.32	1.32	0.0	1.32
4	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0.0	0.0	0.0	0.0
11	1	1	2	1.46	1.58	0.12	1.46
12	0	1	1	1.3	1.3	0.0	1.3
13	1	1	2	1.33	1.66	0.33	1.33
14	1	0	1	1.6	1.6	0.0	1.6
15	0	1	1	1.32	1.32	0.0	1.32
16	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0.0	0.0	0.0	0.0
18	0	1	1	1.04	1.04	0.0	1.04
19	1	1	2	1.46	1.88	0.42	1.46
20	0	0	0	0.0	0.0	0.0	0.0

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 ⓘ

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	%
1	2	3	1	5.0
0	0	0	2	10.0
0	0	0	3	15.0
1	0	1	4	20.0
0	0	0	5	25.0
0	1	1	6	30.0
0	0	0	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

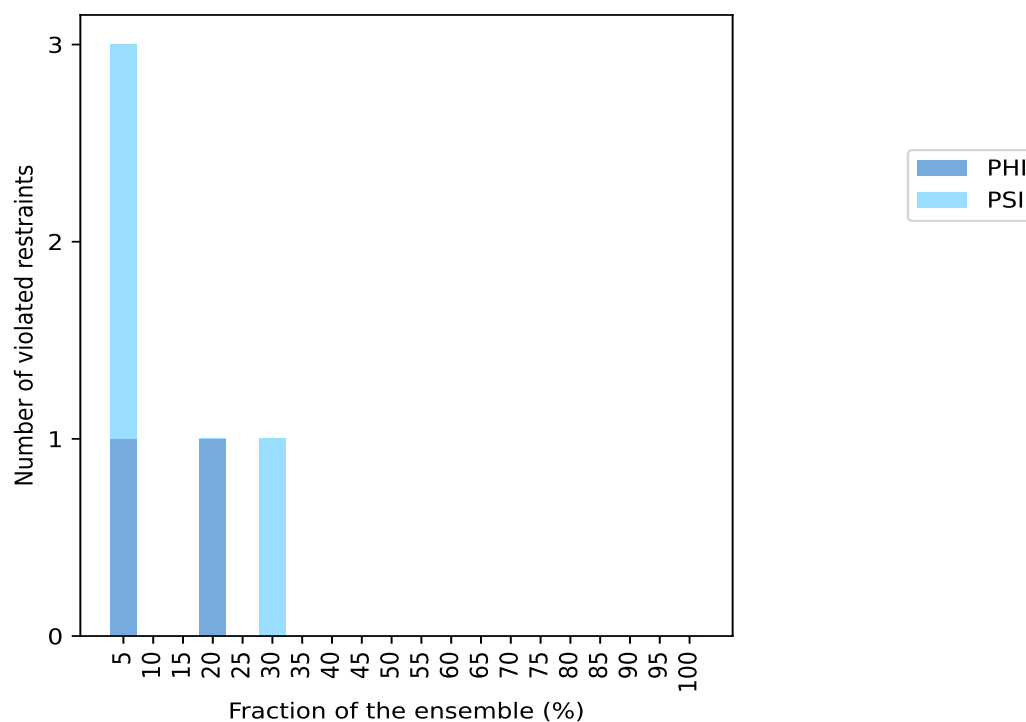
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

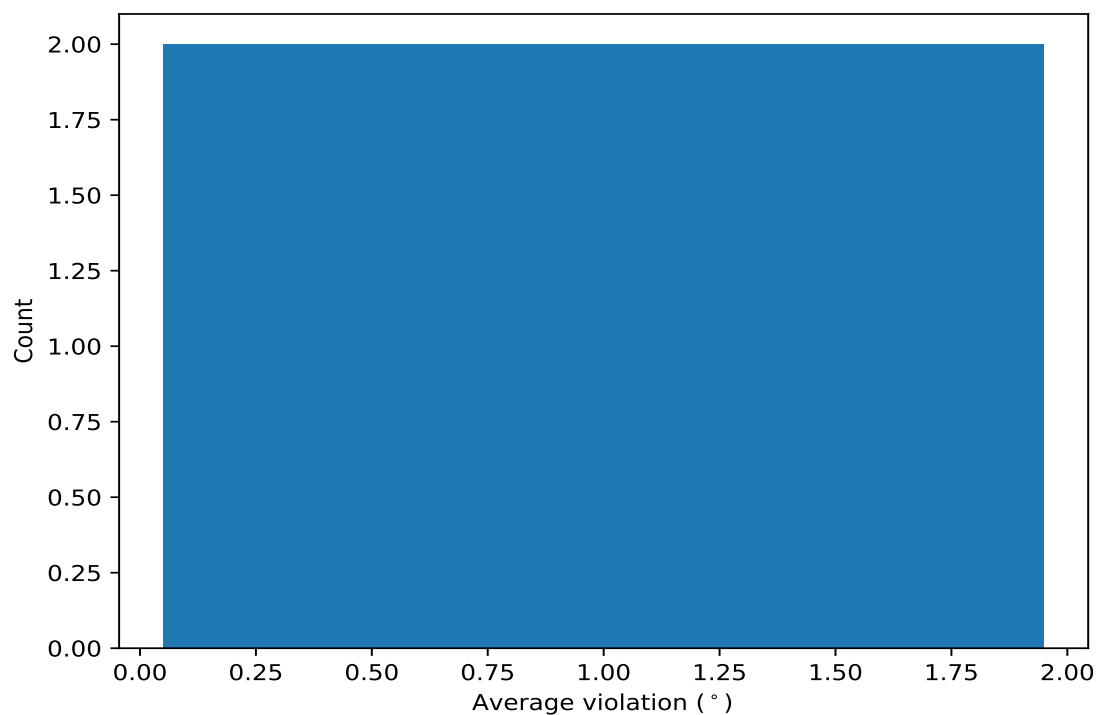


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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.

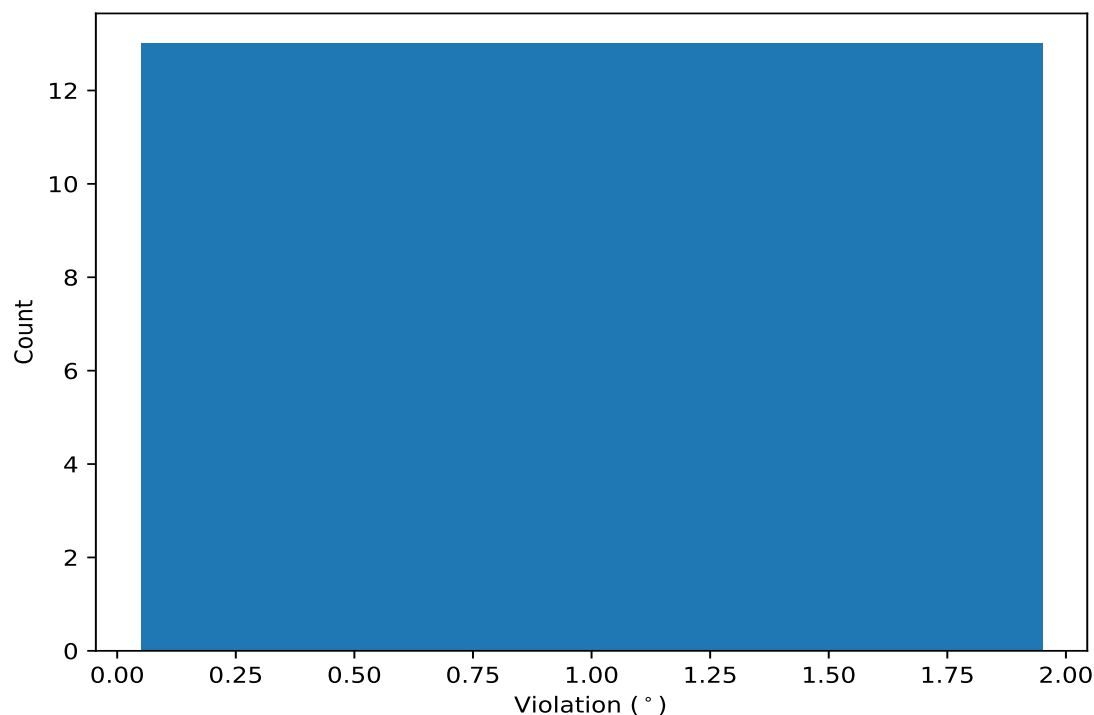
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,154)	1:105:A:LYS:N	1:105:A:LYS:CA	1:105:A:LYS:C	1:106:A:GLY:N	6	1.37	0.25	1.32
(1,49)	1:46:A:PRO:C	1:47:A:TYR:N	1:47:A:TYR:CA	1:47:A:TYR:C	4	1.5	0.2	1.59

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 (°)
(1,154)	1:105:A:LYS:N	1:105:A:LYS:CA	1:105:A:LYS:C	1:106:A:GLY:N	19	1.88
(1,49)	1:46:A:PRO:C	1:47:A:TYR:N	1:47:A:TYR:CA	1:47:A:TYR:C	13	1.66
(1,49)	1:46:A:PRO:C	1:47:A:TYR:N	1:47:A:TYR:CA	1:47:A:TYR:C	14	1.6
(1,49)	1:46:A:PRO:C	1:47:A:TYR:N	1:47:A:TYR:CA	1:47:A:TYR:C	11	1.58
(1,154)	1:105:A:LYS:N	1:105:A:LYS:CA	1:105:A:LYS:C	1:106:A:GLY:N	11	1.33
(1,154)	1:105:A:LYS:N	1:105:A:LYS:CA	1:105:A:LYS:C	1:106:A:GLY:N	3	1.32
(1,154)	1:105:A:LYS:N	1:105:A:LYS:CA	1:105:A:LYS:C	1:106:A:GLY:N	15	1.32
(1,154)	1:105:A:LYS:N	1:105:A:LYS:CA	1:105:A:LYS:C	1:106:A:GLY:N	12	1.3
(1,174)	1:115:A:MET:N	1:115:A:MET:CA	1:115:A:MET:C	1:116:A:GLN:N	1	1.18
(1,49)	1:46:A:PRO:C	1:47:A:TYR:N	1:47:A:TYR:CA	1:47:A:TYR:C	2	1.16
(1,154)	1:105:A:LYS:N	1:105:A:LYS:CA	1:105:A:LYS:C	1:106:A:GLY:N	18	1.04
(1,57)	1:50:A:SER:C	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	19	1.03
(1,58)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:GLU:N	13	1.0