



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 11:09 AM UTC

PDB ID : 9CCH / pdb_00009cch
BMRB ID : 16492
Title : Solution structure of the Bsu Anti-TRAP trimer
Authors : Foster, M.P.; McElroy, C.A.; Ihms, E.C.; Kumar Yadav, D.
Deposited on : 2024-06-21

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 : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
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, SOLUTION SCATTERING

The overall completeness of chemical shifts assignment is 31%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 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:2-A:53, B:2-B:53, C:2-C:53 (156)	0.42	13

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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2370 atoms, of which 1185 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Anti-TRAP regulator.

Mol	Chain	Residues	Atoms						Trace
1	A	53	Total	C	H	N	O	S	0
			789	246	395	65	78	5	
1	B	53	Total	C	H	N	O	S	0
			789	246	395	65	78	5	
1	C	53	Total	C	H	N	O	S	0
			789	246	395	65	78	5	

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

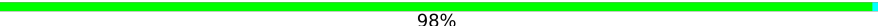
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1
2	B	1	Total	Zn
			1	1
2	C	1	Total	Zn
			1	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

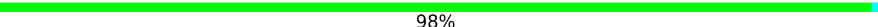
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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: Anti-TRAP regulator

Chain A:  98% .

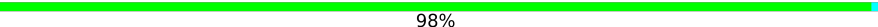


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



- Molecule 1: Anti-TRAP regulator

Chain C:  98% .

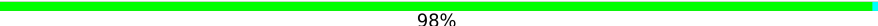


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

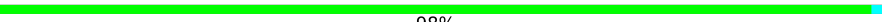
4.2.1 Score per residue for model 1

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

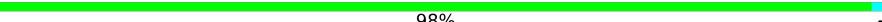


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



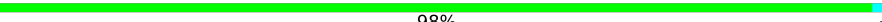
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



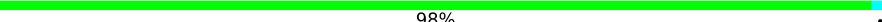
4.2.2 Score per residue for model 2

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

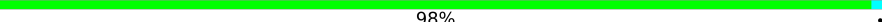


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



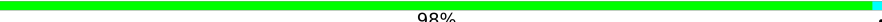
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



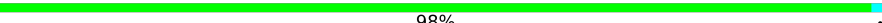
4.2.3 Score per residue for model 3

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

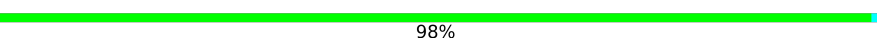


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



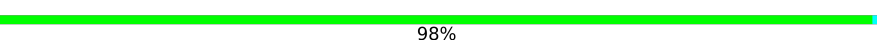
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



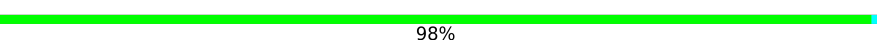
4.2.4 Score per residue for model 4

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

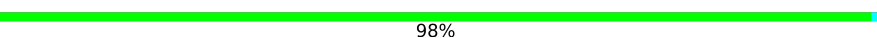


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



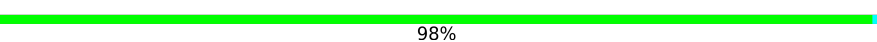
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



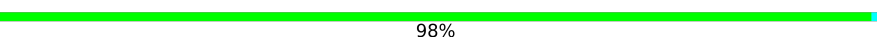
4.2.5 Score per residue for model 5

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

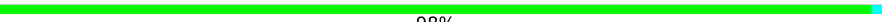


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



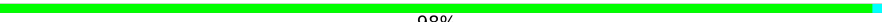
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



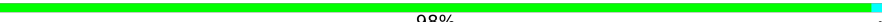
4.2.6 Score per residue for model 6

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

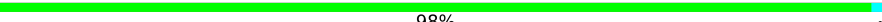


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



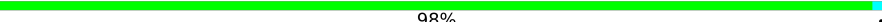
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



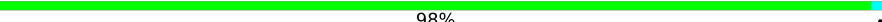
4.2.7 Score per residue for model 7

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

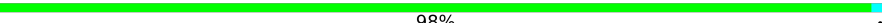


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



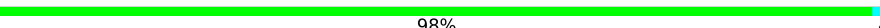
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



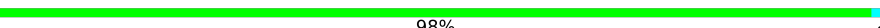
4.2.8 Score per residue for model 8

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

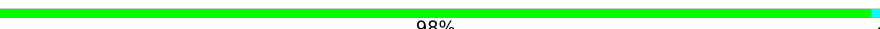


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



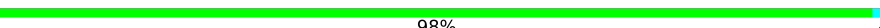
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



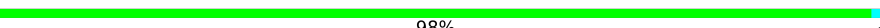
4.2.9 Score per residue for model 9

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

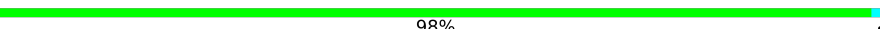


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



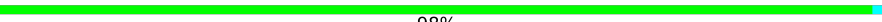
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



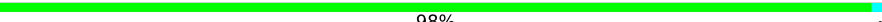
4.2.10 Score per residue for model 10

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

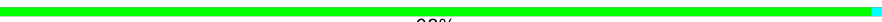


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



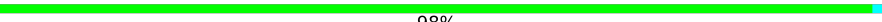
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



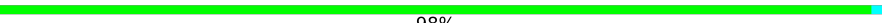
4.2.11 Score per residue for model 11

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

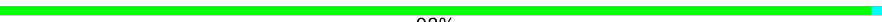


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



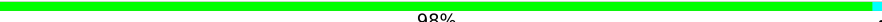
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



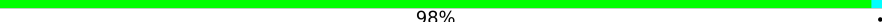
4.2.12 Score per residue for model 12

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

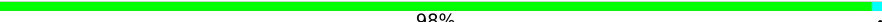


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



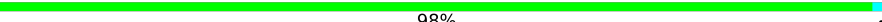
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



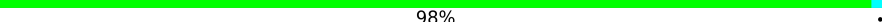
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

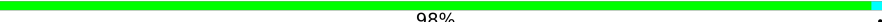


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



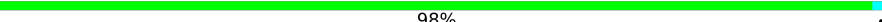
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



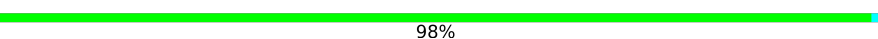
4.2.14 Score per residue for model 14

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

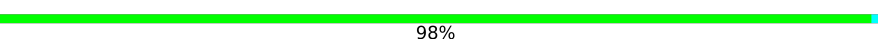


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



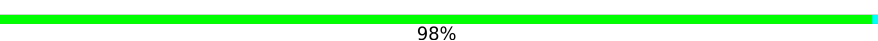
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



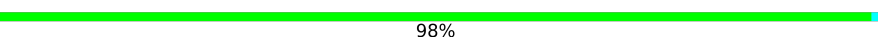
4.2.15 Score per residue for model 15

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

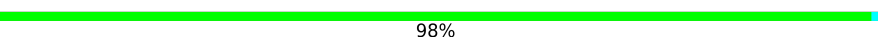


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



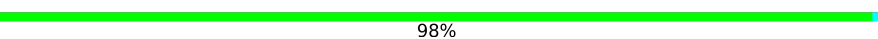
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



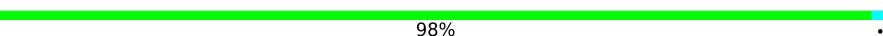
4.2.16 Score per residue for model 16

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

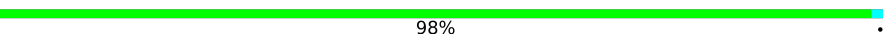


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



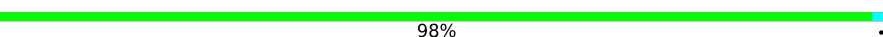
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



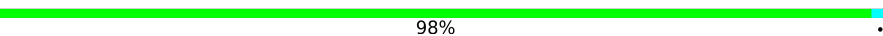
4.2.17 Score per residue for model 17

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

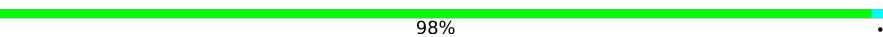


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



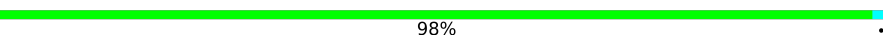
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



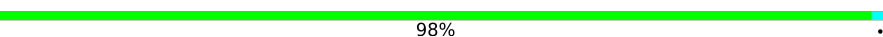
4.2.18 Score per residue for model 18

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

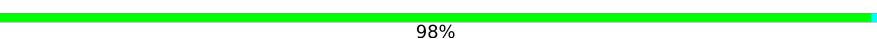


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



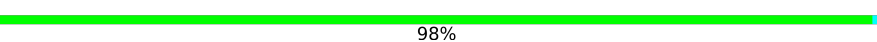
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



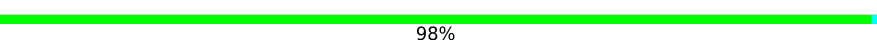
4.2.19 Score per residue for model 19

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

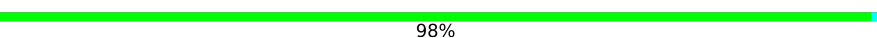


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



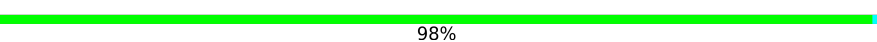
- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



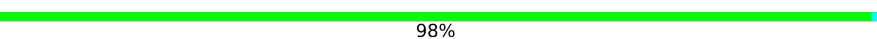
4.2.20 Score per residue for model 20

- Molecule 1: Anti-TRAP regulator

Chain A:  98% .

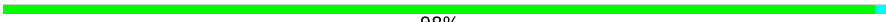


- Molecule 1: Anti-TRAP regulator

Chain B:  98% .



- Molecule 1: Anti-TRAP regulator

Chain C:  98% .



5 Refinement protocol and experimental data overview

The models were refined using the following method: *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
X-PLOR NIH	structure calculation	

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	629
Number of shifts mapped to atoms	629
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	31%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

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

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

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 31% for the well-defined parts and 31% 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	629
Number of shifts mapped to atoms	629
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	52	-0.63 ± 0.13	Should be applied
$^{13}\text{C}_\beta$	47	-0.27 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}'$	48	-0.18 ± 0.25	None needed (< 0.5 ppm)
^{15}N	49	0.69 ± 0.64	None needed (imprecise)

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 31%, i.e. 614 atoms were assigned a chemical shift out of a possible 1995. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	255/777 (33%)	106/318 (33%)	100/312 (32%)	49/147 (33%)
Sidechain	345/1137 (30%)	232/744 (31%)	110/363 (30%)	3/30 (10%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	14/81 (17%)	7/39 (18%)	7/36 (19%)	0/6 (0%)
Overall	614/1995 (31%)	345/1101 (31%)	217/711 (31%)	52/183 (28%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 31%, i.e. 614 atoms were assigned a chemical shift out of a possible 1995. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	255/777 (33%)	106/318 (33%)	100/312 (32%)	49/147 (33%)
Sidechain	345/1137 (30%)	232/744 (31%)	110/363 (30%)	3/30 (10%)
Aromatic	14/81 (17%)	7/39 (18%)	7/36 (19%)	0/6 (0%)
Overall	614/1995 (31%)	345/1101 (31%)	217/711 (31%)	52/183 (28%)

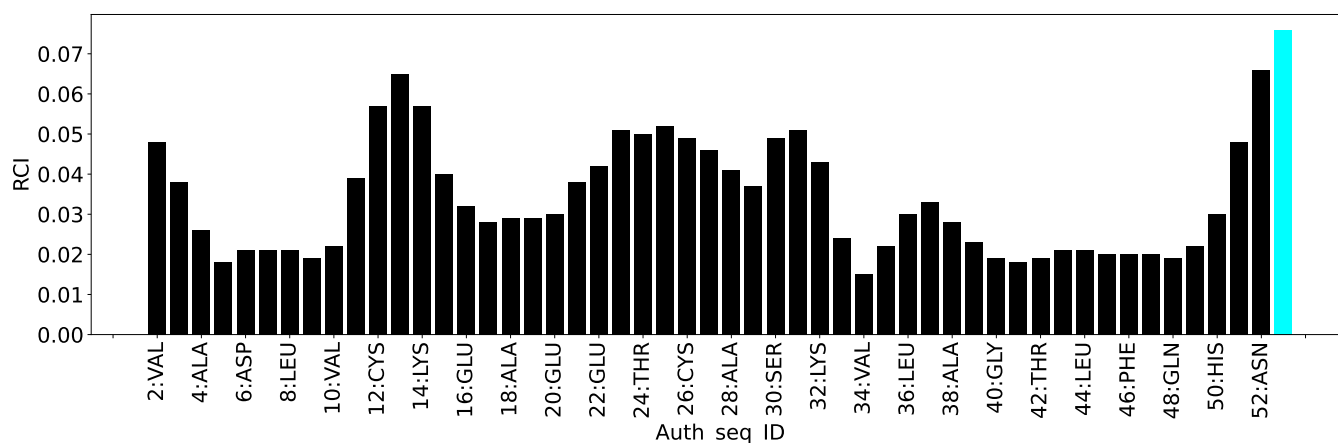
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



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	6897
Intra-residue ($ i-j =0$)	2154
Sequential ($ i-j =1$)	1730
Medium range ($ i-j >1$ and $ i-j <5$)	1303
Long range ($ i-j \geq 5$)	1183
Inter-chain	527
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	315
Number of unmapped restraints	0
Number of restraints per residue	44.5
Number of long range restraints per residue ¹	7.3

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)	68.2	0.2
0.2-0.5 (Medium)	42.3	0.5
>0.5 (Large)	33.9	1.74

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)	57.5	10.0
10.0-20.0 (Medium)	14.5	18.88
>20.0 (Large)	0.1	20.56

9 Distance violation analysis ⓘ

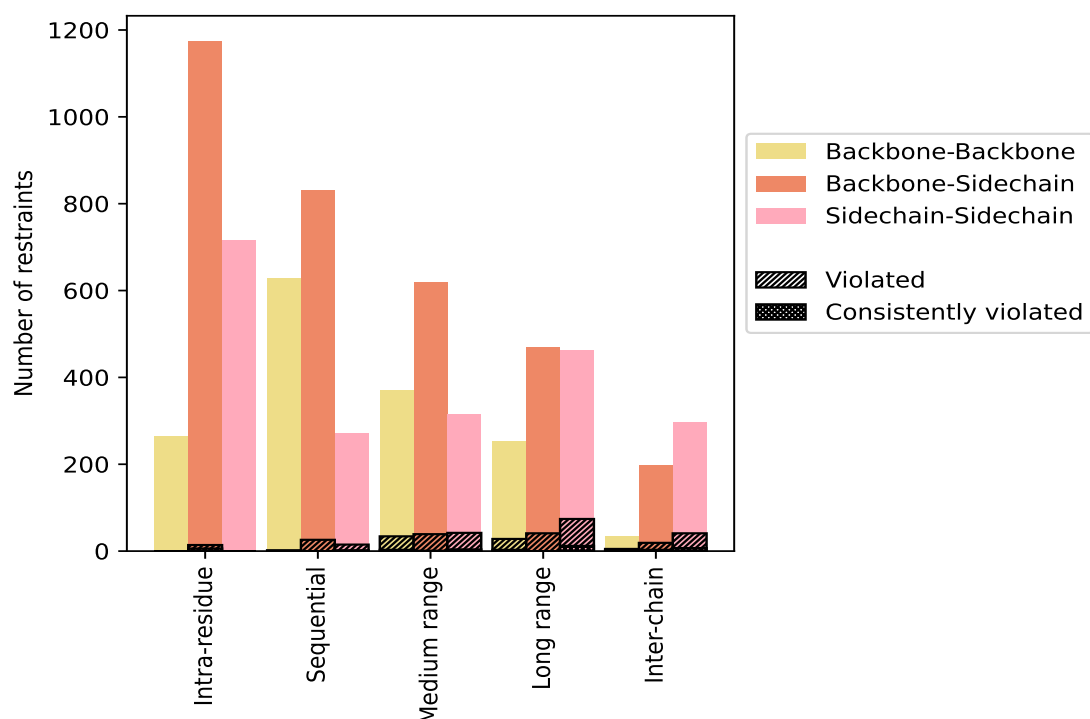
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	2154	31.2	14	0.6	0.2	6	0.3	0.1
Backbone-Backbone	264	3.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1174	17.0	14	1.2	0.2	6	0.5	0.1
Sidechain-Sidechain	716	10.4	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	1730	25.1	43	2.5	0.6	2	0.1	0.0
Backbone-Backbone	628	9.1	2	0.3	0.0	0	0.0	0.0
Backbone-Sidechain	830	12.0	26	3.1	0.4	0	0.0	0.0
Sidechain-Sidechain	272	3.9	15	5.5	0.2	2	0.7	0.0
Medium range ($i-j >1$ & $i-j <5$)	1303	18.9	115	8.8	1.7	8	0.6	0.1
Backbone-Backbone	369	5.4	34	9.2	0.5	3	0.8	0.0
Backbone-Sidechain	619	9.0	39	6.3	0.6	1	0.2	0.0
Sidechain-Sidechain	315	4.6	42	13.3	0.6	4	1.3	0.1
Long range ($i-j \geq 5$)	1183	17.2	143	12.1	2.1	15	1.3	0.2
Backbone-Backbone	252	3.7	28	11.1	0.4	3	1.2	0.0
Backbone-Sidechain	469	6.8	41	8.7	0.6	0	0.0	0.0
Sidechain-Sidechain	462	6.7	74	16.0	1.1	12	2.6	0.2
Inter-chain	527	7.6	65	12.3	0.9	13	2.5	0.2
Backbone-Backbone	33	0.5	5	15.2	0.1	3	9.1	0.0
Backbone-Sidechain	198	2.9	19	9.6	0.3	3	1.5	0.0
Sidechain-Sidechain	296	4.3	41	13.9	0.6	7	2.4	0.1
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	6897	100.0	380	5.5	5.5	44	0.6	0.6
Backbone-Backbone	1546	22.4	69	4.5	1.0	9	0.6	0.1
Backbone-Sidechain	3290	47.7	139	4.2	2.0	10	0.3	0.1
Sidechain-Sidechain	2061	29.9	172	8.3	2.5	25	1.2	0.4

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 disulfid 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	10	26	53	44	17	150	0.32	1.31	0.3	0.19
2	8	20	43	57	17	145	0.34	1.6	0.31	0.21
3	6	16	46	56	23	147	0.35	1.21	0.31	0.2
4	8	15	45	59	18	145	0.36	1.62	0.33	0.21
5	8	23	40	61	21	153	0.34	1.28	0.29	0.21
6	8	25	50	62	18	163	0.34	1.35	0.31	0.21
7	8	17	44	63	17	149	0.33	1.24	0.29	0.21
8	8	21	42	52	17	140	0.35	1.2	0.3	0.22
9	8	16	47	57	19	147	0.39	1.53	0.34	0.22
10	8	14	42	49	23	136	0.38	1.56	0.33	0.24

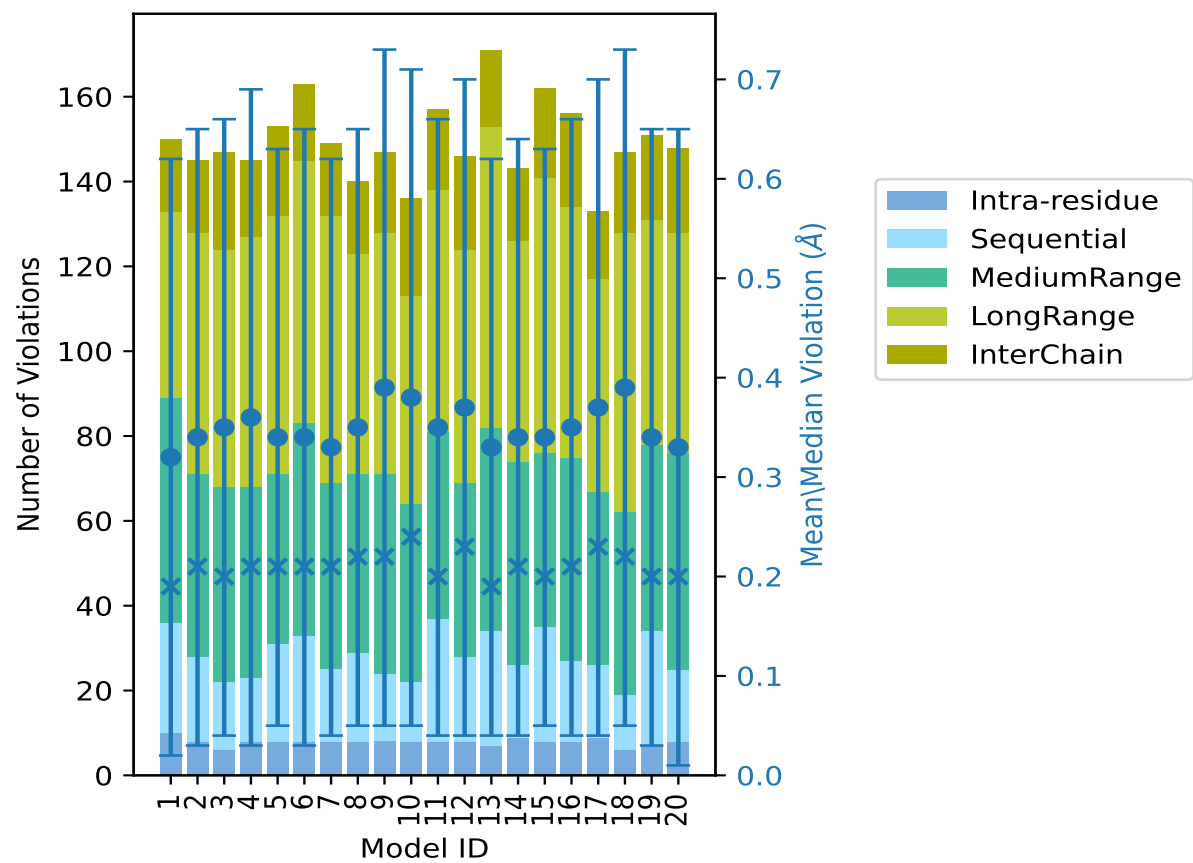
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	8	29	44	57	19	157	0.35	1.22	0.31	0.2
12	8	20	41	55	22	146	0.37	1.59	0.33	0.23
13	7	27	48	71	18	171	0.33	1.2	0.29	0.19
14	9	17	48	52	17	143	0.34	1.33	0.3	0.21
15	8	27	41	65	21	162	0.34	1.18	0.29	0.2
16	8	19	48	59	22	156	0.35	1.21	0.31	0.21
17	9	17	41	50	16	133	0.37	1.56	0.33	0.23
18	6	13	43	66	19	147	0.39	1.32	0.34	0.22
19	7	27	44	53	20	151	0.34	1.28	0.31	0.2
20	8	17	51	52	20	148	0.33	1.74	0.32	0.2

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

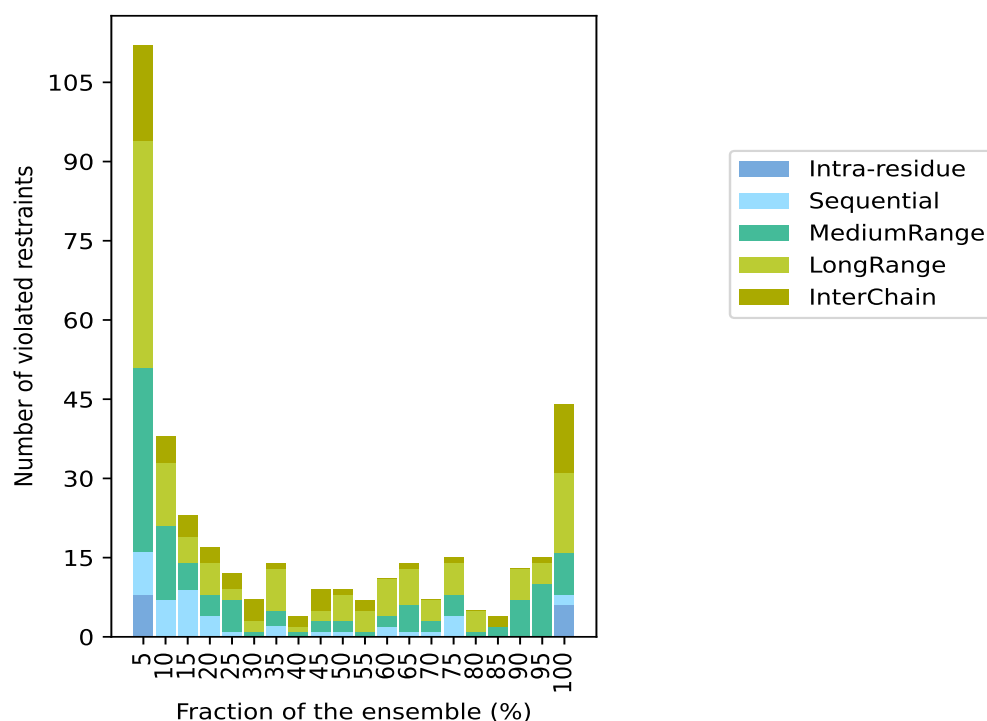
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 6517(IR:2140, SQ:1687, MR:1188, LR:1040, IC:462) restraints 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	%
8	8	35	43	18	112	1	5.0
0	7	14	12	5	38	2	10.0
0	9	5	5	4	23	3	15.0
0	4	4	6	3	17	4	20.0
0	1	6	2	3	12	5	25.0
0	0	1	2	4	7	6	30.0
0	2	3	8	1	14	7	35.0
0	0	1	1	2	4	8	40.0
0	1	2	2	4	9	9	45.0
0	1	2	5	1	9	10	50.0
0	0	1	4	2	7	11	55.0
0	2	2	7	0	11	12	60.0
0	1	5	7	1	14	13	65.0
0	1	2	4	0	7	14	70.0
0	4	4	6	1	15	15	75.0
0	0	1	4	0	5	16	80.0
0	0	2	0	2	4	17	85.0
0	0	7	6	0	13	18	90.0
0	0	10	4	1	15	19	95.0
6	2	8	15	13	44	20	100.0

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

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

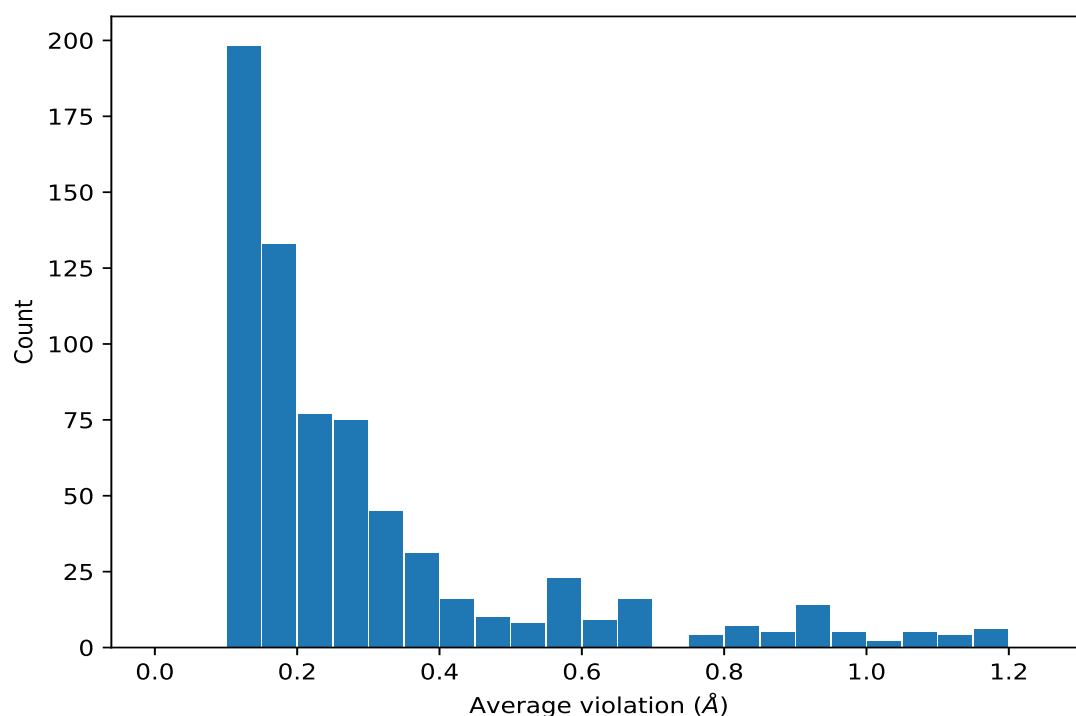
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	20	1.2	0.06	1.19
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	20	1.2	0.06	1.19
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	20	1.2	0.1	1.18
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	20	1.2	0.1	1.18
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	20	1.18	0.03	1.18
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	20	1.18	0.03	1.18
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	20	1.11	0.08	1.12
(2,277)	1:21:C:ILE:HB	1:13:C:PRO:HB2	20	1.11	0.08	1.12
(2,276)	1:21:B:ILE:HB	1:13:B:PRO:HB2	20	1.1	0.25	1.13
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	20	1.1	0.25	1.13
(2,275)	1:21:A:ILE:HB	1:13:A:PRO:HB2	20	1.09	0.2	1.13
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	20	1.09	0.2	1.13
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG3	20	0.95	0.34	1.04
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG2	20	0.95	0.34	1.04
(2,1161)	1:35:A:ILE:HG12	1:13:A:PRO:HG3	20	0.95	0.34	1.04
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG2	20	0.86	0.27	0.94

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG3	20	0.86	0.27	0.94
(2,1162)	1:35:B:ILE:HG13	1:13:B:PRO:HG3	20	0.86	0.27	0.94
(2,1162)	1:35:B:ILE:HG12	1:13:B:PRO:HG3	20	0.86	0.27	0.94
(2,1162)	1:35:B:ILE:HG13	1:16:B:GLU:HG3	20	0.86	0.27	0.94
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG2	20	0.85	0.44	0.68
(2,1163)	1:35:C:ILE:HG12	1:13:C:PRO:HG3	20	0.85	0.44	0.68
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG3	20	0.85	0.44	0.68
(2,1163)	1:35:C:ILE:HG13	1:13:C:PRO:HG3	20	0.85	0.44	0.68
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	20	0.84	0.02	0.84
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	20	0.81	0.1	0.84
(2,603)	1:50:A:HIS:HA	1:32:C:LYS:HD3	20	0.81	0.1	0.84
(2,604)	1:50:B:HIS:HA	1:32:A:LYS:HD3	20	0.77	0.14	0.81
(2,604)	1:50:B:HIS:HA	1:51:B:LEU:HB2	20	0.77	0.14	0.81
(2,604)	1:50:B:HIS:HA	1:32:A:LYS:HD2	20	0.77	0.14	0.81
(2,604)	1:50:B:HIS:HA	1:49:B:LYS:HB2	20	0.77	0.14	0.81
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	20	0.62	0.12	0.66
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	20	0.62	0.12	0.66
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	20	0.6	0.14	0.62
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	20	0.6	0.14	0.62
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	20	0.5	0.1	0.52
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	20	0.5	0.11	0.52
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	20	0.43	0.17	0.39
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	20	0.43	0.12	0.46
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA3	20	0.43	0.12	0.46
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	20	0.4	0.15	0.36
(2,380)	1:43:C:LEU:HG	1:43:A:LEU:HG	20	0.4	0.08	0.42
(2,380)	1:43:B:LEU:HG	1:43:C:LEU:HG	20	0.4	0.08	0.42
(2,380)	1:43:A:LEU:HG	1:43:B:LEU:HG	20	0.4	0.08	0.42
(2,1151)	1:43:C:LEU:HG	1:43:A:LEU:HG	20	0.4	0.08	0.42
(2,1151)	1:43:B:LEU:HG	1:43:C:LEU:HG	20	0.4	0.08	0.42
(2,1151)	1:43:A:LEU:HG	1:43:B:LEU:HG	20	0.4	0.08	0.42
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	20	0.39	0.08	0.36
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	20	0.37	0.05	0.38
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	20	0.29	0.08	0.26
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	20	0.29	0.08	0.26
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	20	0.27	0.07	0.27
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	20	0.27	0.07	0.27
(2,509)	1:43:C:LEU:HD23	1:43:C:LEU:HA	20	0.26	0.03	0.26
(2,509)	1:43:C:LEU:HD21	1:43:C:LEU:HA	20	0.26	0.03	0.26
(2,509)	1:43:C:LEU:HD22	1:43:C:LEU:HA	20	0.26	0.03	0.26
(2,509)	1:43:C:LEU:HD23	1:43:A:LEU:HA	20	0.26	0.03	0.26
(2,1322)	1:43:C:LEU:HD23	1:43:C:LEU:HA	20	0.26	0.03	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1322)	1:43:C:LEU:HD21	1:43:C:LEU:HA	20	0.26	0.03	0.26
(2,1322)	1:43:C:LEU:HD22	1:43:C:LEU:HA	20	0.26	0.03	0.26
(2,1322)	1:43:C:LEU:HD23	1:43:A:LEU:HA	20	0.26	0.03	0.26
(2,507)	1:43:A:LEU:HD22	1:43:A:LEU:HA	20	0.25	0.02	0.25
(2,507)	1:43:A:LEU:HD23	1:43:A:LEU:HA	20	0.25	0.02	0.25
(2,507)	1:43:A:LEU:HD21	1:43:A:LEU:HA	20	0.25	0.02	0.25
(2,1320)	1:43:A:LEU:HD22	1:43:A:LEU:HA	20	0.25	0.02	0.25
(2,1320)	1:43:A:LEU:HD23	1:43:A:LEU:HA	20	0.25	0.02	0.25
(2,1320)	1:43:A:LEU:HD21	1:43:A:LEU:HA	20	0.25	0.02	0.25
(2,508)	1:43:B:LEU:HD21	1:43:B:LEU:HA	20	0.25	0.04	0.26
(2,508)	1:43:B:LEU:HD23	1:43:B:LEU:HA	20	0.25	0.04	0.26
(2,508)	1:43:B:LEU:HD21	1:43:C:LEU:HA	20	0.25	0.04	0.26
(2,508)	1:43:B:LEU:HD22	1:43:B:LEU:HA	20	0.25	0.04	0.26
(2,1321)	1:43:B:LEU:HD21	1:43:B:LEU:HA	20	0.25	0.04	0.26
(2,1321)	1:43:B:LEU:HD23	1:43:B:LEU:HA	20	0.25	0.04	0.26
(2,1321)	1:43:B:LEU:HD21	1:43:C:LEU:HA	20	0.25	0.04	0.26
(2,1321)	1:43:B:LEU:HD22	1:43:B:LEU:HA	20	0.25	0.04	0.26
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	20	0.23	0.08	0.2
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	20	0.23	0.08	0.2
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	20	0.2	0.18	0.16
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	20	0.2	0.05	0.2
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	20	0.2	0.05	0.2
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	20	0.2	0.05	0.2
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	20	0.2	0.04	0.2
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	20	0.2	0.04	0.2
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	20	0.2	0.04	0.2
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	20	0.18	0.04	0.18
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	20	0.18	0.04	0.18
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	20	0.18	0.04	0.18
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	20	0.17	0.04	0.16
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	20	0.17	0.04	0.16
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	20	0.17	0.02	0.17
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	20	0.17	0.02	0.16
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	20	0.16	0.03	0.15
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG23	19	0.98	0.16	0.96
(2,1193)	1:27:C:PRO:HG3	1:21:C:ILE:HG23	19	0.98	0.16	0.96
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG21	19	0.98	0.16	0.96
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG22	19	0.98	0.16	0.96
(2,1193)	1:27:C:PRO:HG3	1:21:C:ILE:HG21	19	0.98	0.16	0.96
(2,1192)	1:27:B:PRO:HG3	1:21:B:ILE:HG23	19	0.93	0.27	0.97
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	19	0.93	0.27	0.97
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG23	19	0.93	0.27	0.97

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1192)	1:27:B:PRO:HG3	1:21:B:ILE:HG21	19	0.93	0.27	0.97
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG21	19	0.93	0.27	0.97
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD12	19	0.68	0.1	0.68
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD11	19	0.68	0.1	0.68
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD13	19	0.68	0.1	0.68
(2,401)	1:27:C:PRO:HG2	1:21:C:ILE:HG23	19	0.68	0.1	0.68
(2,401)	1:27:C:PRO:HG2	1:21:C:ILE:HG21	19	0.68	0.1	0.68
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD11	19	0.67	0.18	0.72
(2,400)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	19	0.67	0.18	0.72
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD13	19	0.67	0.18	0.72
(2,400)	1:27:B:PRO:HG3	1:21:B:ILE:HG21	19	0.67	0.18	0.72
(2,400)	1:27:B:PRO:HG2	1:21:B:ILE:HG21	19	0.67	0.18	0.72
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD12	19	0.67	0.18	0.72
(2,700)	1:15:C:CYS:HA	1:16:C:GLU:HB2	19	0.56	0.06	0.57
(2,700)	1:15:C:CYS:HA	1:12:C:CYS:HB3	19	0.56	0.06	0.57
(2,1409)	1:15:C:CYS:HA	1:16:C:GLU:HB2	19	0.56	0.06	0.57
(2,1409)	1:15:C:CYS:HA	1:12:C:CYS:HB3	19	0.56	0.06	0.57
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	19	0.2	0.03	0.2
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	19	0.2	0.03	0.2
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	19	0.2	0.03	0.2
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	19	0.2	0.08	0.18
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	19	0.2	0.08	0.18
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	19	0.2	0.02	0.2
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	19	0.2	0.02	0.2
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	19	0.2	0.02	0.2
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	19	0.18	0.03	0.18
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	19	0.18	0.05	0.17
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	19	0.17	0.03	0.17
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	19	0.17	0.03	0.17
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	19	0.17	0.03	0.17
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	19	0.16	0.03	0.16
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	19	0.16	0.03	0.16
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG21	18	0.95	0.1	0.94
(2,1191)	1:27:A:PRO:HG3	1:21:A:ILE:HG23	18	0.95	0.1	0.94
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG23	18	0.95	0.1	0.94
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG22	18	0.95	0.1	0.94
(2,1191)	1:27:A:PRO:HG3	1:21:A:ILE:HG22	18	0.95	0.1	0.94
(2,1191)	1:27:A:PRO:HG3	1:21:A:ILE:HG21	18	0.95	0.1	0.94
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD11	18	0.67	0.08	0.66
(2,399)	1:27:A:PRO:HG2	1:21:A:ILE:HG23	18	0.67	0.08	0.66
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD12	18	0.67	0.08	0.66
(2,399)	1:27:A:PRO:HG2	1:21:A:ILE:HG22	18	0.67	0.08	0.66

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD13	18	0.67	0.08	0.66
(2,698)	1:15:A:CYS:HA	1:12:A:CYS:HB3	18	0.57	0.07	0.6
(2,698)	1:15:A:CYS:HA	1:16:A:GLU:HB2	18	0.57	0.07	0.6
(2,1407)	1:15:A:CYS:HA	1:12:A:CYS:HB3	18	0.57	0.07	0.6
(2,1407)	1:15:A:CYS:HA	1:16:A:GLU:HB2	18	0.57	0.07	0.6
(2,699)	1:15:B:CYS:HA	1:16:B:GLU:HB2	18	0.55	0.07	0.56
(2,699)	1:15:B:CYS:HA	1:12:B:CYS:HB3	18	0.55	0.07	0.56
(2,1408)	1:15:B:CYS:HA	1:16:B:GLU:HB2	18	0.55	0.07	0.56
(2,1408)	1:15:B:CYS:HA	1:12:B:CYS:HB3	18	0.55	0.07	0.56
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG3	18	0.46	0.14	0.55
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG2	18	0.46	0.14	0.55
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG2	18	0.45	0.16	0.54
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG3	18	0.45	0.16	0.54
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	18	0.2	0.02	0.2
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	18	0.2	0.03	0.2
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	18	0.2	0.03	0.2
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	18	0.14	0.03	0.14
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	18	0.14	0.03	0.14
(2,484)	1:51:B:LEU:HD12	1:47:A:ILE:HB	17	0.32	0.14	0.28
(2,484)	1:51:B:LEU:HD13	1:47:A:ILE:HB	17	0.32	0.14	0.28
(2,484)	1:51:B:LEU:HD12	1:48:A:GLN:HB3	17	0.32	0.14	0.28
(2,484)	1:51:B:LEU:HD11	1:47:A:ILE:HB	17	0.32	0.14	0.28
(2,484)	1:51:B:LEU:HD13	1:48:A:GLN:HB3	17	0.32	0.14	0.28
(2,485)	1:51:C:LEU:HD12	1:47:B:ILE:HB	17	0.29	0.14	0.26
(2,485)	1:51:C:LEU:HD11	1:48:B:GLN:HB3	17	0.29	0.14	0.26
(2,485)	1:51:C:LEU:HD13	1:47:B:ILE:HB	17	0.29	0.14	0.26
(2,485)	1:51:C:LEU:HD11	1:47:B:ILE:HB	17	0.29	0.14	0.26
(2,485)	1:51:C:LEU:HD12	1:48:B:GLN:HB3	17	0.29	0.14	0.26
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	17	0.13	0.02	0.13
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	17	0.13	0.02	0.13
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	16	0.26	0.09	0.29
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	16	0.26	0.09	0.29
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	16	0.26	0.09	0.29
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	16	0.21	0.04	0.21
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	16	0.21	0.04	0.21
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	16	0.21	0.04	0.21
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	16	0.18	0.04	0.18
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	16	0.18	0.04	0.18
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	16	0.18	0.04	0.18
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	16	0.18	0.04	0.18
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	16	0.16	0.05	0.15
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	16	0.12	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,250)	1:14:C:LYS:HE2	1:22:C:GLU:HB2	15	0.5	0.21	0.44
(2,250)	1:14:C:LYS:HE3	1:22:C:GLU:HB2	15	0.5	0.21	0.44
(2,250)	1:14:C:LYS:HE3	1:20:C:GLU:HG3	15	0.5	0.21	0.44
(2,250)	1:14:C:LYS:HE3	1:20:C:GLU:HG2	15	0.5	0.21	0.44
(2,470)	1:43:C:LEU:HD12	1:8:C:LEU:HD21	15	0.36	0.2	0.27
(2,470)	1:43:C:LEU:HD12	1:8:B:LEU:HD21	15	0.36	0.2	0.27
(2,470)	1:43:C:LEU:HD13	1:8:C:LEU:HD21	15	0.36	0.2	0.27
(2,470)	1:43:C:LEU:HD12	1:8:C:LEU:HD22	15	0.36	0.2	0.27
(2,470)	1:43:C:LEU:HD11	1:8:C:LEU:HD22	15	0.36	0.2	0.27
(2,470)	1:43:C:LEU:HD11	1:8:C:LEU:HD21	15	0.36	0.2	0.27
(2,470)	1:43:C:LEU:HD12	1:8:C:LEU:HD23	15	0.36	0.2	0.27
(2,470)	1:43:C:LEU:HD13	1:8:B:LEU:HD22	15	0.36	0.2	0.27
(2,470)	1:43:C:LEU:HD13	1:8:C:LEU:HD23	15	0.36	0.2	0.27
(2,470)	1:43:C:LEU:HD12	1:8:B:LEU:HD23	15	0.36	0.2	0.27
(2,1556)	1:43:C:LEU:HD12	1:8:C:LEU:HD21	15	0.36	0.2	0.27
(2,1556)	1:43:C:LEU:HD12	1:8:B:LEU:HD21	15	0.36	0.2	0.27
(2,1556)	1:43:C:LEU:HD13	1:8:C:LEU:HD21	15	0.36	0.2	0.27
(2,1556)	1:43:C:LEU:HD12	1:8:C:LEU:HD22	15	0.36	0.2	0.27
(2,1556)	1:43:C:LEU:HD11	1:8:C:LEU:HD22	15	0.36	0.2	0.27
(2,1556)	1:43:C:LEU:HD11	1:8:C:LEU:HD21	15	0.36	0.2	0.27
(2,1556)	1:43:C:LEU:HD12	1:8:C:LEU:HD23	15	0.36	0.2	0.27
(2,1556)	1:43:C:LEU:HD13	1:8:B:LEU:HD22	15	0.36	0.2	0.27
(2,1556)	1:43:C:LEU:HD13	1:8:C:LEU:HD23	15	0.36	0.2	0.27
(2,1556)	1:43:C:LEU:HD12	1:8:B:LEU:HD23	15	0.36	0.2	0.27
(2,483)	1:51:A:LEU:HD12	1:47:C:ILE:HB	15	0.32	0.16	0.31
(2,483)	1:51:A:LEU:HD11	1:47:C:ILE:HB	15	0.32	0.16	0.31
(2,483)	1:51:A:LEU:HD13	1:48:C:GLN:HB3	15	0.32	0.16	0.31
(2,483)	1:51:A:LEU:HD13	1:47:C:ILE:HB	15	0.32	0.16	0.31
(2,483)	1:51:A:LEU:HD11	1:48:C:GLN:HB3	15	0.32	0.16	0.31
(2,483)	1:51:A:LEU:HD12	1:48:C:GLN:HB3	15	0.32	0.16	0.31
(1,338)	1:10:A:VAL:HG11	1:36:A:LEU:HA	15	0.26	0.08	0.28
(1,338)	1:10:A:VAL:HG12	1:36:A:LEU:HA	15	0.26	0.08	0.28
(1,338)	1:10:A:VAL:HG13	1:36:A:LEU:HA	15	0.26	0.08	0.28
(1,2955)	1:37:B:THR:HG21	1:8:B:LEU:HG	15	0.21	0.04	0.21
(1,2955)	1:37:B:THR:HG22	1:8:B:LEU:HG	15	0.21	0.04	0.21
(1,2955)	1:37:B:THR:HG23	1:8:B:LEU:HG	15	0.21	0.04	0.21
(2,60)	1:3:B:ILE:H	1:1:B:FME:HB3	15	0.18	0.06	0.19
(2,60)	1:3:B:ILE:H	1:2:B:VAL:HB	15	0.18	0.06	0.19
(1,3801)	1:8:C:LEU:HD11	1:39:C:GLN:HB2	15	0.14	0.03	0.13
(1,3801)	1:8:C:LEU:HD12	1:39:C:GLN:HB2	15	0.14	0.03	0.13
(1,3801)	1:8:C:LEU:HD13	1:39:C:GLN:HB2	15	0.14	0.03	0.13
(1,3432)	1:49:B:LYS:H	1:53:B:LYS:H	15	0.13	0.03	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3555)	1:53:B:LYS:H	1:49:B:LYS:H	15	0.13	0.03	0.13
(1,3299)	1:46:B:PHE:H	1:48:B:GLN:HB3	15	0.13	0.02	0.12
(1,712)	1:23:A:GLY:HA2	1:24:A:THR:HB	15	0.13	0.02	0.12
(1,712)	1:23:A:GLY:HA3	1:24:A:THR:HB	15	0.13	0.02	0.12
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA2	15	0.13	0.02	0.12
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA3	15	0.13	0.02	0.12
(1,2500)	1:23:B:GLY:HA2	1:24:B:THR:HB	15	0.13	0.02	0.12
(1,2500)	1:23:B:GLY:HA3	1:24:B:THR:HB	15	0.13	0.02	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA2	15	0.13	0.02	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA3	15	0.13	0.02	0.12
(1,3888)	1:10:C:VAL:HG11	1:36:C:LEU:HA	14	0.26	0.08	0.26
(1,3888)	1:10:C:VAL:HG12	1:36:C:LEU:HA	14	0.26	0.08	0.26
(1,3888)	1:10:C:VAL:HG13	1:36:C:LEU:HA	14	0.26	0.08	0.26
(2,868)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	14	0.23	0.14	0.2
(2,868)	1:31:A:GLY:HA2	1:15:A:CYS:HB3	14	0.23	0.14	0.2
(2,871)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	14	0.23	0.14	0.2
(2,871)	1:31:A:GLY:HA2	1:15:A:CYS:HB3	14	0.23	0.14	0.2
(1,4193)	1:21:C:ILE:HD11	1:15:C:CYS:HA	14	0.16	0.04	0.18
(1,4193)	1:21:C:ILE:HD12	1:15:C:CYS:HA	14	0.16	0.04	0.18
(1,4193)	1:21:C:ILE:HD13	1:15:C:CYS:HA	14	0.16	0.04	0.18
(1,2908)	1:36:B:LEU:HD11	1:35:B:ILE:HA	14	0.15	0.02	0.15
(1,2908)	1:36:B:LEU:HD12	1:35:B:ILE:HA	14	0.15	0.02	0.15
(1,2908)	1:36:B:LEU:HD13	1:35:B:ILE:HA	14	0.15	0.02	0.15
(1,1263)	1:40:A:GLY:H	1:43:A:LEU:HB3	14	0.14	0.02	0.15
(1,5057)	1:46:C:PHE:H	1:48:C:GLN:HB3	14	0.13	0.02	0.13
(2,1327)	1:30:B:SER:HB3	1:32:B:LYS:HD3	13	0.38	0.28	0.29
(2,1327)	1:30:B:SER:HB2	1:32:B:LYS:HG3	13	0.38	0.28	0.29
(2,1327)	1:30:B:SER:HB3	1:32:B:LYS:HG3	13	0.38	0.28	0.29
(1,1672)	1:49:A:LYS:H	1:53:A:LYS:H	13	0.26	0.31	0.13
(1,1800)	1:53:A:LYS:H	1:49:A:LYS:H	13	0.26	0.31	0.13
(1,4713)	1:37:C:THR:HG21	1:8:C:LEU:HG	13	0.19	0.05	0.17
(1,4713)	1:37:C:THR:HG22	1:8:C:LEU:HG	13	0.19	0.05	0.17
(1,4713)	1:37:C:THR:HG23	1:8:C:LEU:HG	13	0.19	0.05	0.17
(2,869)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	13	0.18	0.05	0.19
(2,869)	1:31:B:GLY:HA2	1:15:B:CYS:HB3	13	0.18	0.05	0.19
(2,872)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	13	0.18	0.05	0.19
(2,872)	1:31:B:GLY:HA2	1:15:B:CYS:HB3	13	0.18	0.05	0.19
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG12	13	0.18	0.04	0.19
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG13	13	0.18	0.04	0.19
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG12	13	0.18	0.04	0.19
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG13	13	0.18	0.04	0.19
(1,2435)	1:21:B:ILE:HD11	1:15:B:CYS:HA	13	0.17	0.06	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2435)	1:21:B:ILE:HD12	1:15:B:CYS:HA	13	0.17	0.06	0.13
(1,2435)	1:21:B:ILE:HD13	1:15:B:CYS:HA	13	0.17	0.06	0.13
(1,369)	1:11:A:ALA:HA	1:35:A:ILE:HA	13	0.16	0.04	0.16
(1,1052)	1:35:A:ILE:HA	1:11:A:ALA:HA	13	0.16	0.04	0.16
(1,4666)	1:36:C:LEU:HD11	1:35:C:ILE:HA	13	0.14	0.01	0.14
(1,4666)	1:36:C:LEU:HD12	1:35:C:ILE:HA	13	0.14	0.01	0.14
(1,4666)	1:36:C:LEU:HD13	1:35:C:ILE:HA	13	0.14	0.01	0.14
(1,4797)	1:40:C:GLY:H	1:43:C:LEU:HB3	13	0.14	0.02	0.14
(1,3039)	1:40:B:GLY:H	1:43:B:LEU:HB3	13	0.13	0.03	0.13
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB2	13	0.13	0.02	0.12
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB3	13	0.13	0.02	0.12
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB2	13	0.13	0.02	0.12
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB3	13	0.13	0.02	0.12
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB2	13	0.13	0.02	0.12
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB3	13	0.13	0.02	0.12
(2,469)	1:43:B:LEU:HD11	1:8:B:LEU:HD21	12	0.32	0.12	0.36
(2,469)	1:43:B:LEU:HD13	1:8:B:LEU:HD23	12	0.32	0.12	0.36
(2,469)	1:43:B:LEU:HD11	1:8:B:LEU:HD22	12	0.32	0.12	0.36
(2,469)	1:43:B:LEU:HD11	1:8:B:LEU:HD23	12	0.32	0.12	0.36
(2,469)	1:43:B:LEU:HD12	1:8:B:LEU:HD22	12	0.32	0.12	0.36
(2,469)	1:43:B:LEU:HD11	1:8:A:LEU:HD21	12	0.32	0.12	0.36
(2,469)	1:43:B:LEU:HD13	1:8:B:LEU:HD22	12	0.32	0.12	0.36
(2,469)	1:43:B:LEU:HD12	1:8:B:LEU:HD23	12	0.32	0.12	0.36
(2,469)	1:43:B:LEU:HD12	1:8:A:LEU:HD21	12	0.32	0.12	0.36
(2,1555)	1:43:B:LEU:HD11	1:8:B:LEU:HD21	12	0.32	0.12	0.36
(2,1555)	1:43:B:LEU:HD13	1:8:B:LEU:HD23	12	0.32	0.12	0.36
(2,1555)	1:43:B:LEU:HD11	1:8:B:LEU:HD22	12	0.32	0.12	0.36
(2,1555)	1:43:B:LEU:HD11	1:8:B:LEU:HD23	12	0.32	0.12	0.36
(2,1555)	1:43:B:LEU:HD12	1:8:B:LEU:HD22	12	0.32	0.12	0.36
(2,1555)	1:43:B:LEU:HD11	1:8:A:LEU:HD21	12	0.32	0.12	0.36
(2,1555)	1:43:B:LEU:HD13	1:8:B:LEU:HD22	12	0.32	0.12	0.36
(2,1555)	1:43:B:LEU:HD12	1:8:B:LEU:HD23	12	0.32	0.12	0.36
(2,1555)	1:43:B:LEU:HD12	1:8:A:LEU:HD21	12	0.32	0.12	0.36
(2,264)	1:49:B:LYS:HE2	1:53:B:LYS:HB3	12	0.24	0.09	0.26
(2,264)	1:49:B:LYS:HE2	1:53:B:LYS:HD2	12	0.24	0.09	0.26
(1,498)	1:16:A:GLU:H	1:33:A:GLY:H	12	0.23	0.08	0.2
(1,2290)	1:16:B:GLU:H	1:33:B:GLY:H	12	0.22	0.07	0.2
(2,61)	1:3:C:ILE:H	1:2:C:VAL:HB	12	0.18	0.07	0.12
(2,61)	1:3:C:ILE:H	1:1:C:FME:HB3	12	0.18	0.07	0.12
(1,2160)	1:11:B:ALA:HA	1:35:B:ILE:HA	12	0.14	0.03	0.14
(1,2831)	1:35:B:ILE:HA	1:11:B:ALA:HA	12	0.14	0.03	0.14
(1,2044)	1:8:B:LEU:HD11	1:39:B:GLN:HB2	12	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2044)	1:8:B:LEU:HD12	1:39:B:GLN:HB2	12	0.13	0.02	0.12
(1,2044)	1:8:B:LEU:HD13	1:39:B:GLN:HB2	12	0.13	0.02	0.12
(1,4258)	1:23:C:GLY:HA2	1:24:C:THR:HB	12	0.12	0.02	0.12
(1,4258)	1:23:C:GLY:HA3	1:24:C:THR:HB	12	0.12	0.02	0.12
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA2	12	0.12	0.02	0.12
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA3	12	0.12	0.02	0.12
(2,249)	1:14:B:LYS:HE2	1:22:B:GLU:HB2	11	0.49	0.22	0.42
(2,249)	1:14:B:LYS:HE3	1:22:B:GLU:HB2	11	0.49	0.22	0.42
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG12	11	0.16	0.04	0.17
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG13	11	0.16	0.04	0.17
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG12	11	0.16	0.04	0.17
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG13	11	0.16	0.04	0.17
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD2	11	0.16	0.05	0.14
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD3	11	0.16	0.05	0.14
(1,3949)	1:12:C:CYS:H	1:34:C:VAL:HB	11	0.15	0.04	0.15
(1,3107)	1:42:B:THR:HB	1:3:A:ILE:HB	11	0.14	0.03	0.12
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB2	11	0.13	0.03	0.12
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB3	11	0.13	0.03	0.12
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB2	11	0.13	0.03	0.12
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB3	11	0.13	0.03	0.12
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB2	11	0.13	0.03	0.12
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB3	11	0.13	0.03	0.12
(1,1211)	1:38:A:ALA:HA	1:42:A:THR:HA	11	0.12	0.02	0.12
(2,355)	1:32:C:LYS:HD3	1:30:C:SER:HB2	10	0.64	0.16	0.7
(2,355)	1:32:C:LYS:HD3	1:30:C:SER:HB3	10	0.64	0.16	0.7
(2,355)	1:14:C:LYS:HD3	1:21:C:ILE:HA	10	0.64	0.16	0.7
(2,265)	1:49:C:LYS:HE2	1:53:C:LYS:HD2	10	0.24	0.1	0.25
(2,265)	1:49:C:LYS:HE2	1:53:C:LYS:HB3	10	0.24	0.1	0.25
(2,1348)	1:8:B:LEU:HD23	1:43:B:LEU:HG	10	0.2	0.07	0.22
(2,1348)	1:8:B:LEU:HD21	1:43:B:LEU:HG	10	0.2	0.07	0.22
(2,1348)	1:8:B:LEU:HD22	1:43:B:LEU:HG	10	0.2	0.07	0.22
(2,870)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	10	0.2	0.06	0.19
(2,870)	1:31:C:GLY:HA2	1:15:C:CYS:HB3	10	0.2	0.06	0.19
(2,873)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	10	0.2	0.06	0.19
(2,873)	1:31:C:GLY:HA2	1:15:C:CYS:HB3	10	0.2	0.06	0.19
(1,358)	1:10:A:VAL:H	1:36:A:LEU:HA	10	0.17	0.07	0.16
(1,1134)	1:36:A:LEU:HD11	1:35:A:ILE:HA	10	0.14	0.02	0.14
(1,1134)	1:36:A:LEU:HD12	1:35:A:ILE:HA	10	0.14	0.02	0.14
(1,1134)	1:36:A:LEU:HD13	1:35:A:ILE:HA	10	0.14	0.02	0.14
(1,244)	1:8:A:LEU:HD11	1:39:A:GLN:HB2	10	0.13	0.02	0.13
(1,244)	1:8:A:LEU:HD12	1:39:A:GLN:HB2	10	0.13	0.02	0.13
(1,244)	1:8:A:LEU:HD13	1:39:A:GLN:HB2	10	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4743)	1:38:C:ALA:HA	1:42:C:THR:HA	10	0.13	0.02	0.13
(2,270)	1:14:B:LYS:HE2	1:15:B:CYS:HB2	9	0.53	0.26	0.61
(2,270)	1:14:B:LYS:HE3	1:15:B:CYS:HB2	9	0.53	0.26	0.61
(2,248)	1:14:A:LYS:HE2	1:20:A:GLU:HG3	9	0.47	0.24	0.42
(2,248)	1:14:A:LYS:HE2	1:22:A:GLU:HB2	9	0.47	0.24	0.42
(2,248)	1:14:A:LYS:HE3	1:20:A:GLU:HG3	9	0.47	0.24	0.42
(2,1349)	1:8:C:LEU:HD22	1:43:C:LEU:HG	9	0.26	0.08	0.25
(2,1349)	1:8:C:LEU:HD21	1:43:C:LEU:HG	9	0.26	0.08	0.25
(2,1349)	1:8:C:LEU:HD23	1:43:A:LEU:HG	9	0.26	0.08	0.25
(2,1349)	1:8:C:LEU:HD21	1:43:A:LEU:HG	9	0.26	0.08	0.25
(2,1347)	1:8:A:LEU:HD21	1:43:A:LEU:HG	9	0.2	0.07	0.17
(2,1347)	1:8:A:LEU:HD22	1:43:A:LEU:HG	9	0.2	0.07	0.17
(2,1347)	1:8:A:LEU:HD23	1:43:B:LEU:HG	9	0.2	0.07	0.17
(2,1347)	1:8:A:LEU:HD23	1:43:A:LEU:HG	9	0.2	0.07	0.17
(2,1347)	1:8:A:LEU:HD21	1:43:B:LEU:HG	9	0.2	0.07	0.17
(2,263)	1:49:A:LYS:HE2	1:53:A:LYS:HB3	9	0.18	0.08	0.13
(2,263)	1:49:A:LYS:HE2	1:53:A:LYS:HD2	9	0.18	0.08	0.13
(1,2192)	1:12:B:CYS:H	1:34:B:VAL:HB	9	0.18	0.06	0.16
(2,267)	1:51:B:LEU:HB2	1:52:B:ASN:HB2	9	0.16	0.05	0.16
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG2	9	0.16	0.04	0.18
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG3	9	0.16	0.04	0.18
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG2	9	0.16	0.04	0.18
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG3	9	0.16	0.04	0.18
(1,4854)	1:42:C:THR:HB	1:3:B:ILE:HB	9	0.14	0.03	0.15
(2,572)	1:2:C:VAL:HG12	1:1:C:FME:HA	8	0.25	0.16	0.19
(2,572)	1:2:C:VAL:HG11	1:1:C:FME:HA	8	0.25	0.16	0.19
(2,572)	1:2:C:VAL:HG13	1:1:C:FME:HA	8	0.25	0.16	0.19
(2,572)	1:2:C:VAL:HG13	1:39:A:GLN:HA	8	0.25	0.16	0.19
(1,1325)	1:42:A:THR:HB	1:3:C:ILE:HB	8	0.15	0.03	0.15
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD2	8	0.14	0.04	0.13
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD3	8	0.14	0.04	0.13
(1,2985)	1:38:B:ALA:HA	1:42:B:THR:HA	8	0.14	0.02	0.14
(2,353)	1:32:A:LYS:HD3	1:30:A:SER:HB2	7	1.01	0.27	0.89
(2,353)	1:14:A:LYS:HD3	1:21:A:ILE:HA	7	1.01	0.27	0.89
(2,1326)	1:30:A:SER:HB3	1:32:A:LYS:HG3	7	0.56	0.27	0.41
(2,1326)	1:30:A:SER:HB3	1:32:A:LYS:HD3	7	0.56	0.27	0.41
(2,1326)	1:30:A:SER:HB2	1:32:A:LYS:HG3	7	0.56	0.27	0.41
(2,1326)	1:30:A:SER:HB2	1:32:A:LYS:HD3	7	0.56	0.27	0.41
(2,1328)	1:30:C:SER:HB3	1:32:C:LYS:HG3	7	0.56	0.27	0.45
(2,1328)	1:30:C:SER:HB3	1:32:C:LYS:HD3	7	0.56	0.27	0.45
(2,1328)	1:30:C:SER:HB2	1:32:C:LYS:HG3	7	0.56	0.27	0.45
(2,98)	1:35:A:ILE:H	1:9:A:GLU:HG2	7	0.34	0.07	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,98)	1:35:A:ILE:H	1:12:A:CYS:HB2	7	0.34	0.07	0.33
(2,98)	1:35:A:ILE:H	1:9:A:GLU:HG3	7	0.34	0.07	0.33
(2,98)	1:35:A:ILE:H	1:10:A:VAL:HB	7	0.34	0.07	0.33
(2,100)	1:35:C:ILE:H	1:9:C:GLU:HG2	7	0.31	0.05	0.31
(2,1016)	1:13:A:PRO:HB2	1:21:A:ILE:HG22	7	0.29	0.17	0.27
(2,1016)	1:27:A:PRO:HB2	1:21:A:ILE:HG23	7	0.29	0.17	0.27
(2,1016)	1:13:A:PRO:HB2	1:21:A:ILE:HG21	7	0.29	0.17	0.27
(2,1016)	1:13:A:PRO:HB2	1:21:A:ILE:HG23	7	0.29	0.17	0.27
(1,400)	1:12:A:CYS:H	1:34:A:VAL:HB	7	0.25	0.11	0.23
(2,468)	1:43:A:LEU:HD12	1:8:A:LEU:HD23	7	0.2	0.08	0.18
(2,468)	1:43:A:LEU:HD13	1:8:A:LEU:HD21	7	0.2	0.08	0.18
(2,468)	1:43:A:LEU:HD11	1:8:C:LEU:HD23	7	0.2	0.08	0.18
(2,468)	1:43:A:LEU:HD11	1:8:A:LEU:HD23	7	0.2	0.08	0.18
(2,1554)	1:43:A:LEU:HD12	1:8:A:LEU:HD23	7	0.2	0.08	0.18
(2,1554)	1:43:A:LEU:HD13	1:8:A:LEU:HD21	7	0.2	0.08	0.18
(2,1554)	1:43:A:LEU:HD11	1:8:C:LEU:HD23	7	0.2	0.08	0.18
(2,1554)	1:43:A:LEU:HD11	1:8:A:LEU:HD23	7	0.2	0.08	0.18
(1,5298)	1:53:C:LYS:HD2	1:49:C:LYS:HG2	7	0.15	0.03	0.16
(1,5298)	1:53:C:LYS:HD2	1:49:C:LYS:HG3	7	0.15	0.03	0.16
(1,5298)	1:53:C:LYS:HD3	1:49:C:LYS:HG2	7	0.15	0.03	0.16
(1,5298)	1:53:C:LYS:HD3	1:49:C:LYS:HG3	7	0.15	0.03	0.16
(1,2152)	1:10:B:VAL:H	1:36:B:LEU:HA	7	0.15	0.02	0.14
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD11	7	0.12	0.02	0.11
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD12	7	0.12	0.02	0.11
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD13	7	0.12	0.02	0.11
(1,1457)	1:44:A:LEU:HG	1:45:A:ASP:H	7	0.11	0.01	0.11
(1,1491)	1:45:A:ASP:H	1:44:A:LEU:HG	7	0.11	0.01	0.11
(2,581)	1:42:C:THR:HG23	1:4:B:ALA:HB1	6	0.41	0.2	0.35
(2,581)	1:42:C:THR:HG22	1:4:B:ALA:HB2	6	0.41	0.2	0.35
(2,581)	1:42:C:THR:HG21	1:4:B:ALA:HB2	6	0.41	0.2	0.35
(2,581)	1:42:C:THR:HG23	1:4:B:ALA:HB3	6	0.41	0.2	0.35
(2,581)	1:42:C:THR:HG22	1:4:B:ALA:HB3	6	0.41	0.2	0.35
(2,581)	1:42:C:THR:HG23	1:3:B:ILE:HG12	6	0.41	0.2	0.35
(2,1018)	1:13:C:PRO:HB2	1:21:C:ILE:HG23	6	0.29	0.14	0.25
(2,1018)	1:13:C:PRO:HB2	1:21:C:ILE:HG21	6	0.29	0.14	0.25
(2,570)	1:2:A:VAL:HG12	1:1:A:FME:HA	6	0.22	0.1	0.19
(2,570)	1:2:A:VAL:HG11	1:1:A:FME:HA	6	0.22	0.1	0.19
(1,2821)	1:34:B:VAL:H	1:32:B:LYS:HA	6	0.15	0.03	0.14
(1,4140)	1:20:C:GLU:HA	1:27:C:PRO:HD2	6	0.14	0.02	0.14
(1,4140)	1:20:C:GLU:HA	1:27:C:PRO:HD3	6	0.14	0.02	0.14
(2,266)	1:51:A:LEU:HB2	1:52:A:ASN:HB2	6	0.13	0.02	0.12
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD11	6	0.12	0.04	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD12	6	0.12	0.04	0.11
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD13	6	0.12	0.04	0.11
(2,358)	1:14:C:LYS:HD3	1:22:C:GLU:HA	5	0.61	0.41	0.57
(2,358)	1:32:C:LYS:HD2	1:49:A:LYS:HA	5	0.61	0.41	0.57
(2,180)	1:19:B:GLY:H	1:17:B:ARG:HD3	5	0.61	0.42	0.39
(2,180)	1:19:B:GLY:H	1:26:B:CYS:HB2	5	0.61	0.42	0.39
(2,99)	1:35:B:ILE:H	1:9:B:GLU:HG2	5	0.39	0.1	0.36
(2,696)	1:15:B:CYS:HA	1:17:B:ARG:HD2	5	0.29	0.27	0.17
(2,696)	1:15:B:CYS:HA	1:17:B:ARG:HD3	5	0.29	0.27	0.17
(2,1405)	1:15:B:CYS:HA	1:17:B:ARG:HD2	5	0.29	0.27	0.17
(2,1405)	1:15:B:CYS:HA	1:17:B:ARG:HD3	5	0.29	0.27	0.17
(1,4581)	1:34:C:VAL:H	1:32:C:LYS:HG2	5	0.2	0.07	0.22
(1,4581)	1:34:C:VAL:H	1:32:C:LYS:HG3	5	0.2	0.07	0.22
(1,1043)	1:34:A:VAL:H	1:32:A:LYS:HA	5	0.16	0.05	0.17
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD11	5	0.16	0.06	0.12
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD12	5	0.16	0.06	0.12
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD13	5	0.16	0.06	0.12
(1,2672)	1:30:B:SER:HA	1:32:B:LYS:HE2	5	0.13	0.04	0.13
(1,2672)	1:30:B:SER:HA	1:32:B:LYS:HE3	5	0.13	0.04	0.13
(1,3342)	1:48:B:GLN:HB3	1:49:B:LYS:HB3	5	0.12	0.02	0.11
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG21	5	0.12	0.02	0.11
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	5	0.12	0.02	0.11
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG23	5	0.12	0.02	0.11
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG21	5	0.12	0.02	0.11
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG22	5	0.12	0.02	0.11
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG23	5	0.12	0.02	0.11
(1,77)	1:3:A:ILE:HG21	1:39:B:GLN:HG2	5	0.11	0.01	0.11
(1,77)	1:3:A:ILE:HG21	1:39:B:GLN:HG3	5	0.11	0.01	0.11
(1,77)	1:3:A:ILE:HG22	1:39:B:GLN:HG2	5	0.11	0.01	0.11
(1,77)	1:3:A:ILE:HG22	1:39:B:GLN:HG3	5	0.11	0.01	0.11
(1,77)	1:3:A:ILE:HG23	1:39:B:GLN:HG2	5	0.11	0.01	0.11
(1,77)	1:3:A:ILE:HG23	1:39:B:GLN:HG3	5	0.11	0.01	0.11
(2,580)	1:42:B:THR:HG21	1:4:A:ALA:HB1	4	0.32	0.17	0.29
(2,580)	1:42:B:THR:HG22	1:3:A:ILE:HG12	4	0.32	0.17	0.29
(2,580)	1:42:B:THR:HG21	1:3:A:ILE:HG12	4	0.32	0.17	0.29
(2,1017)	1:13:B:PRO:HB2	1:21:B:ILE:HG23	4	0.31	0.21	0.24
(2,1017)	1:27:B:PRO:HB2	1:21:B:ILE:HG21	4	0.31	0.21	0.24
(2,1017)	1:13:B:PRO:HB2	1:21:B:ILE:HG22	4	0.31	0.21	0.24
(1,381)	1:11:A:ALA:H	1:34:A:VAL:HB	4	0.24	0.06	0.22
(1,965)	1:32:A:LYS:H	1:29:A:CYS:HA	4	0.22	0.02	0.22
(2,579)	1:42:A:THR:HG22	1:4:C:ALA:HB2	4	0.2	0.1	0.14
(2,579)	1:42:A:THR:HG23	1:4:C:ALA:HB2	4	0.2	0.1	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,579)	1:42:A:THR:HG21	1:3:C:ILE:HG12	4	0.2	0.1	0.14
(2,579)	1:42:A:THR:HG22	1:4:C:ALA:HB1	4	0.2	0.1	0.14
(1,1782)	1:53:A:LYS:HD2	1:49:A:LYS:HG2	4	0.19	0.01	0.18
(1,1782)	1:53:A:LYS:HD2	1:49:A:LYS:HG3	4	0.19	0.01	0.18
(1,1782)	1:53:A:LYS:HD3	1:49:A:LYS:HG2	4	0.19	0.01	0.18
(1,1782)	1:53:A:LYS:HD3	1:49:A:LYS:HG3	4	0.19	0.01	0.18
(1,2823)	1:34:B:VAL:H	1:32:B:LYS:HG2	4	0.18	0.02	0.18
(1,2823)	1:34:B:VAL:H	1:32:B:LYS:HG3	4	0.18	0.02	0.18
(1,966)	1:32:A:LYS:H	1:29:A:CYS:HB2	4	0.17	0.02	0.17
(1,1152)	1:36:A:LEU:HD21	1:44:A:LEU:HD21	4	0.16	0.03	0.16
(1,1152)	1:36:A:LEU:HD21	1:44:A:LEU:HD22	4	0.16	0.03	0.16
(1,1152)	1:36:A:LEU:HD21	1:44:A:LEU:HD23	4	0.16	0.03	0.16
(1,1152)	1:36:A:LEU:HD22	1:44:A:LEU:HD21	4	0.16	0.03	0.16
(1,1152)	1:36:A:LEU:HD22	1:44:A:LEU:HD22	4	0.16	0.03	0.16
(1,1152)	1:36:A:LEU:HD22	1:44:A:LEU:HD23	4	0.16	0.03	0.16
(1,1152)	1:36:A:LEU:HD23	1:44:A:LEU:HD21	4	0.16	0.03	0.16
(1,1152)	1:36:A:LEU:HD23	1:44:A:LEU:HD22	4	0.16	0.03	0.16
(1,1152)	1:36:A:LEU:HD23	1:44:A:LEU:HD23	4	0.16	0.03	0.16
(1,2222)	1:14:B:LYS:HE2	1:21:B:ILE:HD11	4	0.16	0.05	0.14
(1,2222)	1:14:B:LYS:HE2	1:21:B:ILE:HD12	4	0.16	0.05	0.14
(1,2222)	1:14:B:LYS:HE2	1:21:B:ILE:HD13	4	0.16	0.05	0.14
(1,2222)	1:14:B:LYS:HE3	1:21:B:ILE:HD11	4	0.16	0.05	0.14
(1,2222)	1:14:B:LYS:HE3	1:21:B:ILE:HD12	4	0.16	0.05	0.14
(1,2222)	1:14:B:LYS:HE3	1:21:B:ILE:HD13	4	0.16	0.05	0.14
(2,268)	1:51:C:LEU:HB2	1:52:C:ASN:HB2	4	0.15	0.04	0.16
(1,3909)	1:10:C:VAL:H	1:36:C:LEU:HA	4	0.14	0.03	0.15
(1,2971)	1:37:B:THR:H	1:36:B:LEU:HG	4	0.12	0.0	0.12
(1,5308)	1:53:C:LYS:HG2	1:48:C:GLN:HB2	4	0.12	0.01	0.12
(1,5308)	1:53:C:LYS:HG3	1:48:C:GLN:HB2	4	0.12	0.01	0.12
(1,5015)	1:45:C:ASP:H	1:44:C:LEU:HG	4	0.11	0.01	0.11
(1,3225)	1:44:B:LEU:HG	1:45:B:ASP:H	4	0.11	0.0	0.11
(1,3257)	1:45:B:ASP:H	1:44:B:LEU:HG	4	0.11	0.0	0.11
(2,354)	1:14:B:LYS:HD2	1:21:B:ILE:HA	3	1.07	0.22	0.93
(2,354)	1:14:B:LYS:HD3	1:21:B:ILE:HA	3	1.07	0.22	0.93
(2,354)	1:32:B:LYS:HD3	1:30:B:SER:HB3	3	1.07	0.22	0.93
(1,4456)	1:31:C:GLY:H	1:34:C:VAL:H	3	0.56	0.16	0.61
(1,4578)	1:34:C:VAL:H	1:31:C:GLY:H	3	0.56	0.16	0.61
(2,137)	1:15:A:CYS:H	1:14:A:LYS:HG2	3	0.38	0.17	0.28
(2,137)	1:15:A:CYS:H	1:21:A:ILE:HG13	3	0.38	0.17	0.28
(2,571)	1:2:B:VAL:HG12	1:1:B:FME:HA	3	0.37	0.17	0.32
(2,571)	1:2:B:VAL:HG11	1:1:B:FME:HA	3	0.37	0.17	0.32
(1,2172)	1:11:B:ALA:H	1:34:B:VAL:HB	3	0.22	0.02	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,641)	1:21:A:ILE:HD11	1:13:A:PRO:HD2	3	0.19	0.06	0.23
(1,641)	1:21:A:ILE:HD11	1:13:A:PRO:HD3	3	0.19	0.06	0.23
(1,641)	1:21:A:ILE:HD12	1:13:A:PRO:HD2	3	0.19	0.06	0.23
(1,641)	1:21:A:ILE:HD12	1:13:A:PRO:HD3	3	0.19	0.06	0.23
(1,641)	1:21:A:ILE:HD13	1:13:A:PRO:HD2	3	0.19	0.06	0.23
(1,641)	1:21:A:ILE:HD13	1:13:A:PRO:HD3	3	0.19	0.06	0.23
(2,697)	1:15:C:CYS:HA	1:17:C:ARG:HD3	3	0.19	0.07	0.17
(2,697)	1:15:C:CYS:HA	1:17:C:ARG:HD2	3	0.19	0.07	0.17
(2,1406)	1:15:C:CYS:HA	1:17:C:ARG:HD3	3	0.19	0.07	0.17
(2,1406)	1:15:C:CYS:HA	1:17:C:ARG:HD2	3	0.19	0.07	0.17
(1,1080)	1:35:A:ILE:HG12	1:29:A:CYS:HA	3	0.17	0.07	0.13
(1,1080)	1:35:A:ILE:HG13	1:29:A:CYS:HA	3	0.17	0.07	0.13
(1,1798)	1:53:A:LYS:H	1:51:B:LEU:HD11	3	0.17	0.02	0.17
(1,1798)	1:53:A:LYS:H	1:51:B:LEU:HD12	3	0.17	0.02	0.17
(1,1798)	1:53:A:LYS:H	1:51:B:LEU:HD13	3	0.17	0.02	0.17
(1,3594)	1:2:C:VAL:HG11	1:1:C:FME:HG2	3	0.16	0.02	0.16
(1,3594)	1:2:C:VAL:HG11	1:1:C:FME:HG3	3	0.16	0.02	0.16
(1,3594)	1:2:C:VAL:HG12	1:1:C:FME:HG2	3	0.16	0.02	0.16
(1,3594)	1:2:C:VAL:HG12	1:1:C:FME:HG3	3	0.16	0.02	0.16
(1,3594)	1:2:C:VAL:HG13	1:1:C:FME:HG2	3	0.16	0.02	0.16
(1,3594)	1:2:C:VAL:HG13	1:1:C:FME:HG3	3	0.16	0.02	0.16
(1,4729)	1:37:C:THR:H	1:36:C:LEU:HG	3	0.16	0.02	0.16
(1,4430)	1:30:C:SER:HA	1:32:C:LYS:HE2	3	0.16	0.05	0.13
(1,4430)	1:30:C:SER:HA	1:32:C:LYS:HE3	3	0.16	0.05	0.13
(1,1841)	1:2:B:VAL:HG11	1:3:B:ILE:HG21	3	0.15	0.07	0.11
(1,1841)	1:2:B:VAL:HG11	1:3:B:ILE:HG22	3	0.15	0.07	0.11
(1,1841)	1:2:B:VAL:HG11	1:3:B:ILE:HG23	3	0.15	0.07	0.11
(1,1841)	1:2:B:VAL:HG12	1:3:B:ILE:HG21	3	0.15	0.07	0.11
(1,1841)	1:2:B:VAL:HG12	1:3:B:ILE:HG22	3	0.15	0.07	0.11
(1,1841)	1:2:B:VAL:HG12	1:3:B:ILE:HG23	3	0.15	0.07	0.11
(1,1841)	1:2:B:VAL:HG13	1:3:B:ILE:HG21	3	0.15	0.07	0.11
(1,1841)	1:2:B:VAL:HG13	1:3:B:ILE:HG22	3	0.15	0.07	0.11
(1,1841)	1:2:B:VAL:HG13	1:3:B:ILE:HG23	3	0.15	0.07	0.11
(1,32)	1:2:A:VAL:HG11	1:1:A:FME:HG2	3	0.14	0.02	0.13
(1,32)	1:2:A:VAL:HG11	1:1:A:FME:HG3	3	0.14	0.02	0.13
(1,32)	1:2:A:VAL:HG12	1:1:A:FME:HG2	3	0.14	0.02	0.13
(1,32)	1:2:A:VAL:HG12	1:1:A:FME:HG3	3	0.14	0.02	0.13
(1,32)	1:2:A:VAL:HG13	1:1:A:FME:HG2	3	0.14	0.02	0.13
(1,32)	1:2:A:VAL:HG13	1:1:A:FME:HG3	3	0.14	0.02	0.13
(1,1581)	1:48:A:GLN:HB3	1:49:A:LYS:HB3	3	0.12	0.01	0.11
(1,444)	1:15:A:CYS:HA	1:14:A:LYS:HG2	3	0.11	0.01	0.11
(1,444)	1:15:A:CYS:HA	1:14:A:LYS:HG3	3	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1193)	1:37:A:THR:H	1:36:A:LEU:HG	3	0.11	0.01	0.11
(1,1886)	1:3:B:ILE:HG21	1:39:C:GLN:HG2	3	0.11	0.0	0.11
(1,1886)	1:3:B:ILE:HG21	1:39:C:GLN:HG3	3	0.11	0.0	0.11
(1,1886)	1:3:B:ILE:HG22	1:39:C:GLN:HG2	3	0.11	0.0	0.11
(1,1886)	1:3:B:ILE:HG22	1:39:C:GLN:HG3	3	0.11	0.0	0.11
(1,1886)	1:3:B:ILE:HG23	1:39:C:GLN:HG2	3	0.11	0.0	0.11
(1,1886)	1:3:B:ILE:HG23	1:39:C:GLN:HG3	3	0.11	0.0	0.11
(1,5100)	1:48:C:GLN:HB3	1:49:C:LYS:HB3	3	0.11	0.01	0.11
(1,5110)	1:48:C:GLN:HB2	1:51:A:LEU:HD11	3	0.11	0.01	0.11
(1,5110)	1:48:C:GLN:HB2	1:51:A:LEU:HD12	3	0.11	0.01	0.11
(1,5110)	1:48:C:GLN:HB2	1:51:A:LEU:HD13	3	0.11	0.01	0.11
(1,4983)	1:44:C:LEU:HG	1:45:C:ASP:H	3	0.1	0.0	0.1
(2,356)	1:14:A:LYS:HD3	1:22:A:GLU:HA	2	0.46	0.34	0.46
(1,636)	1:21:A:ILE:HB	1:22:A:GLU:HB2	2	0.37	0.0	0.37
(1,2428)	1:21:B:ILE:HB	1:22:B:GLU:HB2	2	0.32	0.02	0.32
(2,786)	1:20:B:GLU:HG2	1:26:B:CYS:HB2	2	0.31	0.17	0.31
(2,786)	1:20:B:GLU:HG2	1:26:B:CYS:HB3	2	0.31	0.17	0.31
(2,786)	1:20:B:GLU:HG3	1:26:B:CYS:HB2	2	0.31	0.17	0.31
(2,786)	1:20:B:GLU:HG3	1:26:B:CYS:HB3	2	0.31	0.17	0.31
(2,658)	1:21:B:ILE:HD11	1:26:B:CYS:HA	2	0.26	0.01	0.26
(2,658)	1:21:B:ILE:HD12	1:14:B:LYS:HA	2	0.26	0.01	0.26
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD11	2	0.25	0.04	0.25
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD12	2	0.25	0.04	0.25
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD13	2	0.25	0.04	0.25
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD11	2	0.25	0.04	0.25
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD12	2	0.25	0.04	0.25
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD13	2	0.25	0.04	0.25
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD21	2	0.25	0.04	0.25
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD22	2	0.25	0.04	0.25
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD23	2	0.25	0.04	0.25
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD21	2	0.25	0.04	0.25
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD22	2	0.25	0.04	0.25
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD23	2	0.25	0.04	0.25
(2,657)	1:21:A:ILE:HD13	1:26:A:CYS:HA	2	0.24	0.01	0.24
(2,657)	1:21:A:ILE:HD11	1:26:A:CYS:HA	2	0.24	0.01	0.24
(1,2865)	1:35:B:ILE:HG21	1:12:B:CYS:HB2	2	0.2	0.08	0.2
(1,2865)	1:35:B:ILE:HG22	1:12:B:CYS:HB2	2	0.2	0.08	0.2
(1,2865)	1:35:B:ILE:HG23	1:12:B:CYS:HB2	2	0.2	0.08	0.2
(1,2746)	1:32:B:LYS:H	1:29:B:CYS:HA	2	0.2	0.0	0.2
(1,1755)	1:52:A:ASN:H	1:53:A:LYS:H	2	0.2	0.01	0.2
(1,1805)	1:53:A:LYS:H	1:52:A:ASN:H	2	0.2	0.01	0.2
(1,2857)	1:35:B:ILE:HG12	1:29:B:CYS:HA	2	0.2	0.09	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2857)	1:35:B:ILE:HG13	1:29:B:CYS:HA	2	0.2	0.09	0.2
(1,2433)	1:21:B:ILE:HD11	1:13:B:PRO:HD2	2	0.18	0.03	0.18
(1,2433)	1:21:B:ILE:HD11	1:13:B:PRO:HD3	2	0.18	0.03	0.18
(1,2433)	1:21:B:ILE:HD12	1:13:B:PRO:HD2	2	0.18	0.03	0.18
(1,2433)	1:21:B:ILE:HD12	1:13:B:PRO:HD3	2	0.18	0.03	0.18
(1,2433)	1:21:B:ILE:HD13	1:13:B:PRO:HD2	2	0.18	0.03	0.18
(1,2433)	1:21:B:ILE:HD13	1:13:B:PRO:HD3	2	0.18	0.03	0.18
(1,2747)	1:32:B:LYS:H	1:29:B:CYS:HB2	2	0.18	0.03	0.18
(1,4504)	1:32:C:LYS:H	1:29:C:CYS:HA	2	0.17	0.0	0.17
(2,1070)	1:29:A:CYS:HB3	1:32:A:LYS:HD2	2	0.17	0.06	0.17
(2,1070)	1:29:A:CYS:HB3	1:32:A:LYS:HG3	2	0.17	0.06	0.17
(1,3979)	1:14:C:LYS:HE2	1:21:C:ILE:HD11	2	0.17	0.01	0.17
(1,3979)	1:14:C:LYS:HE2	1:21:C:ILE:HD12	2	0.17	0.01	0.17
(1,3979)	1:14:C:LYS:HE2	1:21:C:ILE:HD13	2	0.17	0.01	0.17
(1,3979)	1:14:C:LYS:HE3	1:21:C:ILE:HD11	2	0.17	0.01	0.17
(1,3979)	1:14:C:LYS:HE3	1:21:C:ILE:HD12	2	0.17	0.01	0.17
(1,3979)	1:14:C:LYS:HE3	1:21:C:ILE:HD13	2	0.17	0.01	0.17
(1,1343)	1:42:A:THR:HG21	1:8:C:LEU:HD11	2	0.16	0.03	0.16
(1,1343)	1:42:A:THR:HG21	1:8:C:LEU:HD12	2	0.16	0.03	0.16
(1,1343)	1:42:A:THR:HG21	1:8:C:LEU:HD13	2	0.16	0.03	0.16
(1,1343)	1:42:A:THR:HG22	1:8:C:LEU:HD11	2	0.16	0.03	0.16
(1,1343)	1:42:A:THR:HG22	1:8:C:LEU:HD12	2	0.16	0.03	0.16
(1,1343)	1:42:A:THR:HG22	1:8:C:LEU:HD13	2	0.16	0.03	0.16
(1,1343)	1:42:A:THR:HG23	1:8:C:LEU:HD11	2	0.16	0.03	0.16
(1,1343)	1:42:A:THR:HG23	1:8:C:LEU:HD12	2	0.16	0.03	0.16
(1,1343)	1:42:A:THR:HG23	1:8:C:LEU:HD13	2	0.16	0.03	0.16
(1,4172)	1:20:C:GLU:H	1:31:C:GLY:H	2	0.15	0.03	0.15
(1,4450)	1:31:C:GLY:H	1:20:C:GLU:H	2	0.15	0.03	0.15
(1,1487)	1:45:A:ASP:HB2	1:48:A:GLN:HG2	2	0.15	0.03	0.15
(1,1487)	1:45:A:ASP:HB2	1:48:A:GLN:HG3	2	0.15	0.03	0.15
(1,1487)	1:45:A:ASP:HB3	1:48:A:GLN:HG2	2	0.15	0.03	0.15
(1,1487)	1:45:A:ASP:HB3	1:48:A:GLN:HG3	2	0.15	0.03	0.15
(1,1598)	1:48:A:GLN:HG2	1:45:A:ASP:HB2	2	0.15	0.03	0.15
(1,1598)	1:48:A:GLN:HG2	1:45:A:ASP:HB3	2	0.15	0.03	0.15
(1,1598)	1:48:A:GLN:HG3	1:45:A:ASP:HB2	2	0.15	0.03	0.15
(1,1598)	1:48:A:GLN:HG3	1:45:A:ASP:HB3	2	0.15	0.03	0.15
(2,961)	1:47:A:ILE:HB	1:47:B:ILE:HB	2	0.14	0.03	0.14
(2,961)	1:47:B:ILE:HB	1:47:C:ILE:HB	2	0.14	0.03	0.14
(1,4685)	1:36:C:LEU:HD21	1:44:C:LEU:HD21	2	0.14	0.04	0.14
(1,4685)	1:36:C:LEU:HD21	1:44:C:LEU:HD22	2	0.14	0.04	0.14
(1,4685)	1:36:C:LEU:HD21	1:44:C:LEU:HD23	2	0.14	0.04	0.14
(1,4685)	1:36:C:LEU:HD22	1:44:C:LEU:HD21	2	0.14	0.04	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4685)	1:36:C:LEU:HD22	1:44:C:LEU:HD22	2	0.14	0.04	0.14
(1,4685)	1:36:C:LEU:HD22	1:44:C:LEU:HD23	2	0.14	0.04	0.14
(1,4685)	1:36:C:LEU:HD23	1:44:C:LEU:HD21	2	0.14	0.04	0.14
(1,4685)	1:36:C:LEU:HD23	1:44:C:LEU:HD22	2	0.14	0.04	0.14
(1,4685)	1:36:C:LEU:HD23	1:44:C:LEU:HD23	2	0.14	0.04	0.14
(2,69)	1:51:B:LEU:H	1:51:B:LEU:HD11	2	0.14	0.02	0.14
(2,69)	1:51:B:LEU:H	1:51:C:LEU:HD12	2	0.14	0.02	0.14
(1,331)	1:10:A:VAL:HB	1:11:A:ALA:H	2	0.13	0.01	0.13
(1,377)	1:11:A:ALA:H	1:10:A:VAL:HB	2	0.13	0.01	0.13
(1,1837)	1:2:B:VAL:HG11	1:1:B:FME:HG2	2	0.13	0.01	0.13
(1,1837)	1:2:B:VAL:HG11	1:1:B:FME:HG3	2	0.13	0.01	0.13
(1,1837)	1:2:B:VAL:HG12	1:1:B:FME:HG2	2	0.13	0.01	0.13
(1,1837)	1:2:B:VAL:HG12	1:1:B:FME:HG3	2	0.13	0.01	0.13
(1,1837)	1:2:B:VAL:HG13	1:1:B:FME:HG2	2	0.13	0.01	0.13
(1,1837)	1:2:B:VAL:HG13	1:1:B:FME:HG3	2	0.13	0.01	0.13
(1,2528)	1:24:B:THR:HG21	1:22:B:GLU:HG2	2	0.12	0.01	0.12
(1,2528)	1:24:B:THR:HG21	1:22:B:GLU:HG3	2	0.12	0.01	0.12
(1,2528)	1:24:B:THR:HG22	1:22:B:GLU:HG2	2	0.12	0.01	0.12
(1,2528)	1:24:B:THR:HG22	1:22:B:GLU:HG3	2	0.12	0.01	0.12
(1,2528)	1:24:B:THR:HG23	1:22:B:GLU:HG2	2	0.12	0.01	0.12
(1,2528)	1:24:B:THR:HG23	1:22:B:GLU:HG3	2	0.12	0.01	0.12
(1,3735)	1:6:C:ASP:HA	1:9:C:GLU:HG2	2	0.12	0.01	0.12
(1,3735)	1:6:C:ASP:HA	1:9:C:GLU:HG3	2	0.12	0.01	0.12
(1,5299)	1:53:C:LYS:HE2	1:45:C:ASP:HA	2	0.12	0.01	0.12
(1,5299)	1:53:C:LYS:HE3	1:45:C:ASP:HA	2	0.12	0.01	0.12
(1,4166)	1:20:C:GLU:H	1:18:C:ALA:H	2	0.12	0.0	0.12
(1,1499)	1:45:A:ASP:H	1:48:A:GLN:HB3	2	0.11	0.0	0.11
(2,568)	1:24:B:THR:HG22	1:22:B:GLU:HB2	2	0.11	0.01	0.11
(2,568)	1:24:B:THR:HG23	1:22:B:GLU:HB2	2	0.11	0.01	0.11
(2,1375)	1:24:B:THR:HG22	1:22:B:GLU:HB2	2	0.11	0.01	0.11
(2,1375)	1:24:B:THR:HG23	1:22:B:GLU:HB2	2	0.11	0.01	0.11
(1,2408)	1:20:B:GLU:H	1:18:B:ALA:H	2	0.11	0.0	0.11
(1,2927)	1:36:B:LEU:HD21	1:44:B:LEU:HD21	2	0.11	0.0	0.11
(1,2927)	1:36:B:LEU:HD21	1:44:B:LEU:HD22	2	0.11	0.0	0.11
(1,2927)	1:36:B:LEU:HD21	1:44:B:LEU:HD23	2	0.11	0.0	0.11
(1,2927)	1:36:B:LEU:HD22	1:44:B:LEU:HD21	2	0.11	0.0	0.11
(1,2927)	1:36:B:LEU:HD22	1:44:B:LEU:HD22	2	0.11	0.0	0.11
(1,2927)	1:36:B:LEU:HD22	1:44:B:LEU:HD23	2	0.11	0.0	0.11
(1,2927)	1:36:B:LEU:HD23	1:44:B:LEU:HD21	2	0.11	0.0	0.11
(1,2927)	1:36:B:LEU:HD23	1:44:B:LEU:HD22	2	0.11	0.0	0.11
(1,2927)	1:36:B:LEU:HD23	1:44:B:LEU:HD23	2	0.11	0.0	0.11
(1,3643)	1:3:C:ILE:HG21	1:39:A:GLN:HG2	2	0.1	0.0	0.1

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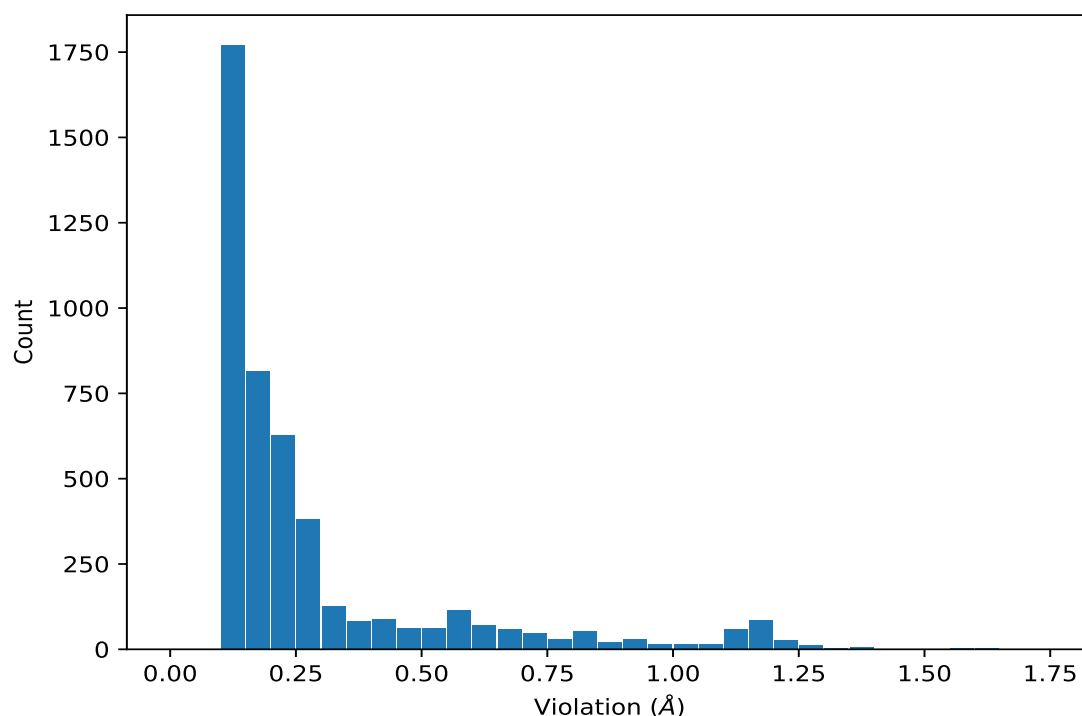
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3643)	1:3:C:ILE:HG21	1:39:A:GLN:HG3	2	0.1	0.0	0.1
(1,3643)	1:3:C:ILE:HG22	1:39:A:GLN:HG2	2	0.1	0.0	0.1
(1,3643)	1:3:C:ILE:HG22	1:39:A:GLN:HG3	2	0.1	0.0	0.1
(1,3643)	1:3:C:ILE:HG23	1:39:A:GLN:HG2	2	0.1	0.0	0.1
(1,3643)	1:3:C:ILE:HG23	1:39:A:GLN:HG3	2	0.1	0.0	0.1

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)
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG2	20	1.74
(2,1163)	1:35:C:ILE:HG12	1:13:C:PRO:HG3	4	1.62
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	2	1.6
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG3	12	1.59
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	17	1.56
(2,1163)	1:35:C:ILE:HG12	1:13:C:PRO:HG3	10	1.56
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	17	1.56
(2,353)	1:14:A:LYS:HD3	1:21:A:ILE:HA	9	1.53
(2,354)	1:14:B:LYS:HD2	1:21:B:ILE:HA	9	1.38
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	20	1.37
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	20	1.37
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	12	1.36
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	12	1.36
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG21	17	1.35
(2,180)	1:19:B:GLY:H	1:26:B:CYS:HB2	6	1.35
(2,1193)	1:27:C:PRO:HG3	1:21:C:ILE:HG21	14	1.33
(2,358)	1:32:C:LYS:HD2	1:49:A:LYS:HA	18	1.32
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	1	1.31
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	1	1.31
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG23	5	1.28
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG23	19	1.28
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	4	1.28
(2,1161)	1:35:A:ILE:HG12	1:13:A:PRO:HG3	5	1.28
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	4	1.28
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG2	10	1.27
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG2	19	1.26
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	5	1.25
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG3	10	1.25
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	5	1.25
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	12	1.25
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	7	1.24
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	1	1.24
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	7	1.24
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	1	1.24
(2,353)	1:32:A:LYS:HD3	1:30:A:SER:HB2	17	1.24
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	1	1.23
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	19	1.23
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG2	7	1.23
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	1	1.23
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	19	1.23
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	9	1.23
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	20	1.23
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	11	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	10	1.22
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	11	1.22
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	10	1.22
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	19	1.22
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	9	1.21
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	3	1.21
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	12	1.21
(2,1163)	1:35:C:ILE:HG13	1:13:C:PRO:HG3	9	1.21
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	9	1.21
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	3	1.21
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	12	1.21
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	16	1.21
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	17	1.21
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	13	1.2
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	18	1.2
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	8	1.2
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	13	1.2
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	18	1.2
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	19	1.2
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG2	12	1.2
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	13	1.2
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	18	1.2
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	8	1.2
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	13	1.2
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	18	1.2
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	19	1.2
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	8	1.2
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	13	1.2
(2,1192)	1:27:B:PRO:HG3	1:21:B:ILE:HG23	1	1.19
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	2	1.19
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	5	1.19
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	6	1.19
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	9	1.19
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	10	1.19
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	11	1.19
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	16	1.19
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	16	1.19
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	20	1.19
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG2	18	1.19
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	2	1.19
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	5	1.19
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	6	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	9	1.19
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	10	1.19
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	11	1.19
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	16	1.19
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	16	1.19
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	20	1.19
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	18	1.19
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	12	1.19
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	18	1.19
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	3	1.19
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	16	1.19
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	4	1.18
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	19	1.18
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	2	1.18
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	8	1.18
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	11	1.18
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	14	1.18
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	15	1.18
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG3	6	1.18
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	4	1.18
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	19	1.18
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	2	1.18
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	8	1.18
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	11	1.18
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	14	1.18
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	15	1.18
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	1	1.18
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	6	1.18
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	4	1.18
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	15	1.17
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	15	1.17
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	5	1.17
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	9	1.17
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	17	1.17
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG2	3	1.17
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG3	8	1.17
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	15	1.17
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	15	1.17
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	5	1.17
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	9	1.17
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	17	1.17
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	15	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	18	1.17
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	3	1.16
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	12	1.16
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	16	1.16
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	3	1.16
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	7	1.16
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG2	15	1.16
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG3	6	1.16
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	3	1.16
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	12	1.16
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	16	1.16
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	3	1.16
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	7	1.16
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	3	1.16
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	17	1.15
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	2	1.15
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	4	1.15
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	17	1.15
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	2	1.15
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	4	1.15
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	6	1.15
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	9	1.15
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	13	1.15
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	15	1.15
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	7	1.15
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	12	1.15
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG23	8	1.14
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	8	1.14
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	7	1.14
(2,1162)	1:35:B:ILE:HG13	1:13:B:PRO:HG3	16	1.14
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	8	1.14
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	7	1.14
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	11	1.14
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	11	1.14
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	14	1.14
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG23	12	1.13
(2,1191)	1:27:A:PRO:HG3	1:21:A:ILE:HG22	9	1.13
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	14	1.13
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	6	1.13
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	14	1.13
(2,1186)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	20	1.13
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG3	6	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG2	18	1.13
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	14	1.13
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	6	1.13
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	14	1.13
(2,394)	1:13:B:PRO:HG2	1:27:B:PRO:HG2	20	1.13
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	11	1.13
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	13	1.13
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	16	1.13
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	6	1.13
(2,1193)	1:27:C:PRO:HG3	1:21:C:ILE:HG23	2	1.12
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG23	7	1.12
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	10	1.12
(2,1185)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	6	1.12
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	10	1.12
(2,393)	1:13:A:PRO:HG2	1:27:A:PRO:HG2	6	1.12
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	2	1.12
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	9	1.12
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	4	1.11
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG21	11	1.11
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG3	4	1.11
(2,1161)	1:35:A:ILE:HG12	1:13:A:PRO:HG3	16	1.11
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	4	1.11
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	19	1.11
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	10	1.11
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	15	1.11
(2,1191)	1:27:A:PRO:HG3	1:21:A:ILE:HG22	16	1.1
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	18	1.1
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	18	1.1
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	5	1.1
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	4	1.1
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	15	1.09
(2,1191)	1:27:A:PRO:HG3	1:21:A:ILE:HG23	3	1.09
(2,1187)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	13	1.09
(2,395)	1:13:C:PRO:HG2	1:27:C:PRO:HG2	13	1.09
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	8	1.09
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	10	1.09
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	14	1.09
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	5	1.09
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	2	1.08
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	17	1.08
(2,1327)	1:30:B:SER:HB2	1:32:B:LYS:HG3	20	1.07
(2,277)	1:21:C:ILE:HB	1:13:C:PRO:HB2	20	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	20	1.07
(2,1326)	1:30:A:SER:HB2	1:32:A:LYS:HD3	9	1.05
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG3	9	1.05
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	14	1.05
(2,1328)	1:30:C:SER:HB2	1:32:C:LYS:HG3	19	1.04
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG23	3	1.04
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	6	1.04
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG2	14	1.04
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG3	18	1.04
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG22	10	1.03
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG22	10	1.03
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG22	13	1.03
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	3	1.03
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG3	8	1.01
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG3	13	1.01
(2,1162)	1:35:B:ILE:HG12	1:13:B:PRO:HG3	15	1.01
(2,353)	1:32:A:LYS:HD3	1:30:A:SER:HB2	16	1.01
(2,276)	1:21:B:ILE:HB	1:13:B:PRO:HB2	1	1.0
(1,1800)	1:53:A:LYS:H	1:49:A:LYS:H	18	1.0
(1,1672)	1:49:A:LYS:H	1:53:A:LYS:H	18	1.0
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG22	12	0.99
(2,1191)	1:27:A:PRO:HG3	1:21:A:ILE:HG21	14	0.99
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	7	0.98
(2,1327)	1:30:B:SER:HB2	1:32:B:LYS:HG3	14	0.97
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG23	9	0.97
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG23	9	0.97
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG23	18	0.97
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG22	18	0.97
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG21	11	0.96
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG22	15	0.96
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG3	2	0.96
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	16	0.96
(1,1800)	1:53:A:LYS:H	1:49:A:LYS:H	11	0.96
(1,1672)	1:49:A:LYS:H	1:53:A:LYS:H	11	0.96
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG22	17	0.95
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	19	0.95
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG21	2	0.94
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG21	7	0.94
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG21	19	0.94
(2,277)	1:21:C:ILE:HB	1:27:C:PRO:HB2	17	0.94
(2,276)	1:21:B:ILE:HB	1:27:B:PRO:HB2	5	0.94
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG23	1	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,604)	1:50:B:HIS:HA	1:49:B:LYS:HB2	18	0.93
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	11	0.93
(2,354)	1:14:B:LYS:HD3	1:21:B:ILE:HA	14	0.93
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	4	0.93
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG21	3	0.92
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG21	18	0.92
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG3	7	0.92
(2,275)	1:21:A:ILE:HB	1:27:A:PRO:HB2	8	0.92
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	13	0.91
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG22	12	0.91
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG22	15	0.91
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	18	0.91
(2,357)	1:32:B:LYS:HD2	1:49:C:LYS:HA	7	0.91
(2,248)	1:14:A:LYS:HE3	1:20:A:GLU:HG3	18	0.91
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG23	4	0.9
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG23	13	0.9
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG21	20	0.9
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG2	9	0.9
(2,604)	1:50:B:HIS:HA	1:49:B:LYS:HB2	11	0.9
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD11	18	0.9
(2,270)	1:14:B:LYS:HE2	1:15:B:CYS:HB2	19	0.9
(2,270)	1:14:B:LYS:HE3	1:15:B:CYS:HB2	19	0.9
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	2	0.89
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG21	11	0.89
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG3	5	0.89
(2,400)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	2	0.89
(2,354)	1:32:B:LYS:HD3	1:30:B:SER:HB3	7	0.89
(2,353)	1:32:A:LYS:HD3	1:30:A:SER:HB2	3	0.89
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	4	0.88
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	18	0.88
(2,353)	1:32:A:LYS:HD3	1:30:A:SER:HB2	13	0.88
(2,248)	1:14:A:LYS:HE2	1:20:A:GLU:HG3	1	0.88
(1,4994)	1:45:C:ASP:HA	1:44:C:LEU:HD11	11	0.88
(1,4994)	1:45:C:ASP:HA	1:44:C:LEU:HD12	11	0.88
(1,4994)	1:45:C:ASP:HA	1:44:C:LEU:HD13	11	0.88
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	11	0.88
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	2	0.87
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	14	0.87
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG22	20	0.86
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG22	5	0.86
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	7	0.86
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	17	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,604)	1:50:B:HIS:HA	1:51:B:LEU:HB2	13	0.86
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	3	0.86
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG21	16	0.85
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG21	20	0.85
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	8	0.85
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	10	0.85
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	9	0.85
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	12	0.85
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	13	0.85
(2,401)	1:27:C:PRO:HG2	1:21:C:ILE:HG21	16	0.85
(2,400)	1:27:B:PRO:HG2	1:21:B:ILE:HG21	20	0.85
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	3	0.84
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	9	0.84
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	16	0.84
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	1	0.84
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	2	0.84
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	16	0.84
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	17	0.84
(2,1405)	1:15:B:CYS:HA	1:17:B:ARG:HD2	6	0.83
(2,696)	1:15:B:CYS:HA	1:17:B:ARG:HD2	6	0.83
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	1	0.83
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	5	0.83
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	6	0.83
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	11	0.83
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	12	0.83
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	13	0.83
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	15	0.83
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	20	0.83
(2,604)	1:50:B:HIS:HA	1:51:B:LEU:HB2	4	0.83
(2,604)	1:50:B:HIS:HA	1:51:B:LEU:HB2	7	0.83
(2,604)	1:50:B:HIS:HA	1:51:B:LEU:HB2	12	0.83
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	4	0.83
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	8	0.83
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD13	12	0.83
(2,276)	1:21:B:ILE:HB	1:13:B:PRO:HB2	10	0.83
(1,4594)	1:35:C:ILE:HA	1:36:C:LEU:HG	19	0.83
(2,605)	1:50:C:HIS:HA	1:51:C:LEU:HB2	19	0.82
(2,604)	1:50:B:HIS:HA	1:51:B:LEU:HB2	3	0.82
(2,604)	1:50:B:HIS:HA	1:51:B:LEU:HB2	6	0.82
(2,604)	1:50:B:HIS:HA	1:51:B:LEU:HB2	20	0.82
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	6	0.82
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD11	3	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,250)	1:14:C:LYS:HE2	1:22:C:GLU:HB2	8	0.82
(2,604)	1:50:B:HIS:HA	1:51:B:LEU:HB2	5	0.81
(2,604)	1:50:B:HIS:HA	1:51:B:LEU:HB2	10	0.81
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	19	0.81
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD12	11	0.81
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG21	17	0.8
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG23	4	0.8
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG3	17	0.8
(2,604)	1:50:B:HIS:HA	1:51:B:LEU:HB2	2	0.8
(2,604)	1:50:B:HIS:HA	1:51:B:LEU:HB2	19	0.8
(2,399)	1:27:A:PRO:HG2	1:21:A:ILE:HG23	4	0.8
(2,355)	1:14:C:LYS:HD3	1:21:C:ILE:HA	10	0.8
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	16	0.8
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	16	0.8
(2,604)	1:50:B:HIS:HA	1:51:B:LEU:HB2	15	0.79
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	7	0.79
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	14	0.79
(2,603)	1:50:A:HIS:HA	1:32:C:LYS:HD3	20	0.79
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD11	15	0.79
(2,356)	1:14:A:LYS:HD3	1:22:A:GLU:HA	4	0.79
(2,353)	1:32:A:LYS:HD3	1:30:A:SER:HB2	18	0.79
(2,270)	1:14:B:LYS:HE2	1:15:B:CYS:HB2	12	0.79
(2,270)	1:14:B:LYS:HE3	1:15:B:CYS:HB2	12	0.79
(2,250)	1:14:C:LYS:HE2	1:22:C:GLU:HB2	1	0.79
(2,604)	1:50:B:HIS:HA	1:51:B:LEU:HB2	17	0.78
(2,1328)	1:30:C:SER:HB3	1:32:C:LYS:HG3	10	0.77
(2,1326)	1:30:A:SER:HB2	1:32:A:LYS:HG3	14	0.77
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD13	11	0.77
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD12	17	0.77
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD11	19	0.77
(2,249)	1:14:B:LYS:HE2	1:22:B:GLU:HB2	1	0.77
(2,249)	1:14:B:LYS:HE2	1:22:B:GLU:HB2	9	0.77
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG3	2	0.76
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG2	15	0.76
(2,604)	1:50:B:HIS:HA	1:32:A:LYS:HD3	1	0.76
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD13	6	0.76
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	7	0.76
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	7	0.76
(2,180)	1:19:B:GLY:H	1:17:B:ARG:HD3	3	0.76
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG3	4	0.75
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	15	0.75
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD11	5	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,355)	1:32:C:LYS:HD3	1:30:C:SER:HB2	9	0.75
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	18	0.75
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG21	10	0.74
(2,785)	1:20:A:GLU:HG2	1:26:A:CYS:HB2	13	0.74
(2,785)	1:20:A:GLU:HG2	1:26:A:CYS:HB3	13	0.74
(2,785)	1:20:A:GLU:HG3	1:26:A:CYS:HB2	13	0.74
(2,785)	1:20:A:GLU:HG3	1:26:A:CYS:HB3	13	0.74
(2,603)	1:50:A:HIS:HA	1:51:A:LEU:HB2	5	0.74
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD12	9	0.74
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	20	0.74
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	20	0.74
(2,250)	1:14:C:LYS:HE3	1:20:C:GLU:HG3	12	0.74
(2,250)	1:14:C:LYS:HE2	1:22:C:GLU:HB2	14	0.74
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	10	0.74
(2,581)	1:42:C:THR:HG23	1:4:B:ALA:HB1	3	0.73
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD13	4	0.73
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD13	12	0.73
(2,355)	1:32:C:LYS:HD3	1:30:C:SER:HB2	2	0.73
(2,355)	1:32:C:LYS:HD3	1:30:C:SER:HB2	12	0.73
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	3	0.73
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	3	0.73
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	19	0.73
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	19	0.73
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	19	0.73
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	19	0.73
(2,249)	1:14:B:LYS:HE2	1:22:B:GLU:HB2	18	0.73
(2,1556)	1:43:C:LEU:HD12	1:8:C:LEU:HD23	9	0.72
(2,1328)	1:30:C:SER:HB3	1:32:C:LYS:HG3	3	0.72
(2,470)	1:43:C:LEU:HD12	1:8:C:LEU:HD23	9	0.72
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD12	15	0.72
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD13	4	0.72
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD13	18	0.72
(2,355)	1:14:C:LYS:HD3	1:21:C:ILE:HA	17	0.72
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	14	0.72
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	14	0.72
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	10	0.72
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	10	0.72
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	12	0.72
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	12	0.72
(1,4578)	1:34:C:VAL:H	1:31:C:GLY:H	17	0.72
(1,4456)	1:31:C:GLY:H	1:34:C:VAL:H	17	0.72
(2,1326)	1:30:A:SER:HB2	1:32:A:LYS:HG3	8	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1191)	1:27:A:PRO:HG2	1:21:A:ILE:HG22	6	0.71
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG2	19	0.71
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD13	18	0.71
(2,399)	1:27:A:PRO:HG2	1:21:A:ILE:HG22	6	0.71
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD13	14	0.71
(2,249)	1:14:B:LYS:HE2	1:22:B:GLU:HB2	3	0.71
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG2	3	0.7
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD11	13	0.7
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD12	11	0.7
(2,353)	1:32:A:LYS:HD3	1:30:A:SER:HB2	5	0.7
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	8	0.7
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	8	0.7
(2,871)	1:31:A:GLY:HA2	1:15:A:CYS:HB3	13	0.69
(2,868)	1:31:A:GLY:HA2	1:15:A:CYS:HB3	13	0.69
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD12	3	0.69
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD13	14	0.69
(2,358)	1:14:C:LYS:HD3	1:22:C:GLU:HA	4	0.69
(2,355)	1:32:C:LYS:HD3	1:30:C:SER:HB3	4	0.69
(2,355)	1:32:C:LYS:HD3	1:30:C:SER:HB2	11	0.69
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	4	0.69
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	4	0.69
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	15	0.69
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	15	0.69
(2,270)	1:14:B:LYS:HE2	1:15:B:CYS:HB2	6	0.69
(2,270)	1:14:B:LYS:HE3	1:15:B:CYS:HB2	6	0.69
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	2	0.69
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	2	0.69
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	14	0.68
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD12	8	0.68
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD11	12	0.68
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD12	17	0.68
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	5	0.68
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	5	0.68
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	7	0.68
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	7	0.68
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	11	0.68
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	11	0.68
(2,250)	1:14:C:LYS:HE2	1:22:C:GLU:HB2	20	0.68
(2,1016)	1:13:A:PRO:HB2	1:21:A:ILE:HG21	19	0.67
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD11	9	0.67
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD11	9	0.67
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD13	13	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	5	0.67
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	5	0.67
(2,270)	1:14:B:LYS:HE2	1:15:B:CYS:HB2	13	0.67
(2,270)	1:14:B:LYS:HE3	1:15:B:CYS:HB2	13	0.67
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	8	0.66
(2,1407)	1:15:A:CYS:HA	1:12:A:CYS:HB3	18	0.66
(2,698)	1:15:A:CYS:HA	1:12:A:CYS:HB3	18	0.66
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD12	1	0.66
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD12	13	0.66
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD13	10	0.66
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	14	0.66
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	14	0.66
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	5	0.66
(2,1556)	1:43:C:LEU:HD12	1:8:B:LEU:HD23	18	0.65
(2,1409)	1:15:C:CYS:HA	1:16:C:GLU:HB2	1	0.65
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG2	13	0.65
(2,700)	1:15:C:CYS:HA	1:16:C:GLU:HB2	1	0.65
(2,470)	1:43:C:LEU:HD12	1:8:B:LEU:HD23	18	0.65
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD13	10	0.65
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD11	14	0.65
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD11	2	0.65
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	4	0.65
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	4	0.65
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	18	0.64
(2,1409)	1:15:C:CYS:HA	1:12:C:CYS:HB3	4	0.64
(2,1408)	1:15:B:CYS:HA	1:12:B:CYS:HB3	13	0.64
(2,1408)	1:15:B:CYS:HA	1:12:B:CYS:HB3	15	0.64
(2,1407)	1:15:A:CYS:HA	1:16:A:GLU:HB2	7	0.64
(2,1407)	1:15:A:CYS:HA	1:12:A:CYS:HB3	10	0.64
(2,1017)	1:27:B:PRO:HB2	1:21:B:ILE:HG21	5	0.64
(2,700)	1:15:C:CYS:HA	1:12:C:CYS:HB3	4	0.64
(2,699)	1:15:B:CYS:HA	1:12:B:CYS:HB3	13	0.64
(2,699)	1:15:B:CYS:HA	1:12:B:CYS:HB3	15	0.64
(2,698)	1:15:A:CYS:HA	1:16:A:GLU:HB2	7	0.64
(2,698)	1:15:A:CYS:HA	1:12:A:CYS:HB3	10	0.64
(2,604)	1:50:B:HIS:HA	1:32:A:LYS:HD3	16	0.64
(2,484)	1:51:B:LEU:HD13	1:48:A:GLN:HB3	16	0.64
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD12	19	0.64
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD13	7	0.64
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	6	0.64
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	6	0.64
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	13	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	13	0.64
(1,2820)	1:34:B:VAL:H	1:31:B:GLY:H	1	0.64
(1,2698)	1:31:B:GLY:H	1:34:B:VAL:H	1	0.64
(2,1509)	1:35:A:ILE:HD11	1:11:A:ALA:HA	16	0.63
(2,1407)	1:15:A:CYS:HA	1:16:A:GLU:HB2	19	0.63
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	16	0.63
(2,698)	1:15:A:CYS:HA	1:16:A:GLU:HB2	19	0.63
(2,663)	1:35:A:ILE:HD11	1:11:A:ALA:HA	16	0.63
(2,604)	1:50:B:HIS:HA	1:32:A:LYS:HD2	9	0.63
(2,484)	1:51:B:LEU:HD13	1:48:A:GLN:HB3	12	0.63
(2,400)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	16	0.63
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD11	15	0.63
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	10	0.62
(2,1409)	1:15:C:CYS:HA	1:12:C:CYS:HB3	6	0.62
(2,1408)	1:15:B:CYS:HA	1:12:B:CYS:HB3	9	0.62
(2,1408)	1:15:B:CYS:HA	1:12:B:CYS:HB3	17	0.62
(2,1407)	1:15:A:CYS:HA	1:12:A:CYS:HB3	9	0.62
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG3	1	0.62
(2,700)	1:15:C:CYS:HA	1:12:C:CYS:HB3	6	0.62
(2,699)	1:15:B:CYS:HA	1:12:B:CYS:HB3	9	0.62
(2,699)	1:15:B:CYS:HA	1:12:B:CYS:HB3	17	0.62
(2,698)	1:15:A:CYS:HA	1:12:A:CYS:HB3	9	0.62
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD11	1	0.62
(2,137)	1:15:A:CYS:H	1:14:A:LYS:HG2	1	0.62
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG3	16	0.62
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	16	0.61
(2,1409)	1:15:C:CYS:HA	1:12:C:CYS:HB3	5	0.61
(2,1408)	1:15:B:CYS:HA	1:12:B:CYS:HB3	8	0.61
(2,1408)	1:15:B:CYS:HA	1:12:B:CYS:HB3	18	0.61
(2,1407)	1:15:A:CYS:HA	1:12:A:CYS:HB3	4	0.61
(2,1407)	1:15:A:CYS:HA	1:12:A:CYS:HB3	6	0.61
(2,1407)	1:15:A:CYS:HA	1:16:A:GLU:HB2	14	0.61
(2,1407)	1:15:A:CYS:HA	1:12:A:CYS:HB3	16	0.61
(2,700)	1:15:C:CYS:HA	1:12:C:CYS:HB3	5	0.61
(2,699)	1:15:B:CYS:HA	1:12:B:CYS:HB3	8	0.61
(2,699)	1:15:B:CYS:HA	1:12:B:CYS:HB3	18	0.61
(2,698)	1:15:A:CYS:HA	1:12:A:CYS:HB3	4	0.61
(2,698)	1:15:A:CYS:HA	1:12:A:CYS:HB3	6	0.61
(2,698)	1:15:A:CYS:HA	1:16:A:GLU:HB2	14	0.61
(2,698)	1:15:A:CYS:HA	1:12:A:CYS:HB3	16	0.61
(2,355)	1:32:C:LYS:HD3	1:30:C:SER:HB2	1	0.61
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	11	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	11	0.61
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	17	0.61
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	17	0.61
(2,270)	1:14:B:LYS:HE2	1:15:B:CYS:HB2	7	0.61
(2,270)	1:14:B:LYS:HE3	1:15:B:CYS:HB2	7	0.61
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	3	0.61
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	3	0.61
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG3	9	0.61
(1,4578)	1:34:C:VAL:H	1:31:C:GLY:H	20	0.61
(1,4456)	1:31:C:GLY:H	1:34:C:VAL:H	20	0.61
(2,1556)	1:43:C:LEU:HD12	1:8:C:LEU:HD21	8	0.6
(2,1409)	1:15:C:CYS:HA	1:16:C:GLU:HB2	2	0.6
(2,1409)	1:15:C:CYS:HA	1:16:C:GLU:HB2	15	0.6
(2,1193)	1:27:C:PRO:HG2	1:21:C:ILE:HG23	6	0.6
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG2	1	0.6
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG3	11	0.6
(2,700)	1:15:C:CYS:HA	1:16:C:GLU:HB2	2	0.6
(2,700)	1:15:C:CYS:HA	1:16:C:GLU:HB2	15	0.6
(2,572)	1:2:C:VAL:HG13	1:1:C:FME:HA	12	0.6
(2,485)	1:51:C:LEU:HD11	1:48:B:GLN:HB3	3	0.6
(2,470)	1:43:C:LEU:HD12	1:8:C:LEU:HD21	8	0.6
(2,401)	1:27:C:PRO:HG2	1:21:C:ILE:HG23	6	0.6
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD11	16	0.6
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	20	0.6
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	20	0.6
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG3	11	0.6
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG3	4	0.6
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	13	0.59
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	19	0.59
(2,1408)	1:15:B:CYS:HA	1:12:B:CYS:HB3	10	0.59
(2,1407)	1:15:A:CYS:HA	1:16:A:GLU:HB2	3	0.59
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG2	12	0.59
(2,699)	1:15:B:CYS:HA	1:12:B:CYS:HB3	10	0.59
(2,698)	1:15:A:CYS:HA	1:16:A:GLU:HB2	3	0.59
(2,581)	1:42:C:THR:HG23	1:3:B:ILE:HG12	15	0.59
(2,571)	1:2:B:VAL:HG12	1:1:B:FME:HA	10	0.59
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD12	20	0.59
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	15	0.59
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	15	0.59
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	16	0.59
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	16	0.59
(2,250)	1:14:C:LYS:HE2	1:22:C:GLU:HB2	9	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,249)	1:14:B:LYS:HE2	1:22:B:GLU:HB2	20	0.59
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG3	9	0.59
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG3	3	0.59
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	12	0.58
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	1	0.58
(2,1409)	1:15:C:CYS:HA	1:16:C:GLU:HB2	11	0.58
(2,1409)	1:15:C:CYS:HA	1:12:C:CYS:HB3	12	0.58
(2,1409)	1:15:C:CYS:HA	1:12:C:CYS:HB3	19	0.58
(2,1407)	1:15:A:CYS:HA	1:16:A:GLU:HB2	11	0.58
(2,700)	1:15:C:CYS:HA	1:16:C:GLU:HB2	11	0.58
(2,700)	1:15:C:CYS:HA	1:12:C:CYS:HB3	12	0.58
(2,700)	1:15:C:CYS:HA	1:12:C:CYS:HB3	19	0.58
(2,698)	1:15:A:CYS:HA	1:16:A:GLU:HB2	11	0.58
(2,580)	1:42:B:THR:HG21	1:3:A:ILE:HG12	14	0.58
(2,483)	1:51:A:LEU:HD12	1:48:C:GLN:HB3	16	0.58
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD11	2	0.58
(2,99)	1:35:B:ILE:H	1:9:B:GLU:HG2	10	0.58
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG3	1	0.58
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG3	2	0.58
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG2	13	0.58
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG3	17	0.58
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG2	6	0.58
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG3	17	0.58
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	3	0.57
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	7	0.57
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	6	0.57
(2,1409)	1:15:C:CYS:HA	1:12:C:CYS:HB3	13	0.57
(2,1409)	1:15:C:CYS:HA	1:12:C:CYS:HB3	14	0.57
(2,1409)	1:15:C:CYS:HA	1:16:C:GLU:HB2	16	0.57
(2,1408)	1:15:B:CYS:HA	1:12:B:CYS:HB3	2	0.57
(2,1407)	1:15:A:CYS:HA	1:12:A:CYS:HB3	1	0.57
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG2	14	0.57
(2,700)	1:15:C:CYS:HA	1:12:C:CYS:HB3	13	0.57
(2,700)	1:15:C:CYS:HA	1:12:C:CYS:HB3	14	0.57
(2,700)	1:15:C:CYS:HA	1:16:C:GLU:HB2	16	0.57
(2,699)	1:15:B:CYS:HA	1:12:B:CYS:HB3	2	0.57
(2,698)	1:15:A:CYS:HA	1:12:A:CYS:HB3	1	0.57
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD11	3	0.57
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD12	5	0.57
(2,358)	1:14:C:LYS:HD3	1:22:C:GLU:HA	6	0.57
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	13	0.57
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	13	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG3	6	0.57
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG3	10	0.57
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG2	15	0.57
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	2	0.56
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	9	0.56
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	10	0.56
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	15	0.56
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	18	0.56
(2,1409)	1:15:C:CYS:HA	1:12:C:CYS:HB3	9	0.56
(2,1408)	1:15:B:CYS:HA	1:12:B:CYS:HB3	16	0.56
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG2	19	0.56
(2,700)	1:15:C:CYS:HA	1:12:C:CYS:HB3	9	0.56
(2,699)	1:15:B:CYS:HA	1:12:B:CYS:HB3	16	0.56
(2,604)	1:50:B:HIS:HA	1:32:A:LYS:HD3	8	0.56
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	8	0.56
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	8	0.56
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	10	0.56
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	10	0.56
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	6	0.56
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	6	0.56
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	17	0.56
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	17	0.56
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG3	8	0.56
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	8	0.56
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	16	0.55
(2,1409)	1:15:C:CYS:HA	1:12:C:CYS:HB3	3	0.55
(2,1409)	1:15:C:CYS:HA	1:12:C:CYS:HB3	18	0.55
(2,1408)	1:15:B:CYS:HA	1:16:B:GLU:HB2	1	0.55
(2,1408)	1:15:B:CYS:HA	1:12:B:CYS:HB3	6	0.55
(2,1408)	1:15:B:CYS:HA	1:12:B:CYS:HB3	7	0.55
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG2	8	0.55
(2,700)	1:15:C:CYS:HA	1:12:C:CYS:HB3	3	0.55
(2,700)	1:15:C:CYS:HA	1:12:C:CYS:HB3	18	0.55
(2,699)	1:15:B:CYS:HA	1:16:B:GLU:HB2	1	0.55
(2,699)	1:15:B:CYS:HA	1:12:B:CYS:HB3	6	0.55
(2,699)	1:15:B:CYS:HA	1:12:B:CYS:HB3	7	0.55
(2,483)	1:51:A:LEU:HD11	1:48:C:GLN:HB3	12	0.55
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD11	20	0.55
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	2	0.55
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	2	0.55
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	15	0.55
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	10	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	1	0.54
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	3	0.54
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	12	0.54
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	12	0.54
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG2	2	0.54
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG3	5	0.54
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG2	11	0.54
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	15	0.54
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	2	0.53
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	12	0.53
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	18	0.53
(2,1409)	1:15:C:CYS:HA	1:16:C:GLU:HB2	20	0.53
(2,1408)	1:15:B:CYS:HA	1:12:B:CYS:HB3	4	0.53
(2,1407)	1:15:A:CYS:HA	1:12:A:CYS:HB3	17	0.53
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG2	11	0.53
(2,700)	1:15:C:CYS:HA	1:16:C:GLU:HB2	20	0.53
(2,699)	1:15:B:CYS:HA	1:12:B:CYS:HB3	4	0.53
(2,698)	1:15:A:CYS:HA	1:12:A:CYS:HB3	17	0.53
(2,485)	1:51:C:LEU:HD12	1:48:B:GLN:HB3	17	0.53
(2,399)	1:13:A:PRO:HG2	1:21:A:ILE:HD12	17	0.53
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	18	0.53
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	18	0.53
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG3	4	0.53
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG2	1	0.53
(1,4686)	1:36:C:LEU:HD22	1:46:A:PHE:HZ	19	0.53
(2,1556)	1:43:C:LEU:HD12	1:8:C:LEU:HD21	13	0.52
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	11	0.52
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	17	0.52
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	9	0.52
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	11	0.52
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	2	0.52
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	10	0.52
(2,1409)	1:15:C:CYS:HA	1:12:C:CYS:HB3	10	0.52
(2,1408)	1:15:B:CYS:HA	1:12:B:CYS:HB3	14	0.52
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG2	1	0.52
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG2	11	0.52
(2,700)	1:15:C:CYS:HA	1:12:C:CYS:HB3	10	0.52
(2,699)	1:15:B:CYS:HA	1:12:B:CYS:HB3	14	0.52
(2,470)	1:43:C:LEU:HD12	1:8:C:LEU:HD21	13	0.52
(2,250)	1:14:C:LYS:HE3	1:20:C:GLU:HG2	18	0.52
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	12	0.52
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	12	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	13	0.51
(2,1407)	1:15:A:CYS:HA	1:16:A:GLU:HB2	8	0.51
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG2	7	0.51
(2,1162)	1:35:B:ILE:HG13	1:16:B:GLU:HG3	20	0.51
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG2	13	0.51
(2,698)	1:15:A:CYS:HA	1:16:A:GLU:HB2	8	0.51
(2,483)	1:51:A:LEU:HD12	1:48:C:GLN:HB3	19	0.51
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	12	0.51
(2,1556)	1:43:C:LEU:HD12	1:8:C:LEU:HD22	5	0.5
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	4	0.5
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	5	0.5
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	4	0.5
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	1	0.5
(2,1408)	1:15:B:CYS:HA	1:12:B:CYS:HB3	11	0.5
(2,1192)	1:27:B:PRO:HG2	1:21:B:ILE:HG21	8	0.5
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG2	16	0.5
(2,699)	1:15:B:CYS:HA	1:12:B:CYS:HB3	11	0.5
(2,470)	1:43:C:LEU:HD12	1:8:C:LEU:HD22	5	0.5
(2,400)	1:27:B:PRO:HG2	1:21:B:ILE:HG21	8	0.5
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	10	0.5
(2,1556)	1:43:C:LEU:HD13	1:8:C:LEU:HD23	16	0.49
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	6	0.49
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	4	0.49
(2,1407)	1:15:A:CYS:HA	1:12:A:CYS:HB3	12	0.49
(2,1162)	1:35:B:ILE:HG12	1:16:B:GLU:HG2	5	0.49
(2,1151)	1:43:A:LEU:HG	1:43:B:LEU:HG	8	0.49
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	8	0.49
(2,698)	1:15:A:CYS:HA	1:12:A:CYS:HB3	12	0.49
(2,470)	1:43:C:LEU:HD13	1:8:C:LEU:HD23	16	0.49
(2,380)	1:43:A:LEU:HG	1:43:B:LEU:HG	8	0.49
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	8	0.49
(2,270)	1:14:B:LYS:HE2	1:15:B:CYS:HB2	5	0.49
(2,270)	1:14:B:LYS:HE3	1:15:B:CYS:HB2	5	0.49
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG3	20	0.49
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	7	0.48
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	17	0.48
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	7	0.48
(2,1151)	1:43:C:LEU:HG	1:43:A:LEU:HG	9	0.48
(2,1151)	1:43:B:LEU:HG	1:43:C:LEU:HG	10	0.48
(2,1151)	1:43:A:LEU:HG	1:43:B:LEU:HG	13	0.48
(2,1018)	1:13:C:PRO:HB2	1:21:C:ILE:HG21	3	0.48
(2,786)	1:20:B:GLU:HG2	1:26:B:CYS:HB2	3	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,786)	1:20:B:GLU:HG2	1:26:B:CYS:HB3	3	0.48
(2,786)	1:20:B:GLU:HG3	1:26:B:CYS:HB2	3	0.48
(2,786)	1:20:B:GLU:HG3	1:26:B:CYS:HB3	3	0.48
(2,483)	1:51:A:LEU:HD11	1:47:C:ILE:HB	2	0.48
(2,380)	1:43:C:LEU:HG	1:43:A:LEU:HG	9	0.48
(2,380)	1:43:B:LEU:HG	1:43:C:LEU:HG	10	0.48
(2,380)	1:43:A:LEU:HG	1:43:B:LEU:HG	13	0.48
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG2	5	0.48
(2,1555)	1:43:B:LEU:HD11	1:8:B:LEU:HD23	9	0.47
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	15	0.47
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	6	0.47
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	5	0.47
(2,1408)	1:15:B:CYS:HA	1:16:B:GLU:HB2	12	0.47
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG2	2	0.47
(2,1151)	1:43:A:LEU:HG	1:43:B:LEU:HG	16	0.47
(2,699)	1:15:B:CYS:HA	1:16:B:GLU:HB2	12	0.47
(2,469)	1:43:B:LEU:HD11	1:8:B:LEU:HD23	9	0.47
(2,380)	1:43:A:LEU:HG	1:43:B:LEU:HG	16	0.47
(2,248)	1:14:A:LYS:HE2	1:22:A:GLU:HB2	17	0.47
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	19	0.47
(1,4186)	1:21:C:ILE:HB	1:22:C:GLU:HB2	19	0.47
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	12	0.47
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	5	0.46
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	20	0.46
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	11	0.46
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	15	0.46
(2,1407)	1:15:A:CYS:HA	1:12:A:CYS:HB3	2	0.46
(2,1151)	1:43:A:LEU:HG	1:43:B:LEU:HG	6	0.46
(2,698)	1:15:A:CYS:HA	1:12:A:CYS:HB3	2	0.46
(2,581)	1:42:C:THR:HG23	1:4:B:ALA:HB3	7	0.46
(2,380)	1:43:A:LEU:HG	1:43:B:LEU:HG	6	0.46
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	16	0.46
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	16	0.46
(2,1555)	1:43:B:LEU:HD11	1:8:B:LEU:HD21	8	0.45
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	16	0.45
(2,1328)	1:30:C:SER:HB3	1:32:C:LYS:HD3	13	0.45
(2,1018)	1:13:C:PRO:HB2	1:21:C:ILE:HG21	18	0.45
(2,484)	1:51:B:LEU:HD12	1:48:A:GLN:HB3	3	0.45
(2,469)	1:43:B:LEU:HD11	1:8:B:LEU:HD21	8	0.45
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	14	0.45
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	8	0.44
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	3	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	20	0.44
(2,1409)	1:15:C:CYS:HA	1:12:C:CYS:HB3	17	0.44
(2,1407)	1:15:A:CYS:HA	1:16:A:GLU:HB2	15	0.44
(2,700)	1:15:C:CYS:HA	1:12:C:CYS:HB3	17	0.44
(2,698)	1:15:A:CYS:HA	1:16:A:GLU:HB2	15	0.44
(2,572)	1:2:C:VAL:HG13	1:39:A:GLN:HA	14	0.44
(2,250)	1:14:C:LYS:HE2	1:22:C:GLU:HB2	17	0.44
(2,98)	1:35:A:ILE:H	1:10:A:VAL:HB	15	0.44
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	9	0.44
(1,3888)	1:10:C:VAL:HG11	1:36:C:LEU:HA	17	0.44
(1,3888)	1:10:C:VAL:HG12	1:36:C:LEU:HA	17	0.44
(1,3888)	1:10:C:VAL:HG13	1:36:C:LEU:HA	17	0.44
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	5	0.44
(2,1555)	1:43:B:LEU:HD12	1:8:B:LEU:HD22	10	0.43
(2,1408)	1:15:B:CYS:HA	1:16:B:GLU:HB2	19	0.43
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG2	14	0.43
(2,1151)	1:43:A:LEU:HG	1:43:B:LEU:HG	5	0.43
(2,1151)	1:43:B:LEU:HG	1:43:C:LEU:HG	11	0.43
(2,699)	1:15:B:CYS:HA	1:16:B:GLU:HB2	19	0.43
(2,570)	1:2:A:VAL:HG11	1:1:A:FME:HA	19	0.43
(2,469)	1:43:B:LEU:HD12	1:8:B:LEU:HD22	10	0.43
(2,401)	1:13:C:PRO:HG2	1:21:C:ILE:HD12	7	0.43
(2,380)	1:43:A:LEU:HG	1:43:B:LEU:HG	5	0.43
(2,380)	1:43:B:LEU:HG	1:43:C:LEU:HG	11	0.43
(2,250)	1:14:C:LYS:HE2	1:22:C:GLU:HB2	2	0.43
(2,250)	1:14:C:LYS:HE2	1:22:C:GLU:HB2	10	0.43
(2,248)	1:14:A:LYS:HE2	1:22:A:GLU:HB2	20	0.43
(2,98)	1:35:A:ILE:H	1:9:A:GLU:HG2	9	0.43
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	18	0.43
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	18	0.43
(2,1555)	1:43:B:LEU:HD12	1:8:B:LEU:HD23	18	0.42
(2,1349)	1:8:C:LEU:HD21	1:43:C:LEU:HG	13	0.42
(2,1151)	1:43:A:LEU:HG	1:43:B:LEU:HG	7	0.42
(2,1151)	1:43:B:LEU:HG	1:43:C:LEU:HG	14	0.42
(2,1151)	1:43:B:LEU:HG	1:43:C:LEU:HG	18	0.42
(2,483)	1:51:A:LEU:HD12	1:47:C:ILE:HB	10	0.42
(2,469)	1:43:B:LEU:HD12	1:8:B:LEU:HD23	18	0.42
(2,380)	1:43:A:LEU:HG	1:43:B:LEU:HG	7	0.42
(2,380)	1:43:B:LEU:HG	1:43:C:LEU:HG	14	0.42
(2,380)	1:43:B:LEU:HG	1:43:C:LEU:HG	18	0.42
(2,355)	1:14:C:LYS:HD3	1:21:C:ILE:HA	6	0.42
(2,249)	1:14:B:LYS:HE2	1:22:B:GLU:HB2	16	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,248)	1:14:A:LYS:HE2	1:22:A:GLU:HB2	9	0.42
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	8	0.42
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	4	0.42
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	12	0.42
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	15	0.42
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	15	0.42
(1,400)	1:12:A:CYS:H	1:34:A:VAL:HB	15	0.42
(2,1555)	1:43:B:LEU:HD11	1:8:A:LEU:HD21	12	0.41
(2,1326)	1:30:A:SER:HB3	1:32:A:LYS:HG3	19	0.41
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG2	20	0.41
(2,1151)	1:43:C:LEU:HG	1:43:A:LEU:HG	15	0.41
(2,469)	1:43:B:LEU:HD11	1:8:A:LEU:HD21	12	0.41
(2,380)	1:43:C:LEU:HG	1:43:A:LEU:HG	15	0.41
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	12	0.41
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	12	0.41
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	9	0.41
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	20	0.41
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	18	0.41
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	18	0.41
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	4	0.41
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	4	0.41
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	4	0.41
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	10	0.41
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	10	0.41
(2,1555)	1:43:B:LEU:HD13	1:8:B:LEU:HD22	13	0.4
(2,1409)	1:15:C:CYS:HA	1:16:C:GLU:HB2	8	0.4
(2,1407)	1:15:A:CYS:HA	1:12:A:CYS:HB3	5	0.4
(2,700)	1:15:C:CYS:HA	1:16:C:GLU:HB2	8	0.4
(2,698)	1:15:A:CYS:HA	1:12:A:CYS:HB3	5	0.4
(2,603)	1:50:A:HIS:HA	1:32:C:LYS:HD3	10	0.4
(2,484)	1:51:B:LEU:HD13	1:47:A:ILE:HB	17	0.4
(2,469)	1:43:B:LEU:HD13	1:8:B:LEU:HD22	13	0.4
(2,270)	1:14:B:LYS:HE2	1:15:B:CYS:HB2	10	0.4
(2,270)	1:14:B:LYS:HE3	1:15:B:CYS:HB2	10	0.4
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	16	0.4
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	18	0.4
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	18	0.4
(1,4908)	1:43:C:LEU:HB3	1:44:C:LEU:HB2	11	0.4
(1,4908)	1:43:C:LEU:HB3	1:44:C:LEU:HB3	11	0.4
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	10	0.4
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	16	0.4
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	16	0.4
(2,1408)	1:15:B:CYS:HA	1:16:B:GLU:HB2	5	0.39
(2,1050)	1:26:B:CYS:HB3	1:15:B:CYS:HB3	3	0.39
(2,699)	1:15:B:CYS:HA	1:16:B:GLU:HB2	5	0.39
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	9	0.39
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	9	0.39
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	9	0.39
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	9	0.39
(2,180)	1:19:B:GLY:H	1:17:B:ARG:HD3	17	0.39
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	3	0.39
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	6	0.39
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	1	0.39
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	2	0.39
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	4	0.39
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	6	0.39
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	8	0.39
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	8	0.39
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	8	0.39
(2,1554)	1:43:A:LEU:HD13	1:8:A:LEU:HD21	15	0.38
(2,1161)	1:35:A:ILE:HG12	1:16:A:GLU:HG3	17	0.38
(2,485)	1:51:C:LEU:HD13	1:47:B:ILE:HB	15	0.38
(2,485)	1:51:C:LEU:HD12	1:47:B:ILE:HB	19	0.38
(2,483)	1:51:A:LEU:HD11	1:47:C:ILE:HB	7	0.38
(2,483)	1:51:A:LEU:HD12	1:47:C:ILE:HB	8	0.38
(2,468)	1:43:A:LEU:HD13	1:8:A:LEU:HD21	15	0.38
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	1	0.38
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	1	0.38
(2,250)	1:14:C:LYS:HE2	1:22:C:GLU:HB2	7	0.38
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	13	0.38
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	11	0.38
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	15	0.38
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	2	0.38
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	12	0.38
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	12	0.38
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	11	0.38
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	11	0.38
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	11	0.38
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	15	0.38
(1,400)	1:12:A:CYS:H	1:34:A:VAL:HB	12	0.38
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	20	0.37
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	13	0.37
(2,1151)	1:43:C:LEU:HG	1:43:A:LEU:HG	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1151)	1:43:A:LEU:HG	1:43:B:LEU:HG	4	0.37
(2,579)	1:42:A:THR:HG23	1:4:C:ALA:HB2	2	0.37
(2,485)	1:51:C:LEU:HD11	1:47:B:ILE:HB	13	0.37
(2,380)	1:43:C:LEU:HG	1:43:A:LEU:HG	1	0.37
(2,380)	1:43:A:LEU:HG	1:43:B:LEU:HG	4	0.37
(2,99)	1:35:B:ILE:H	1:9:B:GLU:HG2	15	0.37
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	14	0.37
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	5	0.37
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	8	0.37
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	17	0.37
(1,636)	1:21:A:ILE:HB	1:22:A:GLU:HB2	1	0.37
(1,636)	1:21:A:ILE:HB	1:22:A:GLU:HB2	8	0.37
(1,338)	1:10:A:VAL:HG11	1:36:A:LEU:HA	12	0.37
(1,338)	1:10:A:VAL:HG12	1:36:A:LEU:HA	12	0.37
(1,338)	1:10:A:VAL:HG13	1:36:A:LEU:HA	12	0.37
(1,338)	1:10:A:VAL:HG11	1:36:A:LEU:HA	17	0.37
(1,338)	1:10:A:VAL:HG12	1:36:A:LEU:HA	17	0.37
(1,338)	1:10:A:VAL:HG13	1:36:A:LEU:HA	17	0.37
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	19	0.36
(2,1151)	1:43:B:LEU:HG	1:43:C:LEU:HG	17	0.36
(2,485)	1:51:C:LEU:HD12	1:48:B:GLN:HB3	18	0.36
(2,380)	1:43:B:LEU:HG	1:43:C:LEU:HG	17	0.36
(2,265)	1:49:C:LYS:HE2	1:53:C:LYS:HD2	1	0.36
(2,264)	1:49:B:LYS:HE2	1:53:B:LYS:HD2	13	0.36
(2,249)	1:14:B:LYS:HE2	1:22:B:GLU:HB2	7	0.36
(2,248)	1:14:A:LYS:HE2	1:22:A:GLU:HB2	5	0.36
(2,248)	1:14:A:LYS:HE2	1:22:A:GLU:HB2	19	0.36
(2,100)	1:35:C:ILE:H	1:9:C:GLU:HG2	10	0.36
(2,99)	1:35:B:ILE:H	1:9:B:GLU:HG2	12	0.36
(2,98)	1:35:A:ILE:H	1:9:A:GLU:HG3	7	0.36
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	11	0.36
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	11	0.36
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	19	0.36
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	5	0.36
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	16	0.36
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	6	0.36
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	17	0.36
(1,338)	1:10:A:VAL:HG11	1:36:A:LEU:HA	2	0.36
(1,338)	1:10:A:VAL:HG12	1:36:A:LEU:HA	2	0.36
(1,338)	1:10:A:VAL:HG13	1:36:A:LEU:HA	2	0.36
(2,1327)	1:30:B:SER:HB3	1:32:B:LYS:HG3	9	0.35
(2,1326)	1:30:A:SER:HB3	1:32:A:LYS:HG3	2	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1326)	1:30:A:SER:HB3	1:32:A:LYS:HD3	7	0.35
(2,1151)	1:43:C:LEU:HG	1:43:A:LEU:HG	12	0.35
(2,484)	1:51:B:LEU:HD12	1:47:A:ILE:HB	7	0.35
(2,484)	1:51:B:LEU:HD11	1:47:A:ILE:HB	19	0.35
(2,380)	1:43:C:LEU:HG	1:43:A:LEU:HG	12	0.35
(2,265)	1:49:C:LYS:HE2	1:53:C:LYS:HD2	4	0.35
(2,265)	1:49:C:LYS:HE2	1:53:C:LYS:HD2	5	0.35
(2,264)	1:49:B:LYS:HE2	1:53:B:LYS:HD2	18	0.35
(2,100)	1:35:C:ILE:H	1:9:C:GLU:HG2	19	0.35
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	7	0.35
(1,4578)	1:34:C:VAL:H	1:31:C:GLY:H	7	0.35
(1,4456)	1:31:C:GLY:H	1:34:C:VAL:H	7	0.35
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	17	0.35
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	20	0.35
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	11	0.35
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	11	0.35
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	19	0.35
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	19	0.35
(1,498)	1:16:A:GLU:H	1:33:A:GLY:H	13	0.35
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	17	0.34
(2,1328)	1:30:C:SER:HB2	1:32:C:LYS:HG3	16	0.34
(2,1327)	1:30:B:SER:HB3	1:32:B:LYS:HG3	12	0.34
(2,1151)	1:43:C:LEU:HG	1:43:A:LEU:HG	2	0.34
(2,580)	1:42:B:THR:HG22	1:3:A:ILE:HG12	10	0.34
(2,380)	1:43:C:LEU:HG	1:43:A:LEU:HG	2	0.34
(2,265)	1:49:C:LYS:HE2	1:53:C:LYS:HD2	19	0.34
(2,264)	1:49:B:LYS:HE2	1:53:B:LYS:HD2	2	0.34
(2,250)	1:14:C:LYS:HE3	1:22:C:GLU:HB2	5	0.34
(2,180)	1:19:B:GLY:H	1:17:B:ARG:HD3	10	0.34
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	11	0.34
(1,4821)	1:41:C:TYR:HB3	1:44:C:LEU:HD21	11	0.34
(1,4821)	1:41:C:TYR:HB3	1:44:C:LEU:HD22	11	0.34
(1,4821)	1:41:C:TYR:HB3	1:44:C:LEU:HD23	11	0.34
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	3	0.34
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	6	0.34
(1,2428)	1:21:B:ILE:HB	1:22:B:GLU:HB2	7	0.34
(1,2290)	1:16:B:GLU:H	1:33:B:GLY:H	3	0.34
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	7	0.34
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	9	0.34
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	18	0.34
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	18	0.34
(1,1042)	1:34:A:VAL:H	1:31:A:GLY:H	20	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,914)	1:31:A:GLY:H	1:34:A:VAL:H	20	0.34
(1,498)	1:16:A:GLU:H	1:33:A:GLY:H	12	0.34
(1,381)	1:11:A:ALA:H	1:34:A:VAL:HB	17	0.34
(2,1555)	1:43:B:LEU:HD13	1:8:B:LEU:HD22	15	0.33
(2,1349)	1:8:C:LEU:HD22	1:43:C:LEU:HG	14	0.33
(2,1327)	1:30:B:SER:HB3	1:32:B:LYS:HD3	8	0.33
(2,1327)	1:30:B:SER:HB3	1:32:B:LYS:HG3	13	0.33
(2,1017)	1:13:B:PRO:HB2	1:21:B:ILE:HG22	14	0.33
(2,871)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	7	0.33
(2,868)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	7	0.33
(2,485)	1:51:C:LEU:HD12	1:47:B:ILE:HB	5	0.33
(2,469)	1:43:B:LEU:HD13	1:8:B:LEU:HD22	15	0.33
(2,358)	1:32:C:LYS:HD2	1:49:A:LYS:HA	11	0.33
(2,250)	1:14:C:LYS:HE2	1:22:C:GLU:HB2	16	0.33
(2,100)	1:35:C:ILE:H	1:9:C:GLU:HG2	15	0.33
(2,98)	1:35:A:ILE:H	1:9:A:GLU:HG2	3	0.33
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	18	0.33
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	9	0.33
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	9	0.33
(1,4830)	1:41:C:TYR:HB2	1:44:C:LEU:HD21	11	0.33
(1,4830)	1:41:C:TYR:HB2	1:44:C:LEU:HD22	11	0.33
(1,4830)	1:41:C:TYR:HB2	1:44:C:LEU:HD23	11	0.33
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	7	0.33
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	9	0.33
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	9	0.33
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	9	0.33
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	14	0.33
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	7	0.33
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	7	0.33
(1,911)	1:31:A:GLY:H	1:32:A:LYS:HG2	9	0.33
(1,911)	1:31:A:GLY:H	1:32:A:LYS:HG3	9	0.33
(1,498)	1:16:A:GLU:H	1:33:A:GLY:H	15	0.33
(2,871)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	17	0.32
(2,868)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	17	0.32
(2,571)	1:2:B:VAL:HG12	1:1:B:FME:HA	11	0.32
(2,265)	1:49:C:LYS:HE2	1:53:C:LYS:HD2	11	0.32
(2,249)	1:14:B:LYS:HE2	1:22:B:GLU:HB2	4	0.32
(2,249)	1:14:B:LYS:HE2	1:22:B:GLU:HB2	11	0.32
(2,99)	1:35:B:ILE:H	1:9:B:GLU:HG2	16	0.32
(2,98)	1:35:A:ILE:H	1:12:A:CYS:HB2	5	0.32
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	15	0.32
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	15	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	19	0.32
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	2	0.32
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	6	0.32
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	6	0.32
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	6	0.32
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	13	0.32
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	13	0.32
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	13	0.32
(1,338)	1:10:A:VAL:HG11	1:36:A:LEU:HA	18	0.32
(1,338)	1:10:A:VAL:HG12	1:36:A:LEU:HA	18	0.32
(1,338)	1:10:A:VAL:HG13	1:36:A:LEU:HA	18	0.32
(2,1347)	1:8:A:LEU:HD23	1:43:A:LEU:HG	9	0.31
(2,1151)	1:43:B:LEU:HG	1:43:C:LEU:HG	20	0.31
(2,1018)	1:13:C:PRO:HB2	1:21:C:ILE:HG21	16	0.31
(2,873)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	5	0.31
(2,870)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	5	0.31
(2,604)	1:50:B:HIS:HA	1:32:A:LYS:HD3	14	0.31
(2,483)	1:51:A:LEU:HD13	1:48:C:GLN:HB3	15	0.31
(2,380)	1:43:B:LEU:HG	1:43:C:LEU:HG	20	0.31
(2,264)	1:49:B:LYS:HE2	1:53:B:LYS:HD2	8	0.31
(2,263)	1:49:A:LYS:HE2	1:53:A:LYS:HD2	13	0.31
(2,100)	1:35:C:ILE:H	1:9:C:GLU:HG2	4	0.31
(2,99)	1:35:B:ILE:H	1:9:B:GLU:HG2	18	0.31
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	19	0.31
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	19	0.31
(1,4581)	1:34:C:VAL:H	1:32:C:LYS:HG2	14	0.31
(1,4581)	1:34:C:VAL:H	1:32:C:LYS:HG3	14	0.31
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	9	0.31
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	1	0.31
(1,2428)	1:21:B:ILE:HB	1:22:B:GLU:HB2	5	0.31
(1,2290)	1:16:B:GLU:H	1:33:B:GLY:H	5	0.31
(1,2192)	1:12:B:CYS:H	1:34:B:VAL:HB	5	0.31
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	3	0.31
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	20	0.31
(1,498)	1:16:A:GLU:H	1:33:A:GLY:H	8	0.31
(1,338)	1:10:A:VAL:HG11	1:36:A:LEU:HA	13	0.31
(1,338)	1:10:A:VAL:HG12	1:36:A:LEU:HA	13	0.31
(1,338)	1:10:A:VAL:HG13	1:36:A:LEU:HA	13	0.31
(1,337)	1:10:A:VAL:HG11	1:35:A:ILE:HB	15	0.31
(1,337)	1:10:A:VAL:HG12	1:35:A:ILE:HB	15	0.31
(1,337)	1:10:A:VAL:HG13	1:35:A:ILE:HB	15	0.31
(2,1322)	1:43:C:LEU:HD22	1:43:C:LEU:HA	18	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1321)	1:43:B:LEU:HD23	1:43:B:LEU:HA	15	0.3
(2,1162)	1:35:B:ILE:HG13	1:13:B:PRO:HG3	3	0.3
(2,1016)	1:27:A:PRO:HB2	1:21:A:ILE:HG23	8	0.3
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	9	0.3
(2,872)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	18	0.3
(2,869)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	18	0.3
(2,509)	1:43:C:LEU:HD22	1:43:C:LEU:HA	18	0.3
(2,508)	1:43:B:LEU:HD23	1:43:B:LEU:HA	15	0.3
(2,485)	1:51:C:LEU:HD11	1:47:B:ILE:HB	9	0.3
(2,484)	1:51:B:LEU:HD13	1:47:A:ILE:HB	20	0.3
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	9	0.3
(2,263)	1:49:A:LYS:HE2	1:53:A:LYS:HD2	19	0.3
(2,100)	1:35:C:ILE:H	1:9:C:GLU:HG2	12	0.3
(2,61)	1:3:C:ILE:H	1:2:C:VAL:HB	17	0.3
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	7	0.3
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	7	0.3
(1,4713)	1:37:C:THR:HG21	1:8:C:LEU:HG	6	0.3
(1,4713)	1:37:C:THR:HG22	1:8:C:LEU:HG	6	0.3
(1,4713)	1:37:C:THR:HG23	1:8:C:LEU:HG	6	0.3
(1,3888)	1:10:C:VAL:HG11	1:36:C:LEU:HA	1	0.3
(1,3888)	1:10:C:VAL:HG12	1:36:C:LEU:HA	1	0.3
(1,3888)	1:10:C:VAL:HG13	1:36:C:LEU:HA	1	0.3
(1,3888)	1:10:C:VAL:HG11	1:36:C:LEU:HA	3	0.3
(1,3888)	1:10:C:VAL:HG12	1:36:C:LEU:HA	3	0.3
(1,3888)	1:10:C:VAL:HG13	1:36:C:LEU:HA	3	0.3
(1,3888)	1:10:C:VAL:HG11	1:36:C:LEU:HA	8	0.3
(1,3888)	1:10:C:VAL:HG12	1:36:C:LEU:HA	8	0.3
(1,3888)	1:10:C:VAL:HG13	1:36:C:LEU:HA	8	0.3
(1,3888)	1:10:C:VAL:HG11	1:36:C:LEU:HA	11	0.3
(1,3888)	1:10:C:VAL:HG12	1:36:C:LEU:HA	11	0.3
(1,3888)	1:10:C:VAL:HG13	1:36:C:LEU:HA	11	0.3
(1,3888)	1:10:C:VAL:HG11	1:36:C:LEU:HA	16	0.3
(1,3888)	1:10:C:VAL:HG12	1:36:C:LEU:HA	16	0.3
(1,3888)	1:10:C:VAL:HG13	1:36:C:LEU:HA	16	0.3
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	13	0.3
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	11	0.3
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	5	0.3
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	5	0.3
(1,2290)	1:16:B:GLU:H	1:33:B:GLY:H	12	0.3
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	1	0.3
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	1	0.3
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	1	0.3
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	4	0.3
(1,358)	1:10:A:VAL:H	1:36:A:LEU:HA	10	0.3
(1,338)	1:10:A:VAL:HG11	1:36:A:LEU:HA	4	0.3
(1,338)	1:10:A:VAL:HG12	1:36:A:LEU:HA	4	0.3
(1,338)	1:10:A:VAL:HG13	1:36:A:LEU:HA	4	0.3
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	13	0.3
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	13	0.3
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	13	0.3
(2,1556)	1:43:C:LEU:HD13	1:8:B:LEU:HD22	10	0.29
(2,1349)	1:8:C:LEU:HD21	1:43:A:LEU:HG	18	0.29
(2,1348)	1:8:B:LEU:HD21	1:43:B:LEU:HG	3	0.29
(2,1347)	1:8:A:LEU:HD21	1:43:A:LEU:HG	6	0.29
(2,1328)	1:30:C:SER:HB3	1:32:C:LYS:HD3	15	0.29
(2,1327)	1:30:B:SER:HB2	1:32:B:LYS:HG3	3	0.29
(2,1327)	1:30:B:SER:HB3	1:32:B:LYS:HD3	7	0.29
(2,1322)	1:43:C:LEU:HD21	1:43:C:LEU:HA	14	0.29
(2,1322)	1:43:C:LEU:HD21	1:43:C:LEU:HA	15	0.29
(2,1188)	1:13:A:PRO:HG2	1:28:A:ALA:HB3	13	0.29
(2,509)	1:43:C:LEU:HD21	1:43:C:LEU:HA	14	0.29
(2,509)	1:43:C:LEU:HD21	1:43:C:LEU:HA	15	0.29
(2,484)	1:51:B:LEU:HD11	1:47:A:ILE:HB	10	0.29
(2,470)	1:43:C:LEU:HD13	1:8:B:LEU:HD22	10	0.29
(2,267)	1:51:B:LEU:HB2	1:52:B:ASN:HB2	2	0.29
(2,100)	1:35:C:ILE:H	1:9:C:GLU:HG2	9	0.29
(2,98)	1:35:A:ILE:H	1:9:A:GLU:HG2	14	0.29
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG2	10	0.29
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	3	0.29
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	14	0.29
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD11	20	0.29
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD12	20	0.29
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD13	20	0.29
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD11	20	0.29
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD12	20	0.29
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD13	20	0.29
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD21	20	0.29
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD22	20	0.29
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD23	20	0.29
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD21	20	0.29
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD22	20	0.29
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD23	20	0.29
(1,2435)	1:21:B:ILE:HD11	1:15:B:CYS:HA	12	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2435)	1:21:B:ILE:HD12	1:15:B:CYS:HA	12	0.29
(1,2435)	1:21:B:ILE:HD13	1:15:B:CYS:HA	12	0.29
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	7	0.29
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	7	0.29
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	7	0.29
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	8	0.29
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	8	0.29
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	8	0.29
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	9	0.29
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	9	0.29
(1,358)	1:10:A:VAL:H	1:36:A:LEU:HA	8	0.29
(2,1406)	1:15:C:CYS:HA	1:17:C:ARG:HD3	12	0.28
(2,1328)	1:30:C:SER:HB3	1:32:C:LYS:HD3	6	0.28
(2,1327)	1:30:B:SER:HB3	1:32:B:LYS:HG3	17	0.28
(2,1322)	1:43:C:LEU:HD22	1:43:C:LEU:HA	4	0.28
(2,1322)	1:43:C:LEU:HD21	1:43:C:LEU:HA	7	0.28
(2,1322)	1:43:C:LEU:HD21	1:43:C:LEU:HA	11	0.28
(2,1322)	1:43:C:LEU:HD21	1:43:C:LEU:HA	13	0.28
(2,1321)	1:43:B:LEU:HD21	1:43:B:LEU:HA	7	0.28
(2,1321)	1:43:B:LEU:HD23	1:43:B:LEU:HA	8	0.28
(2,1320)	1:43:A:LEU:HD22	1:43:A:LEU:HA	5	0.28
(2,1320)	1:43:A:LEU:HD23	1:43:A:LEU:HA	10	0.28
(2,1320)	1:43:A:LEU:HD23	1:43:A:LEU:HA	11	0.28
(2,1016)	1:13:A:PRO:HB2	1:21:A:ILE:HG21	11	0.28
(2,873)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	18	0.28
(2,870)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	18	0.28
(2,697)	1:15:C:CYS:HA	1:17:C:ARG:HD3	12	0.28
(2,509)	1:43:C:LEU:HD22	1:43:C:LEU:HA	4	0.28
(2,509)	1:43:C:LEU:HD21	1:43:C:LEU:HA	7	0.28
(2,509)	1:43:C:LEU:HD21	1:43:C:LEU:HA	11	0.28
(2,509)	1:43:C:LEU:HD21	1:43:C:LEU:HA	13	0.28
(2,508)	1:43:B:LEU:HD21	1:43:B:LEU:HA	7	0.28
(2,508)	1:43:B:LEU:HD23	1:43:B:LEU:HA	8	0.28
(2,507)	1:43:A:LEU:HD22	1:43:A:LEU:HA	5	0.28
(2,507)	1:43:A:LEU:HD23	1:43:A:LEU:HA	10	0.28
(2,507)	1:43:A:LEU:HD23	1:43:A:LEU:HA	11	0.28
(2,484)	1:51:B:LEU:HD12	1:47:A:ILE:HB	1	0.28
(2,264)	1:49:B:LYS:HE2	1:53:B:LYS:HD2	6	0.28
(2,137)	1:15:A:CYS:H	1:21:A:ILE:HG13	4	0.28
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG2	15	0.28
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG2	19	0.28
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG2	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG2	8	0.28
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	1	0.28
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	16	0.28
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	16	0.28
(1,4713)	1:37:C:THR:HG21	1:8:C:LEU:HG	20	0.28
(1,4713)	1:37:C:THR:HG22	1:8:C:LEU:HG	20	0.28
(1,4713)	1:37:C:THR:HG23	1:8:C:LEU:HG	20	0.28
(1,4449)	1:31:C:GLY:H	1:19:C:GLY:H	7	0.28
(1,4128)	1:19:C:GLY:H	1:31:C:GLY:H	7	0.28
(1,2865)	1:35:B:ILE:HG21	1:12:B:CYS:HB2	3	0.28
(1,2865)	1:35:B:ILE:HG22	1:12:B:CYS:HB2	3	0.28
(1,2865)	1:35:B:ILE:HG23	1:12:B:CYS:HB2	3	0.28
(1,2857)	1:35:B:ILE:HG12	1:29:B:CYS:HA	1	0.28
(1,2857)	1:35:B:ILE:HG13	1:29:B:CYS:HA	1	0.28
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	5	0.28
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	5	0.28
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	5	0.28
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	14	0.28
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	14	0.28
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	14	0.28
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	13	0.28
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD11	15	0.28
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD12	15	0.28
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD13	15	0.28
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	12	0.28
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	12	0.28
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	17	0.28
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	17	0.28
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	13	0.28
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	13	0.28
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	13	0.28
(1,907)	1:31:A:GLY:H	1:19:A:GLY:H	20	0.28
(1,577)	1:19:A:GLY:H	1:31:A:GLY:H	20	0.28
(1,400)	1:12:A:CYS:H	1:34:A:VAL:HB	2	0.28
(1,338)	1:10:A:VAL:HG11	1:36:A:LEU:HA	6	0.28
(1,338)	1:10:A:VAL:HG12	1:36:A:LEU:HA	6	0.28
(1,338)	1:10:A:VAL:HG13	1:36:A:LEU:HA	6	0.28
(1,338)	1:10:A:VAL:HG11	1:36:A:LEU:HA	11	0.28
(1,338)	1:10:A:VAL:HG12	1:36:A:LEU:HA	11	0.28
(1,338)	1:10:A:VAL:HG13	1:36:A:LEU:HA	11	0.28
(2,1556)	1:43:C:LEU:HD12	1:8:C:LEU:HD21	2	0.27
(2,1348)	1:8:B:LEU:HD23	1:43:B:LEU:HG	18	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1322)	1:43:C:LEU:HD21	1:43:C:LEU:HA	3	0.27
(2,1322)	1:43:C:LEU:HD21	1:43:C:LEU:HA	8	0.27
(2,1322)	1:43:C:LEU:HD22	1:43:C:LEU:HA	16	0.27
(2,1321)	1:43:B:LEU:HD21	1:43:B:LEU:HA	10	0.27
(2,1321)	1:43:B:LEU:HD23	1:43:B:LEU:HA	12	0.27
(2,1320)	1:43:A:LEU:HD23	1:43:A:LEU:HA	2	0.27
(2,1320)	1:43:A:LEU:HD22	1:43:A:LEU:HA	12	0.27
(2,1016)	1:13:A:PRO:HB2	1:21:A:ILE:HG22	12	0.27
(2,658)	1:21:B:ILE:HD12	1:14:B:LYS:HA	20	0.27
(2,509)	1:43:C:LEU:HD21	1:43:C:LEU:HA	3	0.27
(2,509)	1:43:C:LEU:HD21	1:43:C:LEU:HA	8	0.27
(2,509)	1:43:C:LEU:HD22	1:43:C:LEU:HA	16	0.27
(2,508)	1:43:B:LEU:HD21	1:43:B:LEU:HA	10	0.27
(2,508)	1:43:B:LEU:HD23	1:43:B:LEU:HA	12	0.27
(2,507)	1:43:A:LEU:HD23	1:43:A:LEU:HA	2	0.27
(2,507)	1:43:A:LEU:HD22	1:43:A:LEU:HA	12	0.27
(2,484)	1:51:B:LEU:HD13	1:47:A:ILE:HB	9	0.27
(2,484)	1:51:B:LEU:HD12	1:47:A:ILE:HB	14	0.27
(2,470)	1:43:C:LEU:HD12	1:8:C:LEU:HD21	2	0.27
(2,355)	1:14:C:LYS:HD3	1:21:C:ILE:HA	8	0.27
(2,264)	1:49:B:LYS:HE2	1:53:B:LYS:HB3	7	0.27
(2,263)	1:49:A:LYS:HE2	1:53:A:LYS:HB3	2	0.27
(2,61)	1:3:C:ILE:H	1:2:C:VAL:HB	13	0.27
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	6	0.27
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	6	0.27
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	10	0.27
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	10	0.27
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	14	0.27
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	14	0.27
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	16	0.27
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	16	0.27
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	16	0.27
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	16	0.27
(1,3577)	1:1:C:FME:HE1	1:41:A:TYR:HB3	7	0.27
(1,2955)	1:37:B:THR:HG21	1:8:B:LEU:HG	9	0.27
(1,2955)	1:37:B:THR:HG22	1:8:B:LEU:HG	9	0.27
(1,2955)	1:37:B:THR:HG23	1:8:B:LEU:HG	9	0.27
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD2	20	0.27
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD3	20	0.27
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	2	0.27
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	2	0.27
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	16	0.27
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	16	0.27
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	16	0.27
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	11	0.27
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	11	0.27
(1,1080)	1:35:A:ILE:HG12	1:29:A:CYS:HA	20	0.27
(1,1080)	1:35:A:ILE:HG13	1:29:A:CYS:HA	20	0.27
(1,1052)	1:35:A:ILE:HA	1:11:A:ALA:HA	16	0.27
(1,369)	1:11:A:ALA:HA	1:35:A:ILE:HA	16	0.27
(1,338)	1:10:A:VAL:HG11	1:36:A:LEU:HA	20	0.27
(1,338)	1:10:A:VAL:HG12	1:36:A:LEU:HA	20	0.27
(1,338)	1:10:A:VAL:HG13	1:36:A:LEU:HA	20	0.27
(1,180)	1:6:A:ASP:HA	1:9:A:GLU:HG2	7	0.27
(1,180)	1:6:A:ASP:HA	1:9:A:GLU:HG3	7	0.27
(2,1349)	1:8:C:LEU:HD21	1:43:C:LEU:HG	8	0.26
(2,1348)	1:8:B:LEU:HD23	1:43:B:LEU:HG	7	0.26
(2,1326)	1:30:A:SER:HB3	1:32:A:LYS:HD3	10	0.26
(2,1322)	1:43:C:LEU:HD23	1:43:C:LEU:HA	2	0.26
(2,1322)	1:43:C:LEU:HD23	1:43:C:LEU:HA	12	0.26
(2,1321)	1:43:B:LEU:HD22	1:43:B:LEU:HA	4	0.26
(2,1321)	1:43:B:LEU:HD23	1:43:B:LEU:HA	5	0.26
(2,1321)	1:43:B:LEU:HD22	1:43:B:LEU:HA	6	0.26
(2,1321)	1:43:B:LEU:HD23	1:43:B:LEU:HA	13	0.26
(2,1321)	1:43:B:LEU:HD23	1:43:B:LEU:HA	14	0.26
(2,1320)	1:43:A:LEU:HD22	1:43:A:LEU:HA	8	0.26
(2,1320)	1:43:A:LEU:HD22	1:43:A:LEU:HA	15	0.26
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	5	0.26
(2,873)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	15	0.26
(2,870)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	15	0.26
(2,658)	1:21:B:ILE:HD11	1:26:B:CYS:HA	16	0.26
(2,509)	1:43:C:LEU:HD23	1:43:C:LEU:HA	2	0.26
(2,509)	1:43:C:LEU:HD23	1:43:C:LEU:HA	12	0.26
(2,508)	1:43:B:LEU:HD22	1:43:B:LEU:HA	4	0.26
(2,508)	1:43:B:LEU:HD23	1:43:B:LEU:HA	5	0.26
(2,508)	1:43:B:LEU:HD22	1:43:B:LEU:HA	6	0.26
(2,508)	1:43:B:LEU:HD23	1:43:B:LEU:HA	13	0.26
(2,508)	1:43:B:LEU:HD23	1:43:B:LEU:HA	14	0.26
(2,507)	1:43:A:LEU:HD22	1:43:A:LEU:HA	8	0.26
(2,507)	1:43:A:LEU:HD22	1:43:A:LEU:HA	15	0.26
(2,485)	1:51:C:LEU:HD13	1:47:B:ILE:HB	6	0.26
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	5	0.26
(2,264)	1:49:B:LYS:HE2	1:53:B:LYS:HD2	14	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,248)	1:14:A:LYS:HE2	1:22:A:GLU:HB2	13	0.26
(2,60)	1:3:B:ILE:H	1:2:B:VAL:HB	6	0.26
(2,60)	1:3:B:ILE:H	1:2:B:VAL:HB	11	0.26
(2,60)	1:3:B:ILE:H	1:2:B:VAL:HB	13	0.26
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG2	3	0.26
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	2	0.26
(1,3888)	1:10:C:VAL:HG11	1:36:C:LEU:HA	5	0.26
(1,3888)	1:10:C:VAL:HG12	1:36:C:LEU:HA	5	0.26
(1,3888)	1:10:C:VAL:HG13	1:36:C:LEU:HA	5	0.26
(1,3888)	1:10:C:VAL:HG11	1:36:C:LEU:HA	6	0.26
(1,3888)	1:10:C:VAL:HG12	1:36:C:LEU:HA	6	0.26
(1,3888)	1:10:C:VAL:HG13	1:36:C:LEU:HA	6	0.26
(1,3888)	1:10:C:VAL:HG11	1:36:C:LEU:HA	7	0.26
(1,3888)	1:10:C:VAL:HG12	1:36:C:LEU:HA	7	0.26
(1,3888)	1:10:C:VAL:HG13	1:36:C:LEU:HA	7	0.26
(1,3888)	1:10:C:VAL:HG11	1:36:C:LEU:HA	14	0.26
(1,3888)	1:10:C:VAL:HG12	1:36:C:LEU:HA	14	0.26
(1,3888)	1:10:C:VAL:HG13	1:36:C:LEU:HA	14	0.26
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	3	0.26
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	3	0.26
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	3	0.26
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	5	0.26
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	5	0.26
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	5	0.26
(1,3389)	1:49:B:LYS:HA	1:32:A:LYS:HA	13	0.26
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	14	0.26
(1,2290)	1:16:B:GLU:H	1:33:B:GLY:H	4	0.26
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	2	0.26
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	2	0.26
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	4	0.26
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	4	0.26
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	6	0.26
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	6	0.26
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	4	0.26
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	4	0.26
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	4	0.26
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	12	0.26
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	12	0.26
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	12	0.26
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	20	0.26
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	20	0.26
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	14	0.26
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	14	0.26
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	14	0.26
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	11	0.26
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	11	0.26
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	11	0.26
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	16	0.26
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	16	0.26
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	16	0.26
(2,1556)	1:43:C:LEU:HD13	1:8:C:LEU:HD21	4	0.25
(2,1349)	1:8:C:LEU:HD21	1:43:C:LEU:HG	6	0.25
(2,1348)	1:8:B:LEU:HD21	1:43:B:LEU:HG	13	0.25
(2,1347)	1:8:A:LEU:HD21	1:43:A:LEU:HG	12	0.25
(2,1322)	1:43:C:LEU:HD22	1:43:C:LEU:HA	6	0.25
(2,1322)	1:43:C:LEU:HD22	1:43:C:LEU:HA	10	0.25
(2,1322)	1:43:C:LEU:HD22	1:43:C:LEU:HA	17	0.25
(2,1321)	1:43:B:LEU:HD23	1:43:B:LEU:HA	17	0.25
(2,1320)	1:43:A:LEU:HD21	1:43:A:LEU:HA	3	0.25
(2,1320)	1:43:A:LEU:HD23	1:43:A:LEU:HA	13	0.25
(2,1320)	1:43:A:LEU:HD21	1:43:A:LEU:HA	14	0.25
(2,1320)	1:43:A:LEU:HD22	1:43:A:LEU:HA	16	0.25
(2,1320)	1:43:A:LEU:HD23	1:43:A:LEU:HA	17	0.25
(2,1320)	1:43:A:LEU:HD22	1:43:A:LEU:HA	20	0.25
(2,1192)	1:27:B:PRO:HG3	1:21:B:ILE:HG21	5	0.25
(2,657)	1:21:A:ILE:HD11	1:26:A:CYS:HA	6	0.25
(2,509)	1:43:C:LEU:HD22	1:43:C:LEU:HA	6	0.25
(2,509)	1:43:C:LEU:HD22	1:43:C:LEU:HA	10	0.25
(2,509)	1:43:C:LEU:HD22	1:43:C:LEU:HA	17	0.25
(2,508)	1:43:B:LEU:HD23	1:43:B:LEU:HA	17	0.25
(2,507)	1:43:A:LEU:HD21	1:43:A:LEU:HA	3	0.25
(2,507)	1:43:A:LEU:HD23	1:43:A:LEU:HA	13	0.25
(2,507)	1:43:A:LEU:HD21	1:43:A:LEU:HA	14	0.25
(2,507)	1:43:A:LEU:HD22	1:43:A:LEU:HA	16	0.25
(2,507)	1:43:A:LEU:HD23	1:43:A:LEU:HA	17	0.25
(2,507)	1:43:A:LEU:HD22	1:43:A:LEU:HA	20	0.25
(2,484)	1:51:B:LEU:HD13	1:47:A:ILE:HB	2	0.25
(2,484)	1:51:B:LEU:HD12	1:47:A:ILE:HB	6	0.25
(2,470)	1:43:C:LEU:HD13	1:8:C:LEU:HD21	4	0.25
(2,400)	1:27:B:PRO:HG3	1:21:B:ILE:HG21	5	0.25
(2,269)	1:14:A:LYS:HE2	1:15:A:CYS:HB2	1	0.25
(2,269)	1:14:A:LYS:HE3	1:15:A:CYS:HB2	1	0.25
(2,138)	1:15:B:CYS:H	1:14:B:LYS:HG2	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,61)	1:3:C:ILE:H	1:2:C:VAL:HB	15	0.25
(2,61)	1:3:C:ILE:H	1:2:C:VAL:HB	16	0.25
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG2	7	0.25
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG2	14	0.25
(2,45)	1:14:C:LYS:H	1:14:C:LYS:HG2	16	0.25
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG2	14	0.25
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	5	0.25
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	5	0.25
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	15	0.25
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	15	0.25
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	15	0.25
(1,2955)	1:37:B:THR:HG21	1:8:B:LEU:HG	6	0.25
(1,2955)	1:37:B:THR:HG22	1:8:B:LEU:HG	6	0.25
(1,2955)	1:37:B:THR:HG23	1:8:B:LEU:HG	6	0.25
(1,2955)	1:37:B:THR:HG21	1:8:B:LEU:HG	19	0.25
(1,2955)	1:37:B:THR:HG22	1:8:B:LEU:HG	19	0.25
(1,2955)	1:37:B:THR:HG23	1:8:B:LEU:HG	19	0.25
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	6	0.25
(1,2290)	1:16:B:GLU:H	1:33:B:GLY:H	19	0.25
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG12	6	0.25
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG13	6	0.25
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG12	6	0.25
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG13	6	0.25
(1,2172)	1:11:B:ALA:H	1:34:B:VAL:HB	11	0.25
(1,1841)	1:2:B:VAL:HG11	1:3:B:ILE:HG21	10	0.25
(1,1841)	1:2:B:VAL:HG11	1:3:B:ILE:HG22	10	0.25
(1,1841)	1:2:B:VAL:HG11	1:3:B:ILE:HG23	10	0.25
(1,1841)	1:2:B:VAL:HG12	1:3:B:ILE:HG21	10	0.25
(1,1841)	1:2:B:VAL:HG12	1:3:B:ILE:HG22	10	0.25
(1,1841)	1:2:B:VAL:HG12	1:3:B:ILE:HG23	10	0.25
(1,1841)	1:2:B:VAL:HG13	1:3:B:ILE:HG21	10	0.25
(1,1841)	1:2:B:VAL:HG13	1:3:B:ILE:HG22	10	0.25
(1,1841)	1:2:B:VAL:HG13	1:3:B:ILE:HG23	10	0.25
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	14	0.25
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	14	0.25
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	18	0.25
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	18	0.25
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	18	0.25
(1,965)	1:32:A:LYS:H	1:29:A:CYS:HA	8	0.25
(1,498)	1:16:A:GLU:H	1:33:A:GLY:H	2	0.25
(1,381)	1:11:A:ALA:H	1:34:A:VAL:HB	2	0.25
(1,338)	1:10:A:VAL:HG11	1:36:A:LEU:HA	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:10:A:VAL:HG12	1:36:A:LEU:HA	1	0.25
(1,338)	1:10:A:VAL:HG13	1:36:A:LEU:HA	1	0.25
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	9	0.24
(2,1349)	1:8:C:LEU:HD22	1:43:C:LEU:HG	5	0.24
(2,1327)	1:30:B:SER:HB3	1:32:B:LYS:HD3	5	0.24
(2,1322)	1:43:C:LEU:HD22	1:43:C:LEU:HA	5	0.24
(2,1322)	1:43:C:LEU:HD22	1:43:C:LEU:HA	9	0.24
(2,1321)	1:43:B:LEU:HD23	1:43:B:LEU:HA	2	0.24
(2,1321)	1:43:B:LEU:HD23	1:43:B:LEU:HA	9	0.24
(2,1321)	1:43:B:LEU:HD21	1:43:B:LEU:HA	11	0.24
(2,1321)	1:43:B:LEU:HD22	1:43:B:LEU:HA	16	0.24
(2,1321)	1:43:B:LEU:HD22	1:43:B:LEU:HA	18	0.24
(2,1320)	1:43:A:LEU:HD22	1:43:A:LEU:HA	4	0.24
(2,1320)	1:43:A:LEU:HD23	1:43:A:LEU:HA	6	0.24
(2,1320)	1:43:A:LEU:HD22	1:43:A:LEU:HA	18	0.24
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	1	0.24
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	10	0.24
(2,871)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	10	0.24
(2,868)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	10	0.24
(2,657)	1:21:A:ILE:HD13	1:26:A:CYS:HA	4	0.24
(2,581)	1:42:C:THR:HG21	1:4:B:ALA:HB2	5	0.24
(2,580)	1:42:B:THR:HG21	1:4:A:ALA:HB1	8	0.24
(2,509)	1:43:C:LEU:HD22	1:43:C:LEU:HA	5	0.24
(2,509)	1:43:C:LEU:HD22	1:43:C:LEU:HA	9	0.24
(2,508)	1:43:B:LEU:HD23	1:43:B:LEU:HA	2	0.24
(2,508)	1:43:B:LEU:HD23	1:43:B:LEU:HA	9	0.24
(2,508)	1:43:B:LEU:HD21	1:43:B:LEU:HA	11	0.24
(2,508)	1:43:B:LEU:HD22	1:43:B:LEU:HA	16	0.24
(2,508)	1:43:B:LEU:HD22	1:43:B:LEU:HA	18	0.24
(2,507)	1:43:A:LEU:HD22	1:43:A:LEU:HA	4	0.24
(2,507)	1:43:A:LEU:HD23	1:43:A:LEU:HA	6	0.24
(2,507)	1:43:A:LEU:HD22	1:43:A:LEU:HA	18	0.24
(2,485)	1:51:C:LEU:HD13	1:47:B:ILE:HB	7	0.24
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	1	0.24
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	10	0.24
(2,275)	1:21:A:ILE:HB	1:13:A:PRO:HB2	1	0.24
(2,249)	1:14:B:LYS:HE3	1:22:B:GLU:HB2	13	0.24
(2,137)	1:15:A:CYS:H	1:21:A:ILE:HG13	6	0.24
(2,98)	1:35:A:ILE:H	1:9:A:GLU:HG2	16	0.24
(2,60)	1:3:B:ILE:H	1:2:B:VAL:HB	14	0.24
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	17	0.24
(1,5139)	1:49:C:LYS:HA	1:32:B:LYS:HA	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	4	0.24
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	4	0.24
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	8	0.24
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	8	0.24
(1,4713)	1:37:C:THR:HG21	1:8:C:LEU:HG	16	0.24
(1,4713)	1:37:C:THR:HG22	1:8:C:LEU:HG	16	0.24
(1,4713)	1:37:C:THR:HG23	1:8:C:LEU:HG	16	0.24
(1,4581)	1:34:C:VAL:H	1:32:C:LYS:HG2	13	0.24
(1,4581)	1:34:C:VAL:H	1:32:C:LYS:HG3	13	0.24
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	6	0.24
(1,4193)	1:21:C:ILE:HD11	1:15:C:CYS:HA	14	0.24
(1,4193)	1:21:C:ILE:HD12	1:15:C:CYS:HA	14	0.24
(1,4193)	1:21:C:ILE:HD13	1:15:C:CYS:HA	14	0.24
(1,3949)	1:12:C:CYS:H	1:34:C:VAL:HB	17	0.24
(1,3568)	1:1:C:FME:HA	1:39:A:GLN:HA	18	0.24
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	20	0.24
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	20	0.24
(1,2435)	1:21:B:ILE:HD11	1:15:B:CYS:HA	4	0.24
(1,2435)	1:21:B:ILE:HD12	1:15:B:CYS:HA	4	0.24
(1,2435)	1:21:B:ILE:HD13	1:15:B:CYS:HA	4	0.24
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	14	0.24
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	14	0.24
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	14	0.24
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	6	0.24
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	6	0.24
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	6	0.24
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	1	0.24
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	1	0.24
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	4	0.24
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	4	0.24
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	19	0.24
(1,641)	1:21:A:ILE:HD11	1:13:A:PRO:HD2	6	0.24
(1,641)	1:21:A:ILE:HD11	1:13:A:PRO:HD3	6	0.24
(1,641)	1:21:A:ILE:HD12	1:13:A:PRO:HD2	6	0.24
(1,641)	1:21:A:ILE:HD12	1:13:A:PRO:HD3	6	0.24
(1,641)	1:21:A:ILE:HD13	1:13:A:PRO:HD2	6	0.24
(1,641)	1:21:A:ILE:HD13	1:13:A:PRO:HD3	6	0.24
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	16	0.24
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	16	0.24
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	16	0.24
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	3	0.24
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	3	0.24
(2,1556)	1:43:C:LEU:HD13	1:8:C:LEU:HD21	11	0.23
(2,1322)	1:43:C:LEU:HD21	1:43:C:LEU:HA	20	0.23
(2,1321)	1:43:B:LEU:HD23	1:43:B:LEU:HA	19	0.23
(2,1320)	1:43:A:LEU:HD21	1:43:A:LEU:HA	7	0.23
(2,1320)	1:43:A:LEU:HD23	1:43:A:LEU:HA	9	0.23
(2,1320)	1:43:A:LEU:HD23	1:43:A:LEU:HA	19	0.23
(2,1151)	1:43:B:LEU:HG	1:43:C:LEU:HG	3	0.23
(2,1151)	1:43:C:LEU:HG	1:43:A:LEU:HG	19	0.23
(2,1070)	1:29:A:CYS:HB3	1:32:A:LYS:HG3	14	0.23
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	15	0.23
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	6	0.23
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	11	0.23
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	12	0.23
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	20	0.23
(2,872)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	2	0.23
(2,871)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	12	0.23
(2,869)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	2	0.23
(2,868)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	12	0.23
(2,509)	1:43:C:LEU:HD21	1:43:C:LEU:HA	20	0.23
(2,508)	1:43:B:LEU:HD23	1:43:B:LEU:HA	19	0.23
(2,507)	1:43:A:LEU:HD21	1:43:A:LEU:HA	7	0.23
(2,507)	1:43:A:LEU:HD23	1:43:A:LEU:HA	9	0.23
(2,507)	1:43:A:LEU:HD23	1:43:A:LEU:HA	19	0.23
(2,483)	1:51:A:LEU:HD11	1:47:C:ILE:HB	20	0.23
(2,470)	1:43:C:LEU:HD13	1:8:C:LEU:HD21	11	0.23
(2,380)	1:43:B:LEU:HG	1:43:C:LEU:HG	3	0.23
(2,380)	1:43:C:LEU:HG	1:43:A:LEU:HG	19	0.23
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	15	0.23
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	6	0.23
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	11	0.23
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	12	0.23
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	20	0.23
(2,264)	1:49:B:LYS:HE2	1:53:B:LYS:HD2	11	0.23
(2,61)	1:3:C:ILE:H	1:1:C:FME:HB3	6	0.23
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG2	12	0.23
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG2	19	0.23
(2,43)	1:14:A:LYS:H	1:14:A:LYS:HG2	20	0.23
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	13	0.23
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	13	0.23
(1,4463)	1:32:C:LYS:HB3	1:29:C:CYS:HA	14	0.23
(1,4430)	1:30:C:SER:HA	1:32:C:LYS:HE2	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4430)	1:30:C:SER:HA	1:32:C:LYS:HE3	18	0.23
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	10	0.23
(1,4191)	1:21:C:ILE:HD11	1:13:C:PRO:HD2	6	0.23
(1,4191)	1:21:C:ILE:HD11	1:13:C:PRO:HD3	6	0.23
(1,4191)	1:21:C:ILE:HD12	1:13:C:PRO:HD2	6	0.23
(1,4191)	1:21:C:ILE:HD12	1:13:C:PRO:HD3	6	0.23
(1,4191)	1:21:C:ILE:HD13	1:13:C:PRO:HD2	6	0.23
(1,4191)	1:21:C:ILE:HD13	1:13:C:PRO:HD3	6	0.23
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	10	0.23
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	18	0.23
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	18	0.23
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	18	0.23
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	18	0.23
(1,3888)	1:10:C:VAL:HG11	1:36:C:LEU:HA	20	0.23
(1,3888)	1:10:C:VAL:HG12	1:36:C:LEU:HA	20	0.23
(1,3888)	1:10:C:VAL:HG13	1:36:C:LEU:HA	20	0.23
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	4	0.23
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	4	0.23
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	4	0.23
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	8	0.23
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	8	0.23
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	17	0.23
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	17	0.23
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	16	0.23
(1,2955)	1:37:B:THR:HG21	1:8:B:LEU:HG	2	0.23
(1,2955)	1:37:B:THR:HG22	1:8:B:LEU:HG	2	0.23
(1,2955)	1:37:B:THR:HG23	1:8:B:LEU:HG	2	0.23
(1,2955)	1:37:B:THR:HG21	1:8:B:LEU:HG	7	0.23
(1,2955)	1:37:B:THR:HG22	1:8:B:LEU:HG	7	0.23
(1,2955)	1:37:B:THR:HG23	1:8:B:LEU:HG	7	0.23
(1,2955)	1:37:B:THR:HG21	1:8:B:LEU:HG	13	0.23
(1,2955)	1:37:B:THR:HG22	1:8:B:LEU:HG	13	0.23
(1,2955)	1:37:B:THR:HG23	1:8:B:LEU:HG	13	0.23
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	16	0.23
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	20	0.23
(1,2435)	1:21:B:ILE:HD11	1:15:B:CYS:HA	6	0.23
(1,2435)	1:21:B:ILE:HD12	1:15:B:CYS:HA	6	0.23
(1,2435)	1:21:B:ILE:HD13	1:15:B:CYS:HA	6	0.23
(1,2290)	1:16:B:GLU:H	1:33:B:GLY:H	11	0.23
(1,2222)	1:14:B:LYS:HE2	1:21:B:ILE:HD11	12	0.23
(1,2222)	1:14:B:LYS:HE2	1:21:B:ILE:HD12	12	0.23
(1,2222)	1:14:B:LYS:HE2	1:21:B:ILE:HD13	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2222)	1:14:B:LYS:HE3	1:21:B:ILE:HD11	12	0.23
(1,2222)	1:14:B:LYS:HE3	1:21:B:ILE:HD12	12	0.23
(1,2222)	1:14:B:LYS:HE3	1:21:B:ILE:HD13	12	0.23
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG12	11	0.23
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG13	11	0.23
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG12	11	0.23
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG13	11	0.23
(1,2192)	1:12:B:CYS:H	1:34:B:VAL:HB	4	0.23
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	7	0.23
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	7	0.23
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	7	0.23
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	9	0.23
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	9	0.23
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	9	0.23
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	15	0.23
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	15	0.23
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	15	0.23
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	13	0.23
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	13	0.23
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	13	0.23
(1,1619)	1:49:A:LYS:HA	1:32:C:LYS:HA	19	0.23
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	3	0.23
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	3	0.23
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	2	0.23
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	2	0.23
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	2	0.23
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	3	0.23
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	3	0.23
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	3	0.23
(1,1043)	1:34:A:VAL:H	1:32:A:LYS:HA	17	0.23
(1,965)	1:32:A:LYS:H	1:29:A:CYS:HA	17	0.23
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	3	0.23
(1,641)	1:21:A:ILE:HD11	1:13:A:PRO:HD2	4	0.23
(1,641)	1:21:A:ILE:HD11	1:13:A:PRO:HD3	4	0.23
(1,641)	1:21:A:ILE:HD12	1:13:A:PRO:HD2	4	0.23
(1,641)	1:21:A:ILE:HD12	1:13:A:PRO:HD3	4	0.23
(1,641)	1:21:A:ILE:HD13	1:13:A:PRO:HD2	4	0.23
(1,641)	1:21:A:ILE:HD13	1:13:A:PRO:HD3	4	0.23
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG12	19	0.23
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG13	19	0.23
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG12	19	0.23
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG13	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,400)	1:12:A:CYS:H	1:34:A:VAL:HB	17	0.23
(1,338)	1:10:A:VAL:HG11	1:36:A:LEU:HA	19	0.23
(1,338)	1:10:A:VAL:HG12	1:36:A:LEU:HA	19	0.23
(1,338)	1:10:A:VAL:HG13	1:36:A:LEU:HA	19	0.23
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	4	0.23
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	4	0.23
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	4	0.23
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	18	0.23
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	18	0.23
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	18	0.23
(2,1556)	1:43:C:LEU:HD12	1:8:B:LEU:HD21	3	0.22
(2,1348)	1:8:B:LEU:HD23	1:43:B:LEU:HG	8	0.22
(2,1348)	1:8:B:LEU:HD22	1:43:B:LEU:HG	14	0.22
(2,1322)	1:43:C:LEU:HD23	1:43:C:LEU:HA	1	0.22
(2,1016)	1:13:A:PRO:HB2	1:21:A:ILE:HG23	18	0.22
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	13	0.22
(2,873)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	2	0.22
(2,870)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	2	0.22
(2,572)	1:2:C:VAL:HG12	1:1:C:FME:HA	2	0.22
(2,509)	1:43:C:LEU:HD23	1:43:C:LEU:HA	1	0.22
(2,485)	1:51:C:LEU:HD11	1:47:B:ILE:HB	10	0.22
(2,483)	1:51:A:LEU:HD13	1:47:C:ILE:HB	14	0.22
(2,470)	1:43:C:LEU:HD12	1:8:B:LEU:HD21	3	0.22
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	13	0.22
(2,60)	1:3:B:ILE:H	1:2:B:VAL:HB	18	0.22
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	12	0.22
(1,4581)	1:34:C:VAL:H	1:32:C:LYS:HG2	20	0.22
(1,4581)	1:34:C:VAL:H	1:32:C:LYS:HG3	20	0.22
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	12	0.22
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	18	0.22
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	20	0.22
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	11	0.22
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	16	0.22
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	17	0.22
(1,3801)	1:8:C:LEU:HD11	1:39:C:GLN:HB2	9	0.22
(1,3801)	1:8:C:LEU:HD12	1:39:C:GLN:HB2	9	0.22
(1,3801)	1:8:C:LEU:HD13	1:39:C:GLN:HB2	9	0.22
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	9	0.22
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	9	0.22
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	9	0.22
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	9	0.22
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	9	0.22
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	16	0.22
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	16	0.22
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	16	0.22
(1,3107)	1:42:B:THR:HB	1:3:A:ILE:HB	20	0.22
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	9	0.22
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	8	0.22
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD2	8	0.22
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD3	8	0.22
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG12	9	0.22
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG13	9	0.22
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG12	9	0.22
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG13	9	0.22
(1,2192)	1:12:B:CYS:H	1:34:B:VAL:HB	11	0.22
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	3	0.22
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	3	0.22
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	3	0.22
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	8	0.22
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	8	0.22
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	8	0.22
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	3	0.22
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	3	0.22
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	3	0.22
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	15	0.22
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	15	0.22
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	15	0.22
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	5	0.22
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	5	0.22
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	20	0.22
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	20	0.22
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	17	0.22
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	17	0.22
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	17	0.22
(1,1052)	1:35:A:ILE:HA	1:11:A:ALA:HA	3	0.22
(1,965)	1:32:A:LYS:H	1:29:A:CYS:HA	14	0.22
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	1	0.22
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	6	0.22
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	7	0.22
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	10	0.22
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	18	0.22
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	6	0.22
(1,369)	1:11:A:ALA:HA	1:35:A:ILE:HA	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	8	0.22
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	8	0.22
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	8	0.22
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	6	0.22
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	6	0.22
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	6	0.22
(2,1555)	1:43:B:LEU:HD11	1:8:B:LEU:HD21	2	0.21
(2,1555)	1:43:B:LEU:HD12	1:8:A:LEU:HD21	20	0.21
(2,1554)	1:43:A:LEU:HD13	1:8:A:LEU:HD21	13	0.21
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	19	0.21
(2,1405)	1:15:B:CYS:HA	1:17:B:ARG:HD2	1	0.21
(2,1349)	1:8:C:LEU:HD23	1:43:A:LEU:HG	10	0.21
(2,1347)	1:8:A:LEU:HD22	1:43:A:LEU:HG	4	0.21
(2,1327)	1:30:B:SER:HB3	1:32:B:LYS:HD3	2	0.21
(2,1321)	1:43:B:LEU:HD21	1:43:B:LEU:HA	1	0.21
(2,1321)	1:43:B:LEU:HD23	1:43:B:LEU:HA	20	0.21
(2,1320)	1:43:A:LEU:HD22	1:43:A:LEU:HA	1	0.21
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	14	0.21
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	14	0.21
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	19	0.21
(2,873)	1:31:C:GLY:HA2	1:15:C:CYS:HB3	4	0.21
(2,872)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	15	0.21
(2,872)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	17	0.21
(2,871)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	5	0.21
(2,870)	1:31:C:GLY:HA2	1:15:C:CYS:HB3	4	0.21
(2,869)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	15	0.21
(2,869)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	17	0.21
(2,868)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	5	0.21
(2,696)	1:15:B:CYS:HA	1:17:B:ARG:HD2	1	0.21
(2,581)	1:42:C:THR:HG22	1:4:B:ALA:HB2	4	0.21
(2,581)	1:42:C:THR:HG22	1:4:B:ALA:HB3	11	0.21
(2,508)	1:43:B:LEU:HD21	1:43:B:LEU:HA	1	0.21
(2,508)	1:43:B:LEU:HD23	1:43:B:LEU:HA	20	0.21
(2,507)	1:43:A:LEU:HD22	1:43:A:LEU:HA	1	0.21
(2,485)	1:51:C:LEU:HD12	1:47:B:ILE:HB	20	0.21
(2,483)	1:51:A:LEU:HD13	1:48:C:GLN:HB3	5	0.21
(2,469)	1:43:B:LEU:HD11	1:8:B:LEU:HD21	2	0.21
(2,469)	1:43:B:LEU:HD12	1:8:A:LEU:HD21	20	0.21
(2,468)	1:43:A:LEU:HD13	1:8:A:LEU:HD21	13	0.21
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	14	0.21
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	14	0.21
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,276)	1:21:B:ILE:HB	1:13:B:PRO:HB2	7	0.21
(2,267)	1:51:B:LEU:HB2	1:52:B:ASN:HB2	12	0.21
(2,263)	1:49:A:LYS:HE2	1:53:A:LYS:HB3	4	0.21
(2,100)	1:35:C:ILE:H	1:9:C:GLU:HG2	18	0.21
(2,60)	1:3:B:ILE:H	1:1:B:FME:HB3	1	0.21
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	17	0.21
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	17	0.21
(1,4713)	1:37:C:THR:HG21	1:8:C:LEU:HG	8	0.21
(1,4713)	1:37:C:THR:HG22	1:8:C:LEU:HG	8	0.21
(1,4713)	1:37:C:THR:HG23	1:8:C:LEU:HG	8	0.21
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	4	0.21
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	6	0.21
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	7	0.21
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	9	0.21
(1,4193)	1:21:C:ILE:HD11	1:15:C:CYS:HA	3	0.21
(1,4193)	1:21:C:ILE:HD12	1:15:C:CYS:HA	3	0.21
(1,4193)	1:21:C:ILE:HD13	1:15:C:CYS:HA	3	0.21
(1,4193)	1:21:C:ILE:HD11	1:15:C:CYS:HA	10	0.21
(1,4193)	1:21:C:ILE:HD12	1:15:C:CYS:HA	10	0.21
(1,4193)	1:21:C:ILE:HD13	1:15:C:CYS:HA	10	0.21
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	4	0.21
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	4	0.21
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	4	0.21
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	4	0.21
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	14	0.21
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	14	0.21
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	14	0.21
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	14	0.21
(1,3896)	1:10:C:VAL:HG21	1:11:C:ALA:H	17	0.21
(1,3896)	1:10:C:VAL:HG22	1:11:C:ALA:H	17	0.21
(1,3896)	1:10:C:VAL:HG23	1:11:C:ALA:H	17	0.21
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	1	0.21
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	1	0.21
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	1	0.21
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	6	0.21
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	6	0.21
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	6	0.21
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	13	0.21
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	13	0.21
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	13	0.21
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD11	12	0.21
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD12	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD13	12	0.21
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	3	0.21
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	3	0.21
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	9	0.21
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	9	0.21
(1,3039)	1:40:B:GLY:H	1:43:B:LEU:HB3	13	0.21
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD11	7	0.21
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD12	7	0.21
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD13	7	0.21
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD11	7	0.21
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD12	7	0.21
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD13	7	0.21
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD21	7	0.21
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD22	7	0.21
(1,3003)	1:39:B:GLN:HE21	1:43:B:LEU:HD23	7	0.21
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD21	7	0.21
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD22	7	0.21
(1,3003)	1:39:B:GLN:HE22	1:43:B:LEU:HD23	7	0.21
(1,2955)	1:37:B:THR:HG21	1:8:B:LEU:HG	4	0.21
(1,2955)	1:37:B:THR:HG22	1:8:B:LEU:HG	4	0.21
(1,2955)	1:37:B:THR:HG23	1:8:B:LEU:HG	4	0.21
(1,2955)	1:37:B:THR:HG21	1:8:B:LEU:HG	5	0.21
(1,2955)	1:37:B:THR:HG22	1:8:B:LEU:HG	5	0.21
(1,2955)	1:37:B:THR:HG23	1:8:B:LEU:HG	5	0.21
(1,2831)	1:35:B:ILE:HA	1:11:B:ALA:HA	18	0.21
(1,2672)	1:30:B:SER:HA	1:32:B:LYS:HE2	16	0.21
(1,2672)	1:30:B:SER:HA	1:32:B:LYS:HE3	16	0.21
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	3	0.21
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	7	0.21
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	15	0.21
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	19	0.21
(1,2433)	1:21:B:ILE:HD11	1:13:B:PRO:HD2	16	0.21
(1,2433)	1:21:B:ILE:HD11	1:13:B:PRO:HD3	16	0.21
(1,2433)	1:21:B:ILE:HD12	1:13:B:PRO:HD2	16	0.21
(1,2433)	1:21:B:ILE:HD12	1:13:B:PRO:HD3	16	0.21
(1,2433)	1:21:B:ILE:HD13	1:13:B:PRO:HD2	16	0.21
(1,2433)	1:21:B:ILE:HD13	1:13:B:PRO:HD3	16	0.21
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD2	16	0.21
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD3	16	0.21
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG12	15	0.21
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG13	15	0.21
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG12	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG13	15	0.21
(1,2172)	1:11:B:ALA:H	1:34:B:VAL:HB	5	0.21
(1,2160)	1:11:B:ALA:HA	1:35:B:ILE:HA	18	0.21
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	18	0.21
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	18	0.21
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	18	0.21
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	2	0.21
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	2	0.21
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	2	0.21
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	12	0.21
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	12	0.21
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	12	0.21
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	16	0.21
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	16	0.21
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	16	0.21
(1,1812)	1:1:B:FME:HA	1:39:C:GLN:HA	10	0.21
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	12	0.21
(1,1043)	1:34:A:VAL:H	1:32:A:LYS:HA	20	0.21
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	15	0.21
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	16	0.21
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	9	0.21
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	14	0.21
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD2	6	0.21
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD3	6	0.21
(1,498)	1:16:A:GLU:H	1:33:A:GLY:H	10	0.21
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG12	12	0.21
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG13	12	0.21
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG12	12	0.21
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG13	12	0.21
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG12	18	0.21
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG13	18	0.21
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG12	18	0.21
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG13	18	0.21
(1,391)	1:12:A:CYS:HB3	1:16:A:GLU:HG2	5	0.21
(1,391)	1:12:A:CYS:HB3	1:16:A:GLU:HG3	5	0.21
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	1	0.21
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	1	0.21
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	1	0.21
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	8	0.21
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	8	0.21
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	8	0.21
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	19	0.21
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	19	0.21
(2,1556)	1:43:C:LEU:HD12	1:8:C:LEU:HD23	15	0.2
(2,1555)	1:43:B:LEU:HD13	1:8:B:LEU:HD23	16	0.2
(2,1554)	1:43:A:LEU:HD12	1:8:A:LEU:HD23	5	0.2
(2,1510)	1:35:B:ILE:HD12	1:11:B:ALA:HA	15	0.2
(2,1415)	1:32:C:LYS:HA	1:19:C:GLY:HA2	14	0.2
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	15	0.2
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	20	0.2
(2,872)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	19	0.2
(2,871)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	15	0.2
(2,869)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	19	0.2
(2,868)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	15	0.2
(2,664)	1:35:B:ILE:HD12	1:11:B:ALA:HA	15	0.2
(2,572)	1:2:C:VAL:HG12	1:1:C:FME:HA	8	0.2
(2,570)	1:2:A:VAL:HG12	1:1:A:FME:HA	20	0.2
(2,485)	1:51:C:LEU:HD12	1:47:B:ILE:HB	1	0.2
(2,484)	1:51:B:LEU:HD12	1:47:A:ILE:HB	4	0.2
(2,484)	1:51:B:LEU:HD11	1:47:A:ILE:HB	15	0.2
(2,470)	1:43:C:LEU:HD12	1:8:C:LEU:HD23	15	0.2
(2,469)	1:43:B:LEU:HD13	1:8:B:LEU:HD23	16	0.2
(2,468)	1:43:A:LEU:HD12	1:8:A:LEU:HD23	5	0.2
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	15	0.2
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	20	0.2
(2,271)	1:14:C:LYS:HE2	1:15:C:CYS:HB2	18	0.2
(2,271)	1:14:C:LYS:HE3	1:15:C:CYS:HB2	18	0.2
(2,250)	1:14:C:LYS:HE2	1:22:C:GLU:HB2	3	0.2
(2,60)	1:3:B:ILE:H	1:2:B:VAL:HB	5	0.2
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	8	0.2
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	19	0.2
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	2	0.2
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	5	0.2
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	13	0.2
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	15	0.2
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	8	0.2
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	3	0.2
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	3	0.2
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	3	0.2
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	3	0.2
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	11	0.2
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	11	0.2
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	11	0.2
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	15	0.2
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	15	0.2
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	15	0.2
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	15	0.2
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	19	0.2
(1,3888)	1:10:C:VAL:HG11	1:36:C:LEU:HA	13	0.2
(1,3888)	1:10:C:VAL:HG12	1:36:C:LEU:HA	13	0.2
(1,3888)	1:10:C:VAL:HG13	1:36:C:LEU:HA	13	0.2
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	6	0.2
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	6	0.2
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	6	0.2
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	10	0.2
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	10	0.2
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	10	0.2
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	8	0.2
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	8	0.2
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	8	0.2
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	11	0.2
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	11	0.2
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	11	0.2
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG2	5	0.2
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG3	5	0.2
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG2	5	0.2
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG3	5	0.2
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG2	9	0.2
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG3	9	0.2
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG2	9	0.2
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG3	9	0.2
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	7	0.2
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	9	0.2
(1,2955)	1:37:B:THR:HG21	1:8:B:LEU:HG	8	0.2
(1,2955)	1:37:B:THR:HG22	1:8:B:LEU:HG	8	0.2
(1,2955)	1:37:B:THR:HG23	1:8:B:LEU:HG	8	0.2
(1,2955)	1:37:B:THR:HG21	1:8:B:LEU:HG	16	0.2
(1,2955)	1:37:B:THR:HG22	1:8:B:LEU:HG	16	0.2
(1,2955)	1:37:B:THR:HG23	1:8:B:LEU:HG	16	0.2
(1,2823)	1:34:B:VAL:H	1:32:B:LYS:HG2	1	0.2
(1,2823)	1:34:B:VAL:H	1:32:B:LYS:HG3	1	0.2
(1,2821)	1:34:B:VAL:H	1:32:B:LYS:HA	14	0.2
(1,2747)	1:32:B:LYS:H	1:29:B:CYS:HB2	20	0.2
(1,2746)	1:32:B:LYS:H	1:29:B:CYS:HA	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2746)	1:32:B:LYS:H	1:29:B:CYS:HA	20	0.2
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	4	0.2
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	5	0.2
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	11	0.2
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	13	0.2
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	17	0.2
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	18	0.2
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	1	0.2
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	15	0.2
(1,2435)	1:21:B:ILE:HD11	1:15:B:CYS:HA	19	0.2
(1,2435)	1:21:B:ILE:HD12	1:15:B:CYS:HA	19	0.2
(1,2435)	1:21:B:ILE:HD13	1:15:B:CYS:HA	19	0.2
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG12	17	0.2
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG13	17	0.2
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG12	17	0.2
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG13	17	0.2
(1,2172)	1:11:B:ALA:H	1:34:B:VAL:HB	4	0.2
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	6	0.2
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	6	0.2
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	6	0.2
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	13	0.2
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	13	0.2
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	13	0.2
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	19	0.2
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	19	0.2
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	19	0.2
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	20	0.2
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	20	0.2
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	20	0.2
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	1	0.2
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	1	0.2
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	1	0.2
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	5	0.2
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	5	0.2
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	5	0.2
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	14	0.2
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	14	0.2
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	14	0.2
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	19	0.2
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	19	0.2
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	19	0.2
(1,1805)	1:53:A:LYS:H	1:52:A:ASN:H	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1782)	1:53:A:LYS:HD2	1:49:A:LYS:HG2	20	0.2
(1,1782)	1:53:A:LYS:HD2	1:49:A:LYS:HG3	20	0.2
(1,1782)	1:53:A:LYS:HD3	1:49:A:LYS:HG2	20	0.2
(1,1782)	1:53:A:LYS:HD3	1:49:A:LYS:HG3	20	0.2
(1,1755)	1:52:A:ASN:H	1:53:A:LYS:H	15	0.2
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	19	0.2
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	19	0.2
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	3	0.2
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	9	0.2
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	10	0.2
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	5	0.2
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	5	0.2
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	5	0.2
(1,1152)	1:36:A:LEU:HD21	1:44:A:LEU:HD21	15	0.2
(1,1152)	1:36:A:LEU:HD21	1:44:A:LEU:HD22	15	0.2
(1,1152)	1:36:A:LEU:HD21	1:44:A:LEU:HD23	15	0.2
(1,1152)	1:36:A:LEU:HD22	1:44:A:LEU:HD21	15	0.2
(1,1152)	1:36:A:LEU:HD22	1:44:A:LEU:HD22	15	0.2
(1,1152)	1:36:A:LEU:HD22	1:44:A:LEU:HD23	15	0.2
(1,1152)	1:36:A:LEU:HD23	1:44:A:LEU:HD21	15	0.2
(1,1152)	1:36:A:LEU:HD23	1:44:A:LEU:HD22	15	0.2
(1,1152)	1:36:A:LEU:HD23	1:44:A:LEU:HD23	15	0.2
(1,966)	1:32:A:LYS:H	1:29:A:CYS:HB2	8	0.2
(1,965)	1:32:A:LYS:H	1:29:A:CYS:HA	9	0.2
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	2	0.2
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	11	0.2
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	12	0.2
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD2	1	0.2
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD3	1	0.2
(1,498)	1:16:A:GLU:H	1:33:A:GLY:H	6	0.2
(1,498)	1:16:A:GLU:H	1:33:A:GLY:H	17	0.2
(1,381)	1:11:A:ALA:H	1:34:A:VAL:HB	15	0.2
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	20	0.2
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	20	0.2
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	20	0.2
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	7	0.2
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	7	0.2
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	7	0.2
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	9	0.2
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	9	0.2
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	9	0.2
(2,1018)	1:13:C:PRO:HB2	1:21:C:ILE:HG23	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	7	0.19
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	18	0.19
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	5	0.19
(2,872)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	5	0.19
(2,872)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	11	0.19
(2,872)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	12	0.19
(2,871)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	2	0.19
(2,871)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	19	0.19
(2,869)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	5	0.19
(2,869)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	11	0.19
(2,869)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	12	0.19
(2,868)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	2	0.19
(2,868)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	19	0.19
(2,571)	1:2:B:VAL:HG11	1:1:B:FME:HA	4	0.19
(2,570)	1:2:A:VAL:HG12	1:1:A:FME:HA	3	0.19
(2,570)	1:2:A:VAL:HG11	1:1:A:FME:HA	13	0.19
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	7	0.19
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	18	0.19
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	5	0.19
(2,268)	1:51:C:LEU:HB2	1:52:C:ASN:HB2	3	0.19
(2,180)	1:19:B:GLY:H	1:17:B:ARG:HD3	15	0.19
(2,60)	1:3:B:ILE:H	1:2:B:VAL:HB	3	0.19
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	1	0.19
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	1	0.19
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	2	0.19
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	2	0.19
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	3	0.19
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	3	0.19
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	6	0.19
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	9	0.19
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	16	0.19
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	20	0.19
(1,4854)	1:42:C:THR:HB	1:3:B:ILE:HB	11	0.19
(1,4729)	1:37:C:THR:H	1:36:C:LEU:HG	11	0.19
(1,4713)	1:37:C:THR:HG21	1:8:C:LEU:HG	5	0.19
(1,4713)	1:37:C:THR:HG22	1:8:C:LEU:HG	5	0.19
(1,4713)	1:37:C:THR:HG23	1:8:C:LEU:HG	5	0.19
(1,4713)	1:37:C:THR:HG21	1:8:C:LEU:HG	13	0.19
(1,4713)	1:37:C:THR:HG22	1:8:C:LEU:HG	13	0.19
(1,4713)	1:37:C:THR:HG23	1:8:C:LEU:HG	13	0.19
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	18	0.19
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	3	0.19
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	8	0.19
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	16	0.19
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	18	0.19
(1,4193)	1:21:C:ILE:HD11	1:15:C:CYS:HA	7	0.19
(1,4193)	1:21:C:ILE:HD12	1:15:C:CYS:HA	7	0.19
(1,4193)	1:21:C:ILE:HD13	1:15:C:CYS:HA	7	0.19
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	5	0.19
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	5	0.19
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	5	0.19
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	5	0.19
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	18	0.19
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	13	0.19
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	13	0.19
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	13	0.19
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	16	0.19
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	16	0.19
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	16	0.19
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	10	0.19
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	10	0.19
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	10	0.19
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	12	0.19
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	12	0.19
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	12	0.19
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	18	0.19
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	18	0.19
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	18	0.19
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	19	0.19
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	19	0.19
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	19	0.19
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	20	0.19
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	20	0.19
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	20	0.19
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG2	8	0.19
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG3	8	0.19
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG2	8	0.19
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG3	8	0.19
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	1	0.19
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	1	0.19
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	14	0.19
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	14	0.19
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	13	0.19
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	15	0.19
(1,2955)	1:37:B:THR:HG21	1:8:B:LEU:HG	10	0.19
(1,2955)	1:37:B:THR:HG22	1:8:B:LEU:HG	10	0.19
(1,2955)	1:37:B:THR:HG23	1:8:B:LEU:HG	10	0.19
(1,2823)	1:34:B:VAL:H	1:32:B:LYS:HG2	7	0.19
(1,2823)	1:34:B:VAL:H	1:32:B:LYS:HG3	7	0.19
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	2	0.19
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	12	0.19
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	16	0.19
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG12	3	0.19
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG13	3	0.19
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG12	3	0.19
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG13	3	0.19
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG12	13	0.19
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG13	13	0.19
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG12	13	0.19
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG13	13	0.19
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG12	18	0.19
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG13	18	0.19
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG12	18	0.19
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG13	18	0.19
(1,2192)	1:12:B:CYS:H	1:34:B:VAL:HB	20	0.19
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	10	0.19
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	10	0.19
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	10	0.19
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	20	0.19
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	20	0.19
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	20	0.19
(1,1805)	1:53:A:LYS:H	1:52:A:ASN:H	5	0.19
(1,1798)	1:53:A:LYS:H	1:51:B:LEU:HD11	16	0.19
(1,1798)	1:53:A:LYS:H	1:51:B:LEU:HD12	16	0.19
(1,1798)	1:53:A:LYS:H	1:51:B:LEU:HD13	16	0.19
(1,1782)	1:53:A:LYS:HD2	1:49:A:LYS:HG2	12	0.19
(1,1782)	1:53:A:LYS:HD2	1:49:A:LYS:HG3	12	0.19
(1,1782)	1:53:A:LYS:HD3	1:49:A:LYS:HG2	12	0.19
(1,1782)	1:53:A:LYS:HD3	1:49:A:LYS:HG3	12	0.19
(1,1755)	1:52:A:ASN:H	1:53:A:LYS:H	5	0.19
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	4	0.19
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	13	0.19
(1,1343)	1:42:A:THR:HG21	1:8:C:LEU:HD11	3	0.19
(1,1343)	1:42:A:THR:HG21	1:8:C:LEU:HD12	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1343)	1:42:A:THR:HG21	1:8:C:LEU:HD13	3	0.19
(1,1343)	1:42:A:THR:HG22	1:8:C:LEU:HD11	3	0.19
(1,1343)	1:42:A:THR:HG22	1:8:C:LEU:HD12	3	0.19
(1,1343)	1:42:A:THR:HG22	1:8:C:LEU:HD13	3	0.19
(1,1343)	1:42:A:THR:HG23	1:8:C:LEU:HD11	3	0.19
(1,1343)	1:42:A:THR:HG23	1:8:C:LEU:HD12	3	0.19
(1,1343)	1:42:A:THR:HG23	1:8:C:LEU:HD13	3	0.19
(1,1325)	1:42:A:THR:HB	1:3:C:ILE:HB	9	0.19
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	19	0.19
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	19	0.19
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	19	0.19
(1,1052)	1:35:A:ILE:HA	1:11:A:ALA:HA	20	0.19
(1,1045)	1:34:A:VAL:H	1:32:A:LYS:HG2	1	0.19
(1,1045)	1:34:A:VAL:H	1:32:A:LYS:HG3	1	0.19
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	19	0.19
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	20	0.19
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	16	0.19
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	17	0.19
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG12	1	0.19
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG13	1	0.19
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG12	1	0.19
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG13	1	0.19
(1,381)	1:11:A:ALA:H	1:34:A:VAL:HB	12	0.19
(1,369)	1:11:A:ALA:HA	1:35:A:ILE:HA	20	0.19
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	1	0.19
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	1	0.19
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	1	0.19
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	6	0.19
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	6	0.19
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	6	0.19
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	17	0.19
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	17	0.19
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	17	0.19
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	15	0.19
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	15	0.19
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	15	0.19
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	20	0.19
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	20	0.19
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	20	0.19
(2,1555)	1:43:B:LEU:HD13	1:8:B:LEU:HD23	4	0.18
(2,1554)	1:43:A:LEU:HD11	1:8:A:LEU:HD23	11	0.18
(2,1554)	1:43:A:LEU:HD13	1:8:A:LEU:HD21	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1348)	1:8:B:LEU:HD23	1:43:B:LEU:HG	16	0.18
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	5	0.18
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	10	0.18
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	16	0.18
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	11	0.18
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	16	0.18
(2,961)	1:47:B:ILE:HB	1:47:C:ILE:HB	18	0.18
(2,871)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	8	0.18
(2,868)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	8	0.18
(2,572)	1:2:C:VAL:HG13	1:1:C:FME:HA	9	0.18
(2,469)	1:43:B:LEU:HD13	1:8:B:LEU:HD23	4	0.18
(2,468)	1:43:A:LEU:HD11	1:8:A:LEU:HD23	11	0.18
(2,468)	1:43:A:LEU:HD13	1:8:A:LEU:HD21	18	0.18
(2,440)	1:44:C:LEU:HD11	1:50:A:HIS:HB3	11	0.18
(2,400)	1:13:B:PRO:HG2	1:21:B:ILE:HD11	10	0.18
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	5	0.18
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	10	0.18
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	16	0.18
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	11	0.18
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	16	0.18
(2,268)	1:51:C:LEU:HB2	1:52:C:ASN:HB2	13	0.18
(2,265)	1:49:C:LYS:HE2	1:53:C:LYS:HB3	2	0.18
(2,265)	1:49:C:LYS:HE2	1:53:C:LYS:HB3	10	0.18
(1,5298)	1:53:C:LYS:HD2	1:49:C:LYS:HG2	7	0.18
(1,5298)	1:53:C:LYS:HD2	1:49:C:LYS:HG3	7	0.18
(1,5298)	1:53:C:LYS:HD3	1:49:C:LYS:HG2	7	0.18
(1,5298)	1:53:C:LYS:HD3	1:49:C:LYS:HG3	7	0.18
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB2	7	0.18
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB3	7	0.18
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB2	7	0.18
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB3	7	0.18
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB2	7	0.18
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB3	7	0.18
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB2	15	0.18
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB3	15	0.18
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB2	15	0.18
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB3	15	0.18
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB2	15	0.18
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB3	15	0.18
(1,4743)	1:38:C:ALA:HA	1:42:C:THR:HA	4	0.18
(1,4685)	1:36:C:LEU:HD21	1:44:C:LEU:HD21	18	0.18
(1,4685)	1:36:C:LEU:HD21	1:44:C:LEU:HD22	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4685)	1:36:C:LEU:HD21	1:44:C:LEU:HD23	18	0.18
(1,4685)	1:36:C:LEU:HD22	1:44:C:LEU:HD21	18	0.18
(1,4685)	1:36:C:LEU:HD22	1:44:C:LEU:HD22	18	0.18
(1,4685)	1:36:C:LEU:HD22	1:44:C:LEU:HD23	18	0.18
(1,4685)	1:36:C:LEU:HD23	1:44:C:LEU:HD21	18	0.18
(1,4685)	1:36:C:LEU:HD23	1:44:C:LEU:HD22	18	0.18
(1,4685)	1:36:C:LEU:HD23	1:44:C:LEU:HD23	18	0.18
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	4	0.18
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	15	0.18
(1,4450)	1:31:C:GLY:H	1:20:C:GLU:H	7	0.18
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	3	0.18
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	13	0.18
(1,4193)	1:21:C:ILE:HD11	1:15:C:CYS:HA	2	0.18
(1,4193)	1:21:C:ILE:HD12	1:15:C:CYS:HA	2	0.18
(1,4193)	1:21:C:ILE:HD13	1:15:C:CYS:HA	2	0.18
(1,4193)	1:21:C:ILE:HD11	1:15:C:CYS:HA	8	0.18
(1,4193)	1:21:C:ILE:HD12	1:15:C:CYS:HA	8	0.18
(1,4193)	1:21:C:ILE:HD13	1:15:C:CYS:HA	8	0.18
(1,4193)	1:21:C:ILE:HD11	1:15:C:CYS:HA	13	0.18
(1,4193)	1:21:C:ILE:HD12	1:15:C:CYS:HA	13	0.18
(1,4193)	1:21:C:ILE:HD13	1:15:C:CYS:HA	13	0.18
(1,4172)	1:20:C:GLU:H	1:31:C:GLY:H	7	0.18
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	3	0.18
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	19	0.18
(1,3979)	1:14:C:LYS:HE2	1:21:C:ILE:HD11	18	0.18
(1,3979)	1:14:C:LYS:HE2	1:21:C:ILE:HD12	18	0.18
(1,3979)	1:14:C:LYS:HE2	1:21:C:ILE:HD13	18	0.18
(1,3979)	1:14:C:LYS:HE3	1:21:C:ILE:HD11	18	0.18
(1,3979)	1:14:C:LYS:HE3	1:21:C:ILE:HD12	18	0.18
(1,3979)	1:14:C:LYS:HE3	1:21:C:ILE:HD13	18	0.18
(1,3949)	1:12:C:CYS:H	1:34:C:VAL:HB	19	0.18
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	4	0.18
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	15	0.18
(1,3909)	1:10:C:VAL:H	1:36:C:LEU:HA	6	0.18
(1,3801)	1:8:C:LEU:HD11	1:39:C:GLN:HB2	8	0.18
(1,3801)	1:8:C:LEU:HD12	1:39:C:GLN:HB2	8	0.18
(1,3801)	1:8:C:LEU:HD13	1:39:C:GLN:HB2	8	0.18
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	3	0.18
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	3	0.18
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	3	0.18
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	12	0.18
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	12	0.18
(1,3594)	1:2:C:VAL:HG11	1:1:C:FME:HG2	13	0.18
(1,3594)	1:2:C:VAL:HG11	1:1:C:FME:HG3	13	0.18
(1,3594)	1:2:C:VAL:HG12	1:1:C:FME:HG2	13	0.18
(1,3594)	1:2:C:VAL:HG12	1:1:C:FME:HG3	13	0.18
(1,3594)	1:2:C:VAL:HG13	1:1:C:FME:HG2	13	0.18
(1,3594)	1:2:C:VAL:HG13	1:1:C:FME:HG3	13	0.18
(1,3555)	1:53:B:LYS:H	1:49:B:LYS:H	13	0.18
(1,3555)	1:53:B:LYS:H	1:49:B:LYS:H	14	0.18
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG2	11	0.18
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG3	11	0.18
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG2	11	0.18
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG3	11	0.18
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG2	20	0.18
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG3	20	0.18
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG2	20	0.18
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG3	20	0.18
(1,3432)	1:49:B:LYS:H	1:53:B:LYS:H	13	0.18
(1,3432)	1:49:B:LYS:H	1:53:B:LYS:H	14	0.18
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	4	0.18
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	4	0.18
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	6	0.18
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	6	0.18
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	18	0.18
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB2	18	0.18
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB3	18	0.18
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB2	18	0.18
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB3	18	0.18
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB2	18	0.18
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB3	18	0.18
(1,2831)	1:35:B:ILE:HA	1:11:B:ALA:HA	15	0.18
(1,2821)	1:34:B:VAL:H	1:32:B:LYS:HA	1	0.18
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	8	0.18
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	18	0.18
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA2	12	0.18
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA3	12	0.18
(1,2500)	1:23:B:GLY:HA2	1:24:B:THR:HB	12	0.18
(1,2500)	1:23:B:GLY:HA3	1:24:B:THR:HB	12	0.18
(1,2435)	1:21:B:ILE:HD11	1:15:B:CYS:HA	14	0.18
(1,2435)	1:21:B:ILE:HD12	1:15:B:CYS:HA	14	0.18
(1,2435)	1:21:B:ILE:HD13	1:15:B:CYS:HA	14	0.18
(1,2290)	1:16:B:GLU:H	1:33:B:GLY:H	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG12	14	0.18
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG13	14	0.18
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG12	14	0.18
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG13	14	0.18
(1,2160)	1:11:B:ALA:HA	1:35:B:ILE:HA	15	0.18
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	20	0.18
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	20	0.18
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	20	0.18
(1,2044)	1:8:B:LEU:HD11	1:39:B:GLN:HB2	17	0.18
(1,2044)	1:8:B:LEU:HD12	1:39:B:GLN:HB2	17	0.18
(1,2044)	1:8:B:LEU:HD13	1:39:B:GLN:HB2	17	0.18
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	7	0.18
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	7	0.18
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	7	0.18
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	11	0.18
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	11	0.18
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	11	0.18
(1,1782)	1:53:A:LYS:HD2	1:49:A:LYS:HG2	6	0.18
(1,1782)	1:53:A:LYS:HD2	1:49:A:LYS:HG3	6	0.18
(1,1782)	1:53:A:LYS:HD3	1:49:A:LYS:HG2	6	0.18
(1,1782)	1:53:A:LYS:HD3	1:49:A:LYS:HG3	6	0.18
(1,1782)	1:53:A:LYS:HD2	1:49:A:LYS:HG2	16	0.18
(1,1782)	1:53:A:LYS:HD2	1:49:A:LYS:HG3	16	0.18
(1,1782)	1:53:A:LYS:HD3	1:49:A:LYS:HG2	16	0.18
(1,1782)	1:53:A:LYS:HD3	1:49:A:LYS:HG3	16	0.18
(1,1550)	1:47:A:ILE:HG12	1:50:B:HIS:HB2	13	0.18
(1,1550)	1:47:A:ILE:HG13	1:50:B:HIS:HB2	13	0.18
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	8	0.18
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	16	0.18
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	19	0.18
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	7	0.18
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	7	0.18
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	7	0.18
(1,1134)	1:36:A:LEU:HD11	1:35:A:ILE:HA	20	0.18
(1,1134)	1:36:A:LEU:HD12	1:35:A:ILE:HA	20	0.18
(1,1134)	1:36:A:LEU:HD13	1:35:A:ILE:HA	20	0.18
(1,1052)	1:35:A:ILE:HA	1:11:A:ALA:HA	7	0.18
(1,966)	1:32:A:LYS:H	1:29:A:CYS:HB2	14	0.18
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	12	0.18
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	13	0.18
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	5	0.18
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	20	0.18
(1,498)	1:16:A:GLU:H	1:33:A:GLY:H	5	0.18
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG12	11	0.18
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG13	11	0.18
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG12	11	0.18
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG13	11	0.18
(1,369)	1:11:A:ALA:HA	1:35:A:ILE:HA	7	0.18
(1,358)	1:10:A:VAL:H	1:36:A:LEU:HA	11	0.18
(1,358)	1:10:A:VAL:H	1:36:A:LEU:HA	19	0.18
(1,338)	1:10:A:VAL:HG11	1:36:A:LEU:HA	3	0.18
(1,338)	1:10:A:VAL:HG12	1:36:A:LEU:HA	3	0.18
(1,338)	1:10:A:VAL:HG13	1:36:A:LEU:HA	3	0.18
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	3	0.18
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	3	0.18
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	3	0.18
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	7	0.18
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	7	0.18
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	7	0.18
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	10	0.18
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	10	0.18
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	10	0.18
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	13	0.18
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	13	0.18
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	13	0.18
(2,1554)	1:43:A:LEU:HD11	1:8:C:LEU:HD23	9	0.17
(2,1414)	1:32:B:LYS:HA	1:19:B:GLY:HA2	14	0.17
(2,1406)	1:15:C:CYS:HA	1:17:C:ARG:HD3	8	0.17
(2,1405)	1:15:B:CYS:HA	1:17:B:ARG:HD3	3	0.17
(2,1349)	1:8:C:LEU:HD21	1:43:C:LEU:HG	11	0.17
(2,1347)	1:8:A:LEU:HD22	1:43:A:LEU:HG	14	0.17
(2,1305)	1:51:A:LEU:HD21	1:44:C:LEU:HA	16	0.17
(2,1018)	1:13:C:PRO:HB2	1:21:C:ILE:HG23	1	0.17
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	11	0.17
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	19	0.17
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	18	0.17
(2,873)	1:31:C:GLY:HA2	1:15:C:CYS:HB3	7	0.17
(2,873)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	11	0.17
(2,870)	1:31:C:GLY:HA2	1:15:C:CYS:HB3	7	0.17
(2,870)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	11	0.17
(2,697)	1:15:C:CYS:HA	1:17:C:ARG:HD3	8	0.17
(2,696)	1:15:B:CYS:HA	1:17:B:ARG:HD3	3	0.17
(2,489)	1:51:A:LEU:HD21	1:44:C:LEU:HA	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,468)	1:43:A:LEU:HD11	1:8:C:LEU:HD23	9	0.17
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	11	0.17
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	19	0.17
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	18	0.17
(2,267)	1:51:B:LEU:HB2	1:52:B:ASN:HB2	17	0.17
(2,266)	1:51:A:LEU:HB2	1:52:A:ASN:HB2	14	0.17
(2,248)	1:14:A:LYS:HE2	1:22:A:GLU:HB2	12	0.17
(2,60)	1:3:B:ILE:H	1:2:B:VAL:HB	17	0.17
(2,60)	1:3:B:ILE:H	1:2:B:VAL:HB	19	0.17
(1,5298)	1:53:C:LYS:HD2	1:49:C:LYS:HG2	6	0.17
(1,5298)	1:53:C:LYS:HD2	1:49:C:LYS:HG3	6	0.17
(1,5298)	1:53:C:LYS:HD3	1:49:C:LYS:HG2	6	0.17
(1,5298)	1:53:C:LYS:HD3	1:49:C:LYS:HG3	6	0.17
(1,5298)	1:53:C:LYS:HD2	1:49:C:LYS:HG2	15	0.17
(1,5298)	1:53:C:LYS:HD2	1:49:C:LYS:HG3	15	0.17
(1,5298)	1:53:C:LYS:HD3	1:49:C:LYS:HG2	15	0.17
(1,5298)	1:53:C:LYS:HD3	1:49:C:LYS:HG3	15	0.17
(1,5074)	1:47:C:ILE:HG12	1:50:A:HIS:HB2	20	0.17
(1,5074)	1:47:C:ILE:HG13	1:50:A:HIS:HB2	20	0.17
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	4	0.17
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	15	0.17
(1,4854)	1:42:C:THR:HB	1:3:B:ILE:HB	13	0.17
(1,4713)	1:37:C:THR:HG21	1:8:C:LEU:HG	9	0.17
(1,4713)	1:37:C:THR:HG22	1:8:C:LEU:HG	9	0.17
(1,4713)	1:37:C:THR:HG23	1:8:C:LEU:HG	9	0.17
(1,4713)	1:37:C:THR:HG21	1:8:C:LEU:HG	12	0.17
(1,4713)	1:37:C:THR:HG22	1:8:C:LEU:HG	12	0.17
(1,4713)	1:37:C:THR:HG23	1:8:C:LEU:HG	12	0.17
(1,4713)	1:37:C:THR:HG21	1:8:C:LEU:HG	19	0.17
(1,4713)	1:37:C:THR:HG22	1:8:C:LEU:HG	19	0.17
(1,4713)	1:37:C:THR:HG23	1:8:C:LEU:HG	19	0.17
(1,4666)	1:36:C:LEU:HD11	1:35:C:ILE:HA	16	0.17
(1,4666)	1:36:C:LEU:HD12	1:35:C:ILE:HA	16	0.17
(1,4666)	1:36:C:LEU:HD13	1:35:C:ILE:HA	16	0.17
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	9	0.17
(1,4504)	1:32:C:LYS:H	1:29:C:CYS:HA	14	0.17
(1,4504)	1:32:C:LYS:H	1:29:C:CYS:HA	19	0.17
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	11	0.17
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	5	0.17
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	14	0.17
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	15	0.17
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4193)	1:21:C:ILE:HD11	1:15:C:CYS:HA	5	0.17
(1,4193)	1:21:C:ILE:HD12	1:15:C:CYS:HA	5	0.17
(1,4193)	1:21:C:ILE:HD13	1:15:C:CYS:HA	5	0.17
(1,4140)	1:20:C:GLU:HA	1:27:C:PRO:HD2	6	0.17
(1,4140)	1:20:C:GLU:HA	1:27:C:PRO:HD3	6	0.17
(1,4140)	1:20:C:GLU:HA	1:27:C:PRO:HD2	19	0.17
(1,4140)	1:20:C:GLU:HA	1:27:C:PRO:HD3	19	0.17
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	9	0.17
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	9	0.17
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	9	0.17
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	9	0.17
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	12	0.17
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	12	0.17
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	12	0.17
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	12	0.17
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	13	0.17
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	13	0.17
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	13	0.17
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	13	0.17
(1,3949)	1:12:C:CYS:H	1:34:C:VAL:HB	16	0.17
(1,3949)	1:12:C:CYS:H	1:34:C:VAL:HB	18	0.17
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	9	0.17
(1,3801)	1:8:C:LEU:HD11	1:39:C:GLN:HB2	13	0.17
(1,3801)	1:8:C:LEU:HD12	1:39:C:GLN:HB2	13	0.17
(1,3801)	1:8:C:LEU:HD13	1:39:C:GLN:HB2	13	0.17
(1,3801)	1:8:C:LEU:HD11	1:39:C:GLN:HB2	15	0.17
(1,3801)	1:8:C:LEU:HD12	1:39:C:GLN:HB2	15	0.17
(1,3801)	1:8:C:LEU:HD13	1:39:C:GLN:HB2	15	0.17
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	11	0.17
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	11	0.17
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	11	0.17
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	15	0.17
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	15	0.17
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	15	0.17
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	17	0.17
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	17	0.17
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	17	0.17
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	18	0.17
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	18	0.17
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	18	0.17
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	20	0.17
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	20	0.17
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	2	0.17
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	2	0.17
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	2	0.17
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	14	0.17
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	14	0.17
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	14	0.17
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	15	0.17
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	15	0.17
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	2	0.17
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	6	0.17
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	17	0.17
(1,3107)	1:42:B:THR:HB	1:3:A:ILE:HB	8	0.17
(1,3039)	1:40:B:GLY:H	1:43:B:LEU:HB3	3	0.17
(1,2985)	1:38:B:ALA:HA	1:42:B:THR:HA	16	0.17
(1,2955)	1:37:B:THR:HG21	1:8:B:LEU:HG	18	0.17
(1,2955)	1:37:B:THR:HG22	1:8:B:LEU:HG	18	0.17
(1,2955)	1:37:B:THR:HG23	1:8:B:LEU:HG	18	0.17
(1,2908)	1:36:B:LEU:HD11	1:35:B:ILE:HA	6	0.17
(1,2908)	1:36:B:LEU:HD12	1:35:B:ILE:HA	6	0.17
(1,2908)	1:36:B:LEU:HD13	1:35:B:ILE:HA	6	0.17
(1,2831)	1:35:B:ILE:HA	1:11:B:ALA:HA	16	0.17
(1,2726)	1:32:B:LYS:HE2	1:29:B:CYS:HB3	6	0.17
(1,2726)	1:32:B:LYS:HE3	1:29:B:CYS:HB3	6	0.17
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	10	0.17
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	9	0.17
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	13	0.17
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	17	0.17
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	19	0.17
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD2	1	0.17
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD3	1	0.17
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG12	7	0.17
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG13	7	0.17
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG12	7	0.17
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG13	7	0.17
(1,2160)	1:11:B:ALA:HA	1:35:B:ILE:HA	16	0.17
(1,2152)	1:10:B:VAL:H	1:36:B:LEU:HA	6	0.17
(1,2152)	1:10:B:VAL:H	1:36:B:LEU:HA	9	0.17
(1,2044)	1:8:B:LEU:HD11	1:39:B:GLN:HB2	18	0.17
(1,2044)	1:8:B:LEU:HD12	1:39:B:GLN:HB2	18	0.17
(1,2044)	1:8:B:LEU:HD13	1:39:B:GLN:HB2	18	0.17
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	2	0.17
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	2	0.17
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	5	0.17
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	5	0.17
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	5	0.17
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	10	0.17
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	10	0.17
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	10	0.17
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	12	0.17
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	12	0.17
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	12	0.17
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	17	0.17
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	17	0.17
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	17	0.17
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	4	0.17
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	4	0.17
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	4	0.17
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	8	0.17
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	8	0.17
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	8	0.17
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	9	0.17
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	9	0.17
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	9	0.17
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG21	17	0.17
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG22	17	0.17
(1,1818)	1:1:B:FME:HE1	1:3:B:ILE:HG23	17	0.17
(1,1798)	1:53:A:LYS:H	1:51:B:LEU:HD11	15	0.17
(1,1798)	1:53:A:LYS:H	1:51:B:LEU:HD12	15	0.17
(1,1798)	1:53:A:LYS:H	1:51:B:LEU:HD13	15	0.17
(1,1777)	1:53:A:LYS:HD2	1:48:A:GLN:HB2	15	0.17
(1,1777)	1:53:A:LYS:HD3	1:48:A:GLN:HB2	15	0.17
(1,1598)	1:48:A:GLN:HG2	1:45:A:ASP:HB2	15	0.17
(1,1598)	1:48:A:GLN:HG2	1:45:A:ASP:HB3	15	0.17
(1,1598)	1:48:A:GLN:HG3	1:45:A:ASP:HB2	15	0.17
(1,1598)	1:48:A:GLN:HG3	1:45:A:ASP:HB3	15	0.17
(1,1487)	1:45:A:ASP:HB2	1:48:A:GLN:HG2	15	0.17
(1,1487)	1:45:A:ASP:HB2	1:48:A:GLN:HG3	15	0.17
(1,1487)	1:45:A:ASP:HB3	1:48:A:GLN:HG2	15	0.17
(1,1487)	1:45:A:ASP:HB3	1:48:A:GLN:HG3	15	0.17
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	14	0.17
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	18	0.17
(1,1325)	1:42:A:THR:HB	1:3:C:ILE:HB	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	9	0.17
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	9	0.17
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	9	0.17
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	10	0.17
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	10	0.17
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	10	0.17
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	16	0.17
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	16	0.17
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	16	0.17
(1,1152)	1:36:A:LEU:HD21	1:44:A:LEU:HD21	10	0.17
(1,1152)	1:36:A:LEU:HD21	1:44:A:LEU:HD22	10	0.17
(1,1152)	1:36:A:LEU:HD21	1:44:A:LEU:HD23	10	0.17
(1,1152)	1:36:A:LEU:HD22	1:44:A:LEU:HD21	10	0.17
(1,1152)	1:36:A:LEU:HD22	1:44:A:LEU:HD22	10	0.17
(1,1152)	1:36:A:LEU:HD22	1:44:A:LEU:HD23	10	0.17
(1,1152)	1:36:A:LEU:HD23	1:44:A:LEU:HD21	10	0.17
(1,1152)	1:36:A:LEU:HD23	1:44:A:LEU:HD22	10	0.17
(1,1152)	1:36:A:LEU:HD23	1:44:A:LEU:HD23	10	0.17
(1,1134)	1:36:A:LEU:HD11	1:35:A:ILE:HA	19	0.17
(1,1134)	1:36:A:LEU:HD12	1:35:A:ILE:HA	19	0.17
(1,1134)	1:36:A:LEU:HD13	1:35:A:ILE:HA	19	0.17
(1,1052)	1:35:A:ILE:HA	1:11:A:ALA:HA	13	0.17
(1,1043)	1:34:A:VAL:H	1:32:A:LYS:HA	19	0.17
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	5	0.17
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	8	0.17
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	11	0.17
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	15	0.17
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	18	0.17
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA2	10	0.17
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA3	10	0.17
(1,712)	1:23:A:GLY:HA2	1:24:A:THR:HB	10	0.17
(1,712)	1:23:A:GLY:HA3	1:24:A:THR:HB	10	0.17
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD2	4	0.17
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD3	4	0.17
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG12	14	0.17
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG13	14	0.17
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG12	14	0.17
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG13	14	0.17
(1,400)	1:12:A:CYS:H	1:34:A:VAL:HB	19	0.17
(1,369)	1:11:A:ALA:HA	1:35:A:ILE:HA	13	0.17
(1,244)	1:8:A:LEU:HD11	1:39:A:GLN:HB2	13	0.17
(1,244)	1:8:A:LEU:HD12	1:39:A:GLN:HB2	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:8:A:LEU:HD13	1:39:A:GLN:HB2	13	0.17
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	2	0.17
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	2	0.17
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	2	0.17
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	9	0.17
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	9	0.17
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	9	0.17
(1,32)	1:2:A:VAL:HG11	1:1:A:FME:HG2	9	0.17
(1,32)	1:2:A:VAL:HG11	1:1:A:FME:HG3	9	0.17
(1,32)	1:2:A:VAL:HG12	1:1:A:FME:HG2	9	0.17
(1,32)	1:2:A:VAL:HG12	1:1:A:FME:HG3	9	0.17
(1,32)	1:2:A:VAL:HG13	1:1:A:FME:HG2	9	0.17
(1,32)	1:2:A:VAL:HG13	1:1:A:FME:HG3	9	0.17
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	10	0.17
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	10	0.17
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	10	0.17
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	14	0.17
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	14	0.17
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	14	0.17
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	17	0.17
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	17	0.17
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	17	0.17
(2,1556)	1:43:C:LEU:HD11	1:8:C:LEU:HD21	7	0.16
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA3	8	0.16
(2,1163)	1:35:C:ILE:HG12	1:16:C:GLU:HG2	17	0.16
(2,1017)	1:13:B:PRO:HB2	1:21:B:ILE:HG23	18	0.16
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	2	0.16
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	4	0.16
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	17	0.16
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	3	0.16
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	13	0.16
(2,483)	1:51:A:LEU:HD11	1:47:C:ILE:HB	6	0.16
(2,470)	1:43:C:LEU:HD11	1:8:C:LEU:HD21	7	0.16
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	2	0.16
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	4	0.16
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	17	0.16
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	3	0.16
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	13	0.16
(2,267)	1:51:B:LEU:HB2	1:52:B:ASN:HB2	10	0.16
(2,267)	1:51:B:LEU:HB2	1:52:B:ASN:HB2	19	0.16
(2,69)	1:51:B:LEU:H	1:51:B:LEU:HD11	17	0.16
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD11	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD12	3	0.16
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD13	3	0.16
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	19	0.16
(1,5298)	1:53:C:LYS:HD2	1:49:C:LYS:HG2	5	0.16
(1,5298)	1:53:C:LYS:HD2	1:49:C:LYS:HG3	5	0.16
(1,5298)	1:53:C:LYS:HD3	1:49:C:LYS:HG2	5	0.16
(1,5298)	1:53:C:LYS:HD3	1:49:C:LYS:HG3	5	0.16
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	19	0.16
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	10	0.16
(1,4854)	1:42:C:THR:HB	1:3:B:ILE:HB	5	0.16
(1,4854)	1:42:C:THR:HB	1:3:B:ILE:HB	19	0.16
(1,4797)	1:40:C:GLY:H	1:43:C:LEU:HB3	2	0.16
(1,4797)	1:40:C:GLY:H	1:43:C:LEU:HB3	12	0.16
(1,4797)	1:40:C:GLY:H	1:43:C:LEU:HB3	17	0.16
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB2	2	0.16
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB3	2	0.16
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB2	2	0.16
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB3	2	0.16
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB2	2	0.16
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB3	2	0.16
(1,4729)	1:37:C:THR:H	1:36:C:LEU:HG	16	0.16
(1,4713)	1:37:C:THR:HG21	1:8:C:LEU:HG	10	0.16
(1,4713)	1:37:C:THR:HG22	1:8:C:LEU:HG	10	0.16
(1,4713)	1:37:C:THR:HG23	1:8:C:LEU:HG	10	0.16
(1,4713)	1:37:C:THR:HG21	1:8:C:LEU:HG	15	0.16
(1,4713)	1:37:C:THR:HG22	1:8:C:LEU:HG	15	0.16
(1,4713)	1:37:C:THR:HG23	1:8:C:LEU:HG	15	0.16
(1,4666)	1:36:C:LEU:HD11	1:35:C:ILE:HA	5	0.16
(1,4666)	1:36:C:LEU:HD12	1:35:C:ILE:HA	5	0.16
(1,4666)	1:36:C:LEU:HD13	1:35:C:ILE:HA	5	0.16
(1,4666)	1:36:C:LEU:HD11	1:35:C:ILE:HA	11	0.16
(1,4666)	1:36:C:LEU:HD12	1:35:C:ILE:HA	11	0.16
(1,4666)	1:36:C:LEU:HD13	1:35:C:ILE:HA	11	0.16
(1,4666)	1:36:C:LEU:HD11	1:35:C:ILE:HA	13	0.16
(1,4666)	1:36:C:LEU:HD12	1:35:C:ILE:HA	13	0.16
(1,4666)	1:36:C:LEU:HD13	1:35:C:ILE:HA	13	0.16
(1,4494)	1:32:C:LYS:HG2	1:29:C:CYS:HB3	14	0.16
(1,4494)	1:32:C:LYS:HG3	1:29:C:CYS:HB3	14	0.16
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	14	0.16
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	8	0.16
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	9	0.16
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA2	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA3	12	0.16
(1,4258)	1:23:C:GLY:HA2	1:24:C:THR:HB	12	0.16
(1,4258)	1:23:C:GLY:HA3	1:24:C:THR:HB	12	0.16
(1,3979)	1:14:C:LYS:HE2	1:21:C:ILE:HD11	12	0.16
(1,3979)	1:14:C:LYS:HE2	1:21:C:ILE:HD12	12	0.16
(1,3979)	1:14:C:LYS:HE2	1:21:C:ILE:HD13	12	0.16
(1,3979)	1:14:C:LYS:HE3	1:21:C:ILE:HD11	12	0.16
(1,3979)	1:14:C:LYS:HE3	1:21:C:ILE:HD12	12	0.16
(1,3979)	1:14:C:LYS:HE3	1:21:C:ILE:HD13	12	0.16
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	1	0.16
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	1	0.16
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	1	0.16
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	1	0.16
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	17	0.16
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	17	0.16
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	17	0.16
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	17	0.16
(1,3949)	1:12:C:CYS:H	1:34:C:VAL:HB	3	0.16
(1,3909)	1:10:C:VAL:H	1:36:C:LEU:HA	13	0.16
(1,3801)	1:8:C:LEU:HD11	1:39:C:GLN:HB2	12	0.16
(1,3801)	1:8:C:LEU:HD12	1:39:C:GLN:HB2	12	0.16
(1,3801)	1:8:C:LEU:HD13	1:39:C:GLN:HB2	12	0.16
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	1	0.16
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	1	0.16
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	1	0.16
(1,3594)	1:2:C:VAL:HG11	1:1:C:FME:HG2	15	0.16
(1,3594)	1:2:C:VAL:HG11	1:1:C:FME:HG3	15	0.16
(1,3594)	1:2:C:VAL:HG12	1:1:C:FME:HG2	15	0.16
(1,3594)	1:2:C:VAL:HG12	1:1:C:FME:HG3	15	0.16
(1,3594)	1:2:C:VAL:HG13	1:1:C:FME:HG2	15	0.16
(1,3594)	1:2:C:VAL:HG13	1:1:C:FME:HG3	15	0.16
(1,3555)	1:53:B:LYS:H	1:49:B:LYS:H	12	0.16
(1,3555)	1:53:B:LYS:H	1:49:B:LYS:H	18	0.16
(1,3432)	1:49:B:LYS:H	1:53:B:LYS:H	12	0.16
(1,3432)	1:49:B:LYS:H	1:53:B:LYS:H	18	0.16
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	2	0.16
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	2	0.16
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	7	0.16
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	7	0.16
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	10	0.16
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	10	0.16
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	10	0.16
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	14	0.16
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	20	0.16
(1,3107)	1:42:B:THR:HB	1:3:A:ILE:HB	16	0.16
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB2	19	0.16
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB3	19	0.16
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB2	19	0.16
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB3	19	0.16
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB2	19	0.16
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB3	19	0.16
(1,2985)	1:38:B:ALA:HA	1:42:B:THR:HA	12	0.16
(1,2985)	1:38:B:ALA:HA	1:42:B:THR:HA	15	0.16
(1,2955)	1:37:B:THR:HG21	1:8:B:LEU:HG	12	0.16
(1,2955)	1:37:B:THR:HG22	1:8:B:LEU:HG	12	0.16
(1,2955)	1:37:B:THR:HG23	1:8:B:LEU:HG	12	0.16
(1,2908)	1:36:B:LEU:HD11	1:35:B:ILE:HA	3	0.16
(1,2908)	1:36:B:LEU:HD12	1:35:B:ILE:HA	3	0.16
(1,2908)	1:36:B:LEU:HD13	1:35:B:ILE:HA	3	0.16
(1,2908)	1:36:B:LEU:HD11	1:35:B:ILE:HA	9	0.16
(1,2908)	1:36:B:LEU:HD12	1:35:B:ILE:HA	9	0.16
(1,2908)	1:36:B:LEU:HD13	1:35:B:ILE:HA	9	0.16
(1,2908)	1:36:B:LEU:HD11	1:35:B:ILE:HA	13	0.16
(1,2908)	1:36:B:LEU:HD12	1:35:B:ILE:HA	13	0.16
(1,2908)	1:36:B:LEU:HD13	1:35:B:ILE:HA	13	0.16
(1,2908)	1:36:B:LEU:HD11	1:35:B:ILE:HA	14	0.16
(1,2908)	1:36:B:LEU:HD12	1:35:B:ILE:HA	14	0.16
(1,2908)	1:36:B:LEU:HD13	1:35:B:ILE:HA	14	0.16
(1,2849)	1:35:B:ILE:HD11	1:10:B:VAL:HG21	3	0.16
(1,2849)	1:35:B:ILE:HD11	1:10:B:VAL:HG22	3	0.16
(1,2849)	1:35:B:ILE:HD11	1:10:B:VAL:HG23	3	0.16
(1,2849)	1:35:B:ILE:HD12	1:10:B:VAL:HG21	3	0.16
(1,2849)	1:35:B:ILE:HD12	1:10:B:VAL:HG22	3	0.16
(1,2849)	1:35:B:ILE:HD12	1:10:B:VAL:HG23	3	0.16
(1,2849)	1:35:B:ILE:HD13	1:10:B:VAL:HG21	3	0.16
(1,2849)	1:35:B:ILE:HD13	1:10:B:VAL:HG22	3	0.16
(1,2849)	1:35:B:ILE:HD13	1:10:B:VAL:HG23	3	0.16
(1,2831)	1:35:B:ILE:HA	1:11:B:ALA:HA	10	0.16
(1,2823)	1:34:B:VAL:H	1:32:B:LYS:HG2	2	0.16
(1,2823)	1:34:B:VAL:H	1:32:B:LYS:HG3	2	0.16
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	6	0.16
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	11	0.16
(1,2435)	1:21:B:ILE:HD11	1:15:B:CYS:HA	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2435)	1:21:B:ILE:HD12	1:15:B:CYS:HA	11	0.16
(1,2435)	1:21:B:ILE:HD13	1:15:B:CYS:HA	11	0.16
(1,2290)	1:16:B:GLU:H	1:33:B:GLY:H	6	0.16
(1,2290)	1:16:B:GLU:H	1:33:B:GLY:H	13	0.16
(1,2290)	1:16:B:GLU:H	1:33:B:GLY:H	15	0.16
(1,2290)	1:16:B:GLU:H	1:33:B:GLY:H	16	0.16
(1,2217)	1:14:B:LYS:HB2	1:21:B:ILE:HD11	7	0.16
(1,2217)	1:14:B:LYS:HB2	1:21:B:ILE:HD12	7	0.16
(1,2217)	1:14:B:LYS:HB2	1:21:B:ILE:HD13	7	0.16
(1,2217)	1:14:B:LYS:HB3	1:21:B:ILE:HD11	7	0.16
(1,2217)	1:14:B:LYS:HB3	1:21:B:ILE:HD12	7	0.16
(1,2217)	1:14:B:LYS:HB3	1:21:B:ILE:HD13	7	0.16
(1,2192)	1:12:B:CYS:H	1:34:B:VAL:HB	8	0.16
(1,2160)	1:11:B:ALA:HA	1:35:B:ILE:HA	10	0.16
(1,2141)	1:10:B:VAL:HG21	1:35:B:ILE:HD11	3	0.16
(1,2141)	1:10:B:VAL:HG21	1:35:B:ILE:HD12	3	0.16
(1,2141)	1:10:B:VAL:HG21	1:35:B:ILE:HD13	3	0.16
(1,2141)	1:10:B:VAL:HG22	1:35:B:ILE:HD11	3	0.16
(1,2141)	1:10:B:VAL:HG22	1:35:B:ILE:HD12	3	0.16
(1,2141)	1:10:B:VAL:HG22	1:35:B:ILE:HD13	3	0.16
(1,2141)	1:10:B:VAL:HG23	1:35:B:ILE:HD11	3	0.16
(1,2141)	1:10:B:VAL:HG23	1:35:B:ILE:HD12	3	0.16
(1,2141)	1:10:B:VAL:HG23	1:35:B:ILE:HD13	3	0.16
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	19	0.16
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	19	0.16
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	19	0.16
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	14	0.16
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	5	0.16
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	6	0.16
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	7	0.16
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	11	0.16
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	15	0.16
(1,1325)	1:42:A:THR:HB	1:3:C:ILE:HB	16	0.16
(1,1263)	1:40:A:GLY:H	1:43:A:LEU:HB3	3	0.16
(1,1263)	1:40:A:GLY:H	1:43:A:LEU:HB3	4	0.16
(1,1263)	1:40:A:GLY:H	1:43:A:LEU:HB3	11	0.16
(1,1263)	1:40:A:GLY:H	1:43:A:LEU:HB3	18	0.16
(1,1263)	1:40:A:GLY:H	1:43:A:LEU:HB3	19	0.16
(1,1134)	1:36:A:LEU:HD11	1:35:A:ILE:HA	13	0.16
(1,1134)	1:36:A:LEU:HD12	1:35:A:ILE:HA	13	0.16
(1,1134)	1:36:A:LEU:HD13	1:35:A:ILE:HA	13	0.16
(1,1052)	1:35:A:ILE:HA	1:11:A:ALA:HA	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1052)	1:35:A:ILE:HA	1:11:A:ALA:HA	9	0.16
(1,1052)	1:35:A:ILE:HA	1:11:A:ALA:HA	14	0.16
(1,966)	1:32:A:LYS:H	1:29:A:CYS:HB2	17	0.16
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	2	0.16
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	3	0.16
(1,369)	1:11:A:ALA:HA	1:35:A:ILE:HA	1	0.16
(1,369)	1:11:A:ALA:HA	1:35:A:ILE:HA	9	0.16
(1,369)	1:11:A:ALA:HA	1:35:A:ILE:HA	14	0.16
(1,358)	1:10:A:VAL:H	1:36:A:LEU:HA	18	0.16
(1,358)	1:10:A:VAL:H	1:36:A:LEU:HA	20	0.16
(1,244)	1:8:A:LEU:HD11	1:39:A:GLN:HB2	14	0.16
(1,244)	1:8:A:LEU:HD12	1:39:A:GLN:HB2	14	0.16
(1,244)	1:8:A:LEU:HD13	1:39:A:GLN:HB2	14	0.16
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	4	0.16
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	4	0.16
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	4	0.16
(2,1404)	1:15:A:CYS:HA	1:17:A:ARG:HD3	14	0.15
(2,1322)	1:43:C:LEU:HD23	1:43:A:LEU:HA	19	0.15
(2,1016)	1:13:A:PRO:HB2	1:21:A:ILE:HG22	14	0.15
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	6	0.15
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	2	0.15
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	10	0.15
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	1	0.15
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	2	0.15
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	3	0.15
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	7	0.15
(2,873)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	6	0.15
(2,872)	1:31:B:GLY:HA2	1:15:B:CYS:HB3	8	0.15
(2,872)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	13	0.15
(2,870)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	6	0.15
(2,869)	1:31:B:GLY:HA2	1:15:B:CYS:HB3	8	0.15
(2,869)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	13	0.15
(2,695)	1:15:A:CYS:HA	1:17:A:ARG:HD3	14	0.15
(2,570)	1:2:A:VAL:HG12	1:1:A:FME:HA	7	0.15
(2,509)	1:43:C:LEU:HD23	1:43:A:LEU:HA	19	0.15
(2,483)	1:51:A:LEU:HD12	1:47:C:ILE:HB	1	0.15
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	6	0.15
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	2	0.15
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	10	0.15
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	1	0.15
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	2	0.15
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	7	0.15
(2,249)	1:14:B:LYS:HE2	1:22:B:GLU:HB2	14	0.15
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	1	0.15
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	12	0.15
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	13	0.15
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	1	0.15
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	12	0.15
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	13	0.15
(1,5118)	1:48:C:GLN:HG2	1:45:C:ASP:HB2	11	0.15
(1,5118)	1:48:C:GLN:HG2	1:45:C:ASP:HB3	11	0.15
(1,5118)	1:48:C:GLN:HG3	1:45:C:ASP:HB2	11	0.15
(1,5118)	1:48:C:GLN:HG3	1:45:C:ASP:HB3	11	0.15
(1,5057)	1:46:C:PHE:H	1:48:C:GLN:HB3	6	0.15
(1,5057)	1:46:C:PHE:H	1:48:C:GLN:HB3	14	0.15
(1,5057)	1:46:C:PHE:H	1:48:C:GLN:HB3	15	0.15
(1,5011)	1:45:C:ASP:HB2	1:48:C:GLN:HG2	11	0.15
(1,5011)	1:45:C:ASP:HB2	1:48:C:GLN:HG3	11	0.15
(1,5011)	1:45:C:ASP:HB3	1:48:C:GLN:HG2	11	0.15
(1,5011)	1:45:C:ASP:HB3	1:48:C:GLN:HG3	11	0.15
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	2	0.15
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	5	0.15
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	11	0.15
(1,4854)	1:42:C:THR:HB	1:3:B:ILE:HB	6	0.15
(1,4800)	1:41:C:TYR:HA	1:36:C:LEU:HD11	19	0.15
(1,4800)	1:41:C:TYR:HA	1:36:C:LEU:HD12	19	0.15
(1,4800)	1:41:C:TYR:HA	1:36:C:LEU:HD13	19	0.15
(1,4797)	1:40:C:GLY:H	1:43:C:LEU:HB3	6	0.15
(1,4797)	1:40:C:GLY:H	1:43:C:LEU:HB3	20	0.15
(1,4743)	1:38:C:ALA:HA	1:42:C:THR:HA	9	0.15
(1,4713)	1:37:C:THR:HG21	1:8:C:LEU:HG	4	0.15
(1,4713)	1:37:C:THR:HG22	1:8:C:LEU:HG	4	0.15
(1,4713)	1:37:C:THR:HG23	1:8:C:LEU:HG	4	0.15
(1,4673)	1:36:C:LEU:HD11	1:41:C:TYR:HA	19	0.15
(1,4673)	1:36:C:LEU:HD12	1:41:C:TYR:HA	19	0.15
(1,4673)	1:36:C:LEU:HD13	1:41:C:TYR:HA	19	0.15
(1,4666)	1:36:C:LEU:HD11	1:35:C:ILE:HA	2	0.15
(1,4666)	1:36:C:LEU:HD12	1:35:C:ILE:HA	2	0.15
(1,4666)	1:36:C:LEU:HD13	1:35:C:ILE:HA	2	0.15
(1,4505)	1:32:C:LYS:H	1:29:C:CYS:HB2	19	0.15
(1,4387)	1:28:C:ALA:H	1:30:C:SER:H	20	0.15
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	2	0.15
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	7	0.15
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	12	0.15
(1,4193)	1:21:C:ILE:HD11	1:15:C:CYS:HA	11	0.15
(1,4193)	1:21:C:ILE:HD12	1:15:C:CYS:HA	11	0.15
(1,4193)	1:21:C:ILE:HD13	1:15:C:CYS:HA	11	0.15
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	18	0.15
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	8	0.15
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	8	0.15
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	8	0.15
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	8	0.15
(1,3949)	1:12:C:CYS:H	1:34:C:VAL:HB	5	0.15
(1,3801)	1:8:C:LEU:HD11	1:39:C:GLN:HB2	3	0.15
(1,3801)	1:8:C:LEU:HD12	1:39:C:GLN:HB2	3	0.15
(1,3801)	1:8:C:LEU:HD13	1:39:C:GLN:HB2	3	0.15
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	4	0.15
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	4	0.15
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	4	0.15
(1,3567)	1:1:C:FME:HA	1:3:C:ILE:H	18	0.15
(1,3555)	1:53:B:LYS:H	1:49:B:LYS:H	6	0.15
(1,3432)	1:49:B:LYS:H	1:53:B:LYS:H	6	0.15
(1,3342)	1:48:B:GLN:HB3	1:49:B:LYS:HB3	8	0.15
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	16	0.15
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	16	0.15
(1,3299)	1:46:B:PHE:H	1:48:B:GLN:HB3	6	0.15
(1,3299)	1:46:B:PHE:H	1:48:B:GLN:HB3	13	0.15
(1,3299)	1:46:B:PHE:H	1:48:B:GLN:HB3	14	0.15
(1,3299)	1:46:B:PHE:H	1:48:B:GLN:HB3	20	0.15
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	1	0.15
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	4	0.15
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	12	0.15
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	19	0.15
(1,3107)	1:42:B:THR:HB	1:3:A:ILE:HB	5	0.15
(1,3098)	1:42:B:THR:HB	1:39:B:GLN:HE21	17	0.15
(1,3098)	1:42:B:THR:HB	1:39:B:GLN:HE22	17	0.15
(1,2955)	1:37:B:THR:HG21	1:8:B:LEU:HG	15	0.15
(1,2955)	1:37:B:THR:HG22	1:8:B:LEU:HG	15	0.15
(1,2955)	1:37:B:THR:HG23	1:8:B:LEU:HG	15	0.15
(1,2908)	1:36:B:LEU:HD11	1:35:B:ILE:HA	1	0.15
(1,2908)	1:36:B:LEU:HD12	1:35:B:ILE:HA	1	0.15
(1,2908)	1:36:B:LEU:HD13	1:35:B:ILE:HA	1	0.15
(1,2908)	1:36:B:LEU:HD11	1:35:B:ILE:HA	19	0.15
(1,2908)	1:36:B:LEU:HD12	1:35:B:ILE:HA	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2908)	1:36:B:LEU:HD13	1:35:B:ILE:HA	19	0.15
(1,2823)	1:34:B:VAL:H	1:32:B:LYS:HG2	8	0.15
(1,2823)	1:34:B:VAL:H	1:32:B:LYS:HG3	8	0.15
(1,2821)	1:34:B:VAL:H	1:32:B:LYS:HA	17	0.15
(1,2747)	1:32:B:LYS:H	1:29:B:CYS:HB2	14	0.15
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG21	19	0.15
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	19	0.15
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG23	19	0.15
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG21	19	0.15
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG22	19	0.15
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG23	19	0.15
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	4	0.15
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	5	0.15
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD2	9	0.15
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD3	9	0.15
(1,2290)	1:16:B:GLU:H	1:33:B:GLY:H	2	0.15
(1,2222)	1:14:B:LYS:HE2	1:21:B:ILE:HD11	19	0.15
(1,2222)	1:14:B:LYS:HE2	1:21:B:ILE:HD12	19	0.15
(1,2222)	1:14:B:LYS:HE2	1:21:B:ILE:HD13	19	0.15
(1,2222)	1:14:B:LYS:HE3	1:21:B:ILE:HD11	19	0.15
(1,2222)	1:14:B:LYS:HE3	1:21:B:ILE:HD12	19	0.15
(1,2222)	1:14:B:LYS:HE3	1:21:B:ILE:HD13	19	0.15
(1,2192)	1:12:B:CYS:H	1:34:B:VAL:HB	2	0.15
(1,2192)	1:12:B:CYS:H	1:34:B:VAL:HB	7	0.15
(1,2152)	1:10:B:VAL:H	1:36:B:LEU:HA	1	0.15
(1,2044)	1:8:B:LEU:HD11	1:39:B:GLN:HB2	2	0.15
(1,2044)	1:8:B:LEU:HD12	1:39:B:GLN:HB2	2	0.15
(1,2044)	1:8:B:LEU:HD13	1:39:B:GLN:HB2	2	0.15
(1,2044)	1:8:B:LEU:HD11	1:39:B:GLN:HB2	20	0.15
(1,2044)	1:8:B:LEU:HD12	1:39:B:GLN:HB2	20	0.15
(1,2044)	1:8:B:LEU:HD13	1:39:B:GLN:HB2	20	0.15
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	4	0.15
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	4	0.15
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	4	0.15
(1,1800)	1:53:A:LYS:H	1:49:A:LYS:H	16	0.15
(1,1672)	1:49:A:LYS:H	1:53:A:LYS:H	16	0.15
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD11	16	0.15
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD12	16	0.15
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD13	16	0.15
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	6	0.15
(1,1325)	1:42:A:THR:HB	1:3:C:ILE:HB	6	0.15
(1,1263)	1:40:A:GLY:H	1:43:A:LEU:HB3	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1263)	1:40:A:GLY:H	1:43:A:LEU:HB3	12	0.15
(1,1211)	1:38:A:ALA:HA	1:42:A:THR:HA	12	0.15
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	8	0.15
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	8	0.15
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	8	0.15
(1,1186)	1:37:A:THR:HG21	1:8:A:LEU:HG	15	0.15
(1,1186)	1:37:A:THR:HG22	1:8:A:LEU:HG	15	0.15
(1,1186)	1:37:A:THR:HG23	1:8:A:LEU:HG	15	0.15
(1,1152)	1:36:A:LEU:HD21	1:44:A:LEU:HD21	7	0.15
(1,1152)	1:36:A:LEU:HD21	1:44:A:LEU:HD22	7	0.15
(1,1152)	1:36:A:LEU:HD21	1:44:A:LEU:HD23	7	0.15
(1,1152)	1:36:A:LEU:HD22	1:44:A:LEU:HD21	7	0.15
(1,1152)	1:36:A:LEU:HD22	1:44:A:LEU:HD22	7	0.15
(1,1152)	1:36:A:LEU:HD22	1:44:A:LEU:HD23	7	0.15
(1,1152)	1:36:A:LEU:HD23	1:44:A:LEU:HD21	7	0.15
(1,1152)	1:36:A:LEU:HD23	1:44:A:LEU:HD22	7	0.15
(1,1152)	1:36:A:LEU:HD23	1:44:A:LEU:HD23	7	0.15
(1,1052)	1:35:A:ILE:HA	1:11:A:ALA:HA	11	0.15
(1,966)	1:32:A:LYS:H	1:29:A:CYS:HB2	9	0.15
(1,795)	1:26:A:CYS:HB2	1:20:A:GLU:HA	13	0.15
(1,795)	1:26:A:CYS:HB3	1:20:A:GLU:HA	13	0.15
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA2	3	0.15
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA3	3	0.15
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA2	13	0.15
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA3	13	0.15
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA2	16	0.15
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA3	16	0.15
(1,712)	1:23:A:GLY:HA2	1:24:A:THR:HB	3	0.15
(1,712)	1:23:A:GLY:HA3	1:24:A:THR:HB	3	0.15
(1,712)	1:23:A:GLY:HA2	1:24:A:THR:HB	13	0.15
(1,712)	1:23:A:GLY:HA3	1:24:A:THR:HB	13	0.15
(1,712)	1:23:A:GLY:HA2	1:24:A:THR:HB	16	0.15
(1,712)	1:23:A:GLY:HA3	1:24:A:THR:HB	16	0.15
(1,498)	1:16:A:GLU:H	1:33:A:GLY:H	4	0.15
(1,369)	1:11:A:ALA:HA	1:35:A:ILE:HA	11	0.15
(1,244)	1:8:A:LEU:HD11	1:39:A:GLN:HB2	16	0.15
(1,244)	1:8:A:LEU:HD12	1:39:A:GLN:HB2	16	0.15
(1,244)	1:8:A:LEU:HD13	1:39:A:GLN:HB2	16	0.15
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	11	0.15
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	11	0.15
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	11	0.15
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	12	0.15
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	12	0.15
(2,1555)	1:43:B:LEU:HD11	1:8:B:LEU:HD22	5	0.14
(2,1347)	1:8:A:LEU:HD21	1:43:A:LEU:HG	18	0.14
(2,1347)	1:8:A:LEU:HD21	1:43:B:LEU:HG	19	0.14
(2,1327)	1:30:B:SER:HB3	1:32:B:LYS:HD3	15	0.14
(2,1049)	1:26:A:CYS:HB3	1:15:A:CYS:HB3	13	0.14
(2,1016)	1:13:A:PRO:HB2	1:21:A:ILE:HG22	5	0.14
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	8	0.14
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	9	0.14
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	18	0.14
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	4	0.14
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	7	0.14
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	17	0.14
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	6	0.14
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	8	0.14
(2,871)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	16	0.14
(2,868)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	16	0.14
(2,786)	1:20:B:GLU:HG2	1:26:B:CYS:HB2	1	0.14
(2,786)	1:20:B:GLU:HG2	1:26:B:CYS:HB3	1	0.14
(2,786)	1:20:B:GLU:HG3	1:26:B:CYS:HB2	1	0.14
(2,786)	1:20:B:GLU:HG3	1:26:B:CYS:HB3	1	0.14
(2,638)	1:38:C:ALA:HB1	1:39:C:GLN:HA	11	0.14
(2,579)	1:42:A:THR:HG21	1:3:C:ILE:HG12	5	0.14
(2,579)	1:42:A:THR:HG22	1:4:C:ALA:HB2	9	0.14
(2,572)	1:2:C:VAL:HG13	1:1:C:FME:HA	15	0.14
(2,570)	1:2:A:VAL:HG12	1:1:A:FME:HA	5	0.14
(2,485)	1:51:C:LEU:HD11	1:47:B:ILE:HB	8	0.14
(2,485)	1:51:C:LEU:HD12	1:48:B:GLN:HB3	11	0.14
(2,469)	1:43:B:LEU:HD11	1:8:B:LEU:HD22	5	0.14
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	8	0.14
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	9	0.14
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	18	0.14
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	4	0.14
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	7	0.14
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	17	0.14
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	6	0.14
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	8	0.14
(2,270)	1:14:B:LYS:HE2	1:15:B:CYS:HB2	20	0.14
(2,270)	1:14:B:LYS:HE3	1:15:B:CYS:HB2	20	0.14
(2,266)	1:51:A:LEU:HB2	1:52:A:ASN:HB2	19	0.14
(2,264)	1:49:B:LYS:HE2	1:53:B:LYS:HB3	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,161)	1:37:A:THR:H	1:39:A:GLN:HB2	8	0.14
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	4	0.14
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	11	0.14
(1,5298)	1:53:C:LYS:HD2	1:49:C:LYS:HG2	19	0.14
(1,5298)	1:53:C:LYS:HD2	1:49:C:LYS:HG3	19	0.14
(1,5298)	1:53:C:LYS:HD3	1:49:C:LYS:HG2	19	0.14
(1,5298)	1:53:C:LYS:HD3	1:49:C:LYS:HG3	19	0.14
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	4	0.14
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	11	0.14
(1,5057)	1:46:C:PHE:H	1:48:C:GLN:HB3	1	0.14
(1,5057)	1:46:C:PHE:H	1:48:C:GLN:HB3	4	0.14
(1,5022)	1:45:C:ASP:H	1:48:C:GLN:HB3	19	0.14
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	1	0.14
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	14	0.14
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	17	0.14
(1,4854)	1:42:C:THR:HB	1:3:B:ILE:HB	4	0.14
(1,4797)	1:40:C:GLY:H	1:43:C:LEU:HB3	1	0.14
(1,4797)	1:40:C:GLY:H	1:43:C:LEU:HB3	7	0.14
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB2	3	0.14
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB3	3	0.14
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB2	3	0.14
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB3	3	0.14
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB2	3	0.14
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB3	3	0.14
(1,4743)	1:38:C:ALA:HA	1:42:C:THR:HA	8	0.14
(1,4743)	1:38:C:ALA:HA	1:42:C:THR:HA	12	0.14
(1,4743)	1:38:C:ALA:HA	1:42:C:THR:HA	16	0.14
(1,4725)	1:37:C:THR:H	1:10:C:VAL:HG11	17	0.14
(1,4725)	1:37:C:THR:H	1:10:C:VAL:HG12	17	0.14
(1,4725)	1:37:C:THR:H	1:10:C:VAL:HG13	17	0.14
(1,4713)	1:37:C:THR:HG21	1:8:C:LEU:HG	18	0.14
(1,4713)	1:37:C:THR:HG22	1:8:C:LEU:HG	18	0.14
(1,4713)	1:37:C:THR:HG23	1:8:C:LEU:HG	18	0.14
(1,4680)	1:36:C:LEU:HD21	1:36:C:LEU:H	19	0.14
(1,4680)	1:36:C:LEU:HD22	1:36:C:LEU:H	19	0.14
(1,4680)	1:36:C:LEU:HD23	1:36:C:LEU:H	19	0.14
(1,4666)	1:36:C:LEU:HD11	1:35:C:ILE:HA	1	0.14
(1,4666)	1:36:C:LEU:HD12	1:35:C:ILE:HA	1	0.14
(1,4666)	1:36:C:LEU:HD13	1:35:C:ILE:HA	1	0.14
(1,4666)	1:36:C:LEU:HD11	1:35:C:ILE:HA	3	0.14
(1,4666)	1:36:C:LEU:HD12	1:35:C:ILE:HA	3	0.14
(1,4666)	1:36:C:LEU:HD13	1:35:C:ILE:HA	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4666)	1:36:C:LEU:HD11	1:35:C:ILE:HA	7	0.14
(1,4666)	1:36:C:LEU:HD12	1:35:C:ILE:HA	7	0.14
(1,4666)	1:36:C:LEU:HD13	1:35:C:ILE:HA	7	0.14
(1,4666)	1:36:C:LEU:HD11	1:35:C:ILE:HA	14	0.14
(1,4666)	1:36:C:LEU:HD12	1:35:C:ILE:HA	14	0.14
(1,4666)	1:36:C:LEU:HD13	1:35:C:ILE:HA	14	0.14
(1,4666)	1:36:C:LEU:HD11	1:35:C:ILE:HA	20	0.14
(1,4666)	1:36:C:LEU:HD12	1:35:C:ILE:HA	20	0.14
(1,4666)	1:36:C:LEU:HD13	1:35:C:ILE:HA	20	0.14
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	1	0.14
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	2	0.14
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	5	0.14
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	6	0.14
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	7	0.14
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	8	0.14
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	11	0.14
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	12	0.14
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	1	0.14
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	11	0.14
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA2	1	0.14
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA3	1	0.14
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA2	6	0.14
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA3	6	0.14
(1,4258)	1:23:C:GLY:HA2	1:24:C:THR:HB	1	0.14
(1,4258)	1:23:C:GLY:HA3	1:24:C:THR:HB	1	0.14
(1,4258)	1:23:C:GLY:HA2	1:24:C:THR:HB	6	0.14
(1,4258)	1:23:C:GLY:HA3	1:24:C:THR:HB	6	0.14
(1,4140)	1:20:C:GLU:HA	1:27:C:PRO:HD2	3	0.14
(1,4140)	1:20:C:GLU:HA	1:27:C:PRO:HD3	3	0.14
(1,4140)	1:20:C:GLU:HA	1:27:C:PRO:HD2	12	0.14
(1,4140)	1:20:C:GLU:HA	1:27:C:PRO:HD3	12	0.14
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	5	0.14
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	1	0.14
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	2	0.14
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	5	0.14
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	6	0.14
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	7	0.14
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	8	0.14
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	11	0.14
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	12	0.14
(1,3801)	1:8:C:LEU:HD11	1:39:C:GLN:HB2	2	0.14
(1,3801)	1:8:C:LEU:HD12	1:39:C:GLN:HB2	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3801)	1:8:C:LEU:HD13	1:39:C:GLN:HB2	2	0.14
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	2	0.14
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	2	0.14
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	2	0.14
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	5	0.14
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	5	0.14
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	5	0.14
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	8	0.14
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	8	0.14
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	8	0.14
(1,3594)	1:2:C:VAL:HG11	1:1:C:FME:HG2	16	0.14
(1,3594)	1:2:C:VAL:HG11	1:1:C:FME:HG3	16	0.14
(1,3594)	1:2:C:VAL:HG12	1:1:C:FME:HG2	16	0.14
(1,3594)	1:2:C:VAL:HG12	1:1:C:FME:HG3	16	0.14
(1,3594)	1:2:C:VAL:HG13	1:1:C:FME:HG2	16	0.14
(1,3594)	1:2:C:VAL:HG13	1:1:C:FME:HG3	16	0.14
(1,3555)	1:53:B:LYS:H	1:49:B:LYS:H	19	0.14
(1,3432)	1:49:B:LYS:H	1:53:B:LYS:H	19	0.14
(1,3316)	1:47:B:ILE:HG12	1:50:C:HIS:HB2	13	0.14
(1,3316)	1:47:B:ILE:HG13	1:50:C:HIS:HB2	13	0.14
(1,3299)	1:46:B:PHE:H	1:48:B:GLN:HB3	1	0.14
(1,3299)	1:46:B:PHE:H	1:48:B:GLN:HB3	12	0.14
(1,3107)	1:42:B:THR:HB	1:3:A:ILE:HB	4	0.14
(1,3039)	1:40:B:GLY:H	1:43:B:LEU:HB3	6	0.14
(1,3039)	1:40:B:GLY:H	1:43:B:LEU:HB3	7	0.14
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB2	15	0.14
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB3	15	0.14
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB2	15	0.14
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB3	15	0.14
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB2	15	0.14
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB3	15	0.14
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB2	16	0.14
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB3	16	0.14
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB2	16	0.14
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB3	16	0.14
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB2	16	0.14
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB3	16	0.14
(1,2985)	1:38:B:ALA:HA	1:42:B:THR:HA	9	0.14
(1,2908)	1:36:B:LEU:HD11	1:35:B:ILE:HA	2	0.14
(1,2908)	1:36:B:LEU:HD12	1:35:B:ILE:HA	2	0.14
(1,2908)	1:36:B:LEU:HD13	1:35:B:ILE:HA	2	0.14
(1,2908)	1:36:B:LEU:HD11	1:35:B:ILE:HA	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2908)	1:36:B:LEU:HD12	1:35:B:ILE:HA	7	0.14
(1,2908)	1:36:B:LEU:HD13	1:35:B:ILE:HA	7	0.14
(1,2908)	1:36:B:LEU:HD11	1:35:B:ILE:HA	17	0.14
(1,2908)	1:36:B:LEU:HD12	1:35:B:ILE:HA	17	0.14
(1,2908)	1:36:B:LEU:HD13	1:35:B:ILE:HA	17	0.14
(1,2908)	1:36:B:LEU:HD11	1:35:B:ILE:HA	20	0.14
(1,2908)	1:36:B:LEU:HD12	1:35:B:ILE:HA	20	0.14
(1,2908)	1:36:B:LEU:HD13	1:35:B:ILE:HA	20	0.14
(1,2831)	1:35:B:ILE:HA	1:11:B:ALA:HA	7	0.14
(1,2831)	1:35:B:ILE:HA	1:11:B:ALA:HA	13	0.14
(1,2831)	1:35:B:ILE:HA	1:11:B:ALA:HA	17	0.14
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	12	0.14
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA2	6	0.14
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA3	6	0.14
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA2	19	0.14
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA3	19	0.14
(1,2500)	1:23:B:GLY:HA2	1:24:B:THR:HB	6	0.14
(1,2500)	1:23:B:GLY:HA3	1:24:B:THR:HB	6	0.14
(1,2500)	1:23:B:GLY:HA2	1:24:B:THR:HB	19	0.14
(1,2500)	1:23:B:GLY:HA3	1:24:B:THR:HB	19	0.14
(1,2433)	1:21:B:ILE:HD11	1:13:B:PRO:HD2	20	0.14
(1,2433)	1:21:B:ILE:HD11	1:13:B:PRO:HD3	20	0.14
(1,2433)	1:21:B:ILE:HD12	1:13:B:PRO:HD2	20	0.14
(1,2433)	1:21:B:ILE:HD12	1:13:B:PRO:HD3	20	0.14
(1,2433)	1:21:B:ILE:HD13	1:13:B:PRO:HD2	20	0.14
(1,2433)	1:21:B:ILE:HD13	1:13:B:PRO:HD3	20	0.14
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD2	17	0.14
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD3	17	0.14
(1,2160)	1:11:B:ALA:HA	1:35:B:ILE:HA	7	0.14
(1,2160)	1:11:B:ALA:HA	1:35:B:ILE:HA	13	0.14
(1,2160)	1:11:B:ALA:HA	1:35:B:ILE:HA	17	0.14
(1,2152)	1:10:B:VAL:H	1:36:B:LEU:HA	3	0.14
(1,2152)	1:10:B:VAL:H	1:36:B:LEU:HA	7	0.14
(1,2152)	1:10:B:VAL:H	1:36:B:LEU:HA	20	0.14
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	3	0.14
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	3	0.14
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	3	0.14
(1,2044)	1:8:B:LEU:HD11	1:39:B:GLN:HB2	13	0.14
(1,2044)	1:8:B:LEU:HD12	1:39:B:GLN:HB2	13	0.14
(1,2044)	1:8:B:LEU:HD13	1:39:B:GLN:HB2	13	0.14
(1,1837)	1:2:B:VAL:HG11	1:1:B:FME:HG2	6	0.14
(1,1837)	1:2:B:VAL:HG11	1:1:B:FME:HG3	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1837)	1:2:B:VAL:HG12	1:1:B:FME:HG2	6	0.14
(1,1837)	1:2:B:VAL:HG12	1:1:B:FME:HG3	6	0.14
(1,1837)	1:2:B:VAL:HG13	1:1:B:FME:HG2	6	0.14
(1,1837)	1:2:B:VAL:HG13	1:1:B:FME:HG3	6	0.14
(1,1800)	1:53:A:LYS:H	1:49:A:LYS:H	20	0.14
(1,1798)	1:53:A:LYS:H	1:51:B:LEU:HD11	12	0.14
(1,1798)	1:53:A:LYS:H	1:51:B:LEU:HD12	12	0.14
(1,1798)	1:53:A:LYS:H	1:51:B:LEU:HD13	12	0.14
(1,1672)	1:49:A:LYS:H	1:53:A:LYS:H	20	0.14
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	1	0.14
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	19	0.14
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	1	0.14
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	20	0.14
(1,1325)	1:42:A:THR:HB	1:3:C:ILE:HB	7	0.14
(1,1263)	1:40:A:GLY:H	1:43:A:LEU:HB3	9	0.14
(1,1263)	1:40:A:GLY:H	1:43:A:LEU:HB3	13	0.14
(1,1211)	1:38:A:ALA:HA	1:42:A:THR:HA	15	0.14
(1,1134)	1:36:A:LEU:HD11	1:35:A:ILE:HA	2	0.14
(1,1134)	1:36:A:LEU:HD12	1:35:A:ILE:HA	2	0.14
(1,1134)	1:36:A:LEU:HD13	1:35:A:ILE:HA	2	0.14
(1,1134)	1:36:A:LEU:HD11	1:35:A:ILE:HA	4	0.14
(1,1134)	1:36:A:LEU:HD12	1:35:A:ILE:HA	4	0.14
(1,1134)	1:36:A:LEU:HD13	1:35:A:ILE:HA	4	0.14
(1,1134)	1:36:A:LEU:HD11	1:35:A:ILE:HA	6	0.14
(1,1134)	1:36:A:LEU:HD12	1:35:A:ILE:HA	6	0.14
(1,1134)	1:36:A:LEU:HD13	1:35:A:ILE:HA	6	0.14
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	10	0.14
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD2	8	0.14
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD3	8	0.14
(1,430)	1:14:A:LYS:HE2	1:21:A:ILE:HD11	18	0.14
(1,430)	1:14:A:LYS:HE2	1:21:A:ILE:HD12	18	0.14
(1,430)	1:14:A:LYS:HE2	1:21:A:ILE:HD13	18	0.14
(1,430)	1:14:A:LYS:HE3	1:21:A:ILE:HD11	18	0.14
(1,430)	1:14:A:LYS:HE3	1:21:A:ILE:HD12	18	0.14
(1,430)	1:14:A:LYS:HE3	1:21:A:ILE:HD13	18	0.14
(1,400)	1:12:A:CYS:H	1:34:A:VAL:HB	1	0.14
(1,400)	1:12:A:CYS:H	1:34:A:VAL:HB	20	0.14
(1,377)	1:11:A:ALA:H	1:10:A:VAL:HB	10	0.14
(1,358)	1:10:A:VAL:H	1:36:A:LEU:HA	6	0.14
(1,331)	1:10:A:VAL:HB	1:11:A:ALA:H	10	0.14
(1,244)	1:8:A:LEU:HD11	1:39:A:GLN:HB2	1	0.14
(1,244)	1:8:A:LEU:HD12	1:39:A:GLN:HB2	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:8:A:LEU:HD13	1:39:A:GLN:HB2	1	0.14
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	5	0.14
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	5	0.14
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	5	0.14
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	5	0.14
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	5	0.14
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	5	0.14
(2,1413)	1:32:A:LYS:HA	1:19:A:GLY:HA2	14	0.13
(2,1349)	1:8:C:LEU:HD22	1:43:C:LEU:HG	20	0.13
(2,1347)	1:8:A:LEU:HD21	1:43:A:LEU:HG	3	0.13
(2,1347)	1:8:A:LEU:HD23	1:43:B:LEU:HG	5	0.13
(2,1307)	1:51:C:LEU:HD23	1:44:B:LEU:HA	3	0.13
(2,1018)	1:13:C:PRO:HB2	1:21:C:ILE:HG23	12	0.13
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	20	0.13
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	1	0.13
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	17	0.13
(2,873)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	17	0.13
(2,872)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	14	0.13
(2,871)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	11	0.13
(2,870)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	17	0.13
(2,869)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	14	0.13
(2,868)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	11	0.13
(2,580)	1:42:B:THR:HG22	1:3:A:ILE:HG12	12	0.13
(2,579)	1:42:A:THR:HG22	1:4:C:ALA:HB1	17	0.13
(2,572)	1:2:C:VAL:HG11	1:1:C:FME:HA	4	0.13
(2,491)	1:51:C:LEU:HD23	1:44:B:LEU:HA	3	0.13
(2,484)	1:51:B:LEU:HD12	1:47:A:ILE:HB	5	0.13
(2,460)	1:36:B:LEU:HD12	1:46:C:PHE:HE1	20	0.13
(2,358)	1:14:C:LYS:HD3	1:22:C:GLU:HA	15	0.13
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	20	0.13
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	1	0.13
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	17	0.13
(2,268)	1:51:C:LEU:HB2	1:52:C:ASN:HB2	11	0.13
(2,267)	1:51:B:LEU:HB2	1:52:B:ASN:HB2	5	0.13
(2,267)	1:51:B:LEU:HB2	1:52:B:ASN:HB2	15	0.13
(2,266)	1:51:A:LEU:HB2	1:52:A:ASN:HB2	5	0.13
(2,265)	1:49:C:LYS:HE2	1:53:C:LYS:HB3	9	0.13
(2,263)	1:49:A:LYS:HE2	1:53:A:LYS:HB3	1	0.13
(2,263)	1:49:A:LYS:HE2	1:53:A:LYS:HB3	10	0.13
(2,68)	1:51:A:LEU:H	1:51:A:LEU:HD11	14	0.13
(2,61)	1:3:C:ILE:H	1:2:C:VAL:HB	9	0.13
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD11	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD12	13	0.13
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD13	13	0.13
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	3	0.13
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	14	0.13
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	16	0.13
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	18	0.13
(1,5308)	1:53:C:LYS:HG2	1:48:C:GLN:HB2	15	0.13
(1,5308)	1:53:C:LYS:HG3	1:48:C:GLN:HB2	15	0.13
(1,5299)	1:53:C:LYS:HE2	1:45:C:ASP:HA	2	0.13
(1,5299)	1:53:C:LYS:HE3	1:45:C:ASP:HA	2	0.13
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	3	0.13
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	14	0.13
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	16	0.13
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	18	0.13
(1,5057)	1:46:C:PHE:H	1:48:C:GLN:HB3	7	0.13
(1,5057)	1:46:C:PHE:H	1:48:C:GLN:HB3	9	0.13
(1,5057)	1:46:C:PHE:H	1:48:C:GLN:HB3	11	0.13
(1,5057)	1:46:C:PHE:H	1:48:C:GLN:HB3	20	0.13
(1,5015)	1:45:C:ASP:H	1:44:C:LEU:HG	11	0.13
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	7	0.13
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	13	0.13
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	18	0.13
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	19	0.13
(1,4872)	1:42:C:THR:HG21	1:8:B:LEU:HD11	2	0.13
(1,4872)	1:42:C:THR:HG21	1:8:B:LEU:HD12	2	0.13
(1,4872)	1:42:C:THR:HG21	1:8:B:LEU:HD13	2	0.13
(1,4872)	1:42:C:THR:HG22	1:8:B:LEU:HD11	2	0.13
(1,4872)	1:42:C:THR:HG22	1:8:B:LEU:HD12	2	0.13
(1,4872)	1:42:C:THR:HG22	1:8:B:LEU:HD13	2	0.13
(1,4872)	1:42:C:THR:HG23	1:8:B:LEU:HD11	2	0.13
(1,4872)	1:42:C:THR:HG23	1:8:B:LEU:HD12	2	0.13
(1,4872)	1:42:C:THR:HG23	1:8:B:LEU:HD13	2	0.13
(1,4797)	1:40:C:GLY:H	1:43:C:LEU:HB3	8	0.13
(1,4797)	1:40:C:GLY:H	1:43:C:LEU:HB3	14	0.13
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB2	1	0.13
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB3	1	0.13
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB2	1	0.13
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB3	1	0.13
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB2	1	0.13
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB3	1	0.13
(1,4729)	1:37:C:THR:H	1:36:C:LEU:HG	1	0.13
(1,4666)	1:36:C:LEU:HD11	1:35:C:ILE:HA	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4666)	1:36:C:LEU:HD12	1:35:C:ILE:HA	6	0.13
(1,4666)	1:36:C:LEU:HD13	1:35:C:ILE:HA	6	0.13
(1,4666)	1:36:C:LEU:HD11	1:35:C:ILE:HA	8	0.13
(1,4666)	1:36:C:LEU:HD12	1:35:C:ILE:HA	8	0.13
(1,4666)	1:36:C:LEU:HD13	1:35:C:ILE:HA	8	0.13
(1,4581)	1:34:C:VAL:H	1:32:C:LYS:HG2	3	0.13
(1,4581)	1:34:C:VAL:H	1:32:C:LYS:HG3	3	0.13
(1,4493)	1:32:C:LYS:HE3	1:49:A:LYS:HG2	11	0.13
(1,4442)	1:31:C:GLY:HA2	1:19:C:GLY:HA2	7	0.13
(1,4442)	1:31:C:GLY:HA2	1:19:C:GLY:HA3	7	0.13
(1,4442)	1:31:C:GLY:HA3	1:19:C:GLY:HA2	7	0.13
(1,4442)	1:31:C:GLY:HA3	1:19:C:GLY:HA3	7	0.13
(1,4430)	1:30:C:SER:HA	1:32:C:LYS:HE2	4	0.13
(1,4430)	1:30:C:SER:HA	1:32:C:LYS:HE3	4	0.13
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	10	0.13
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA2	13	0.13
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA3	13	0.13
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA2	15	0.13
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA3	15	0.13
(1,4258)	1:23:C:GLY:HA2	1:24:C:THR:HB	13	0.13
(1,4258)	1:23:C:GLY:HA3	1:24:C:THR:HB	13	0.13
(1,4258)	1:23:C:GLY:HA2	1:24:C:THR:HB	15	0.13
(1,4258)	1:23:C:GLY:HA3	1:24:C:THR:HB	15	0.13
(1,4193)	1:21:C:ILE:HD11	1:15:C:CYS:HA	15	0.13
(1,4193)	1:21:C:ILE:HD12	1:15:C:CYS:HA	15	0.13
(1,4193)	1:21:C:ILE:HD13	1:15:C:CYS:HA	15	0.13
(1,4140)	1:20:C:GLU:HA	1:27:C:PRO:HD2	4	0.13
(1,4140)	1:20:C:GLU:HA	1:27:C:PRO:HD3	4	0.13
(1,4117)	1:19:C:GLY:HA2	1:31:C:GLY:HA2	7	0.13
(1,4117)	1:19:C:GLY:HA2	1:31:C:GLY:HA3	7	0.13
(1,4117)	1:19:C:GLY:HA3	1:31:C:GLY:HA2	7	0.13
(1,4117)	1:19:C:GLY:HA3	1:31:C:GLY:HA3	7	0.13
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	7	0.13
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	14	0.13
(1,3909)	1:10:C:VAL:H	1:36:C:LEU:HA	20	0.13
(1,3887)	1:10:C:VAL:HG11	1:35:C:ILE:HB	8	0.13
(1,3887)	1:10:C:VAL:HG12	1:35:C:ILE:HB	8	0.13
(1,3887)	1:10:C:VAL:HG13	1:35:C:ILE:HB	8	0.13
(1,3801)	1:8:C:LEU:HD11	1:39:C:GLN:HB2	10	0.13
(1,3801)	1:8:C:LEU:HD12	1:39:C:GLN:HB2	10	0.13
(1,3801)	1:8:C:LEU:HD13	1:39:C:GLN:HB2	10	0.13
(1,3801)	1:8:C:LEU:HD11	1:39:C:GLN:HB2	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3801)	1:8:C:LEU:HD12	1:39:C:GLN:HB2	14	0.13
(1,3801)	1:8:C:LEU:HD13	1:39:C:GLN:HB2	14	0.13
(1,3735)	1:6:C:ASP:HA	1:9:C:GLU:HG2	16	0.13
(1,3735)	1:6:C:ASP:HA	1:9:C:GLU:HG3	16	0.13
(1,3704)	1:5:C:THR:HB	1:42:A:THR:HA	18	0.13
(1,3555)	1:53:B:LYS:H	1:49:B:LYS:H	9	0.13
(1,3555)	1:53:B:LYS:H	1:49:B:LYS:H	11	0.13
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG2	2	0.13
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG3	2	0.13
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG2	2	0.13
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG3	2	0.13
(1,3432)	1:49:B:LYS:H	1:53:B:LYS:H	9	0.13
(1,3432)	1:49:B:LYS:H	1:53:B:LYS:H	11	0.13
(1,3299)	1:46:B:PHE:H	1:48:B:GLN:HB3	19	0.13
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	3	0.13
(1,3124)	1:42:B:THR:H	1:38:B:ALA:HA	11	0.13
(1,3039)	1:40:B:GLY:H	1:43:B:LEU:HB3	5	0.13
(1,3039)	1:40:B:GLY:H	1:43:B:LEU:HB3	14	0.13
(1,3039)	1:40:B:GLY:H	1:43:B:LEU:HB3	20	0.13
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB2	5	0.13
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB3	5	0.13
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB2	5	0.13
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB3	5	0.13
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB2	5	0.13
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB3	5	0.13
(1,2985)	1:38:B:ALA:HA	1:42:B:THR:HA	2	0.13
(1,2985)	1:38:B:ALA:HA	1:42:B:THR:HA	10	0.13
(1,2985)	1:38:B:ALA:HA	1:42:B:THR:HA	18	0.13
(1,2971)	1:37:B:THR:H	1:36:B:LEU:HG	19	0.13
(1,2955)	1:37:B:THR:HG21	1:8:B:LEU:HG	14	0.13
(1,2955)	1:37:B:THR:HG22	1:8:B:LEU:HG	14	0.13
(1,2955)	1:37:B:THR:HG23	1:8:B:LEU:HG	14	0.13
(1,2908)	1:36:B:LEU:HD11	1:35:B:ILE:HA	8	0.13
(1,2908)	1:36:B:LEU:HD12	1:35:B:ILE:HA	8	0.13
(1,2908)	1:36:B:LEU:HD13	1:35:B:ILE:HA	8	0.13
(1,2865)	1:35:B:ILE:HG21	1:12:B:CYS:HB2	5	0.13
(1,2865)	1:35:B:ILE:HG22	1:12:B:CYS:HB2	5	0.13
(1,2865)	1:35:B:ILE:HG23	1:12:B:CYS:HB2	5	0.13
(1,2831)	1:35:B:ILE:HA	1:11:B:ALA:HA	9	0.13
(1,2821)	1:34:B:VAL:H	1:32:B:LYS:HA	13	0.13
(1,2687)	1:31:B:GLY:HA2	1:29:B:CYS:HB2	1	0.13
(1,2687)	1:31:B:GLY:HA3	1:29:B:CYS:HB2	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2672)	1:30:B:SER:HA	1:32:B:LYS:HE2	2	0.13
(1,2672)	1:30:B:SER:HA	1:32:B:LYS:HE3	2	0.13
(1,2672)	1:30:B:SER:HA	1:32:B:LYS:HE2	15	0.13
(1,2672)	1:30:B:SER:HA	1:32:B:LYS:HE3	15	0.13
(1,2528)	1:24:B:THR:HG21	1:22:B:GLU:HG2	7	0.13
(1,2528)	1:24:B:THR:HG21	1:22:B:GLU:HG3	7	0.13
(1,2528)	1:24:B:THR:HG22	1:22:B:GLU:HG2	7	0.13
(1,2528)	1:24:B:THR:HG22	1:22:B:GLU:HG3	7	0.13
(1,2528)	1:24:B:THR:HG23	1:22:B:GLU:HG2	7	0.13
(1,2528)	1:24:B:THR:HG23	1:22:B:GLU:HG3	7	0.13
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA2	9	0.13
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA3	9	0.13
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA2	15	0.13
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA3	15	0.13
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA2	16	0.13
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA3	16	0.13
(1,2500)	1:23:B:GLY:HA2	1:24:B:THR:HB	9	0.13
(1,2500)	1:23:B:GLY:HA3	1:24:B:THR:HB	9	0.13
(1,2500)	1:23:B:GLY:HA2	1:24:B:THR:HB	15	0.13
(1,2500)	1:23:B:GLY:HA3	1:24:B:THR:HB	15	0.13
(1,2500)	1:23:B:GLY:HA2	1:24:B:THR:HB	16	0.13
(1,2500)	1:23:B:GLY:HA3	1:24:B:THR:HB	16	0.13
(1,2435)	1:21:B:ILE:HD11	1:15:B:CYS:HA	3	0.13
(1,2435)	1:21:B:ILE:HD12	1:15:B:CYS:HA	3	0.13
(1,2435)	1:21:B:ILE:HD13	1:15:B:CYS:HA	3	0.13
(1,2435)	1:21:B:ILE:HD11	1:15:B:CYS:HA	13	0.13
(1,2435)	1:21:B:ILE:HD12	1:15:B:CYS:HA	13	0.13
(1,2435)	1:21:B:ILE:HD13	1:15:B:CYS:HA	13	0.13
(1,2435)	1:21:B:ILE:HD11	1:15:B:CYS:HA	17	0.13
(1,2435)	1:21:B:ILE:HD12	1:15:B:CYS:HA	17	0.13
(1,2435)	1:21:B:ILE:HD13	1:15:B:CYS:HA	17	0.13
(1,2222)	1:14:B:LYS:HE2	1:21:B:ILE:HD11	18	0.13
(1,2222)	1:14:B:LYS:HE2	1:21:B:ILE:HD12	18	0.13
(1,2222)	1:14:B:LYS:HE2	1:21:B:ILE:HD13	18	0.13
(1,2222)	1:14:B:LYS:HE3	1:21:B:ILE:HD11	18	0.13
(1,2222)	1:14:B:LYS:HE3	1:21:B:ILE:HD12	18	0.13
(1,2222)	1:14:B:LYS:HE3	1:21:B:ILE:HD13	18	0.13
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG12	12	0.13
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG13	12	0.13
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG12	12	0.13
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG13	12	0.13
(1,2160)	1:11:B:ALA:HA	1:35:B:ILE:HA	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2044)	1:8:B:LEU:HD11	1:39:B:GLN:HB2	9	0.13
(1,2044)	1:8:B:LEU:HD12	1:39:B:GLN:HB2	9	0.13
(1,2044)	1:8:B:LEU:HD13	1:39:B:GLN:HB2	9	0.13
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	1	0.13
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	1	0.13
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	1	0.13
(1,1800)	1:53:A:LYS:H	1:49:A:LYS:H	6	0.13
(1,1800)	1:53:A:LYS:H	1:49:A:LYS:H	9	0.13
(1,1800)	1:53:A:LYS:H	1:49:A:LYS:H	12	0.13
(1,1800)	1:53:A:LYS:H	1:49:A:LYS:H	13	0.13
(1,1672)	1:49:A:LYS:H	1:53:A:LYS:H	6	0.13
(1,1672)	1:49:A:LYS:H	1:53:A:LYS:H	9	0.13
(1,1672)	1:49:A:LYS:H	1:53:A:LYS:H	12	0.13
(1,1672)	1:49:A:LYS:H	1:53:A:LYS:H	13	0.13
(1,1581)	1:48:A:GLN:HB3	1:49:A:LYS:HB3	6	0.13
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	20	0.13
(1,1422)	1:44:A:LEU:HA	1:46:B:PHE:HZ	10	0.13
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	2	0.13
(1,1343)	1:42:A:THR:HG21	1:8:C:LEU:HD11	13	0.13
(1,1343)	1:42:A:THR:HG21	1:8:C:LEU:HD12	13	0.13
(1,1343)	1:42:A:THR:HG21	1:8:C:LEU:HD13	13	0.13
(1,1343)	1:42:A:THR:HG22	1:8:C:LEU:HD11	13	0.13
(1,1343)	1:42:A:THR:HG22	1:8:C:LEU:HD12	13	0.13
(1,1343)	1:42:A:THR:HG22	1:8:C:LEU:HD13	13	0.13
(1,1343)	1:42:A:THR:HG23	1:8:C:LEU:HD11	13	0.13
(1,1343)	1:42:A:THR:HG23	1:8:C:LEU:HD12	13	0.13
(1,1343)	1:42:A:THR:HG23	1:8:C:LEU:HD13	13	0.13
(1,1263)	1:40:A:GLY:H	1:43:A:LEU:HB3	1	0.13
(1,1211)	1:38:A:ALA:HA	1:42:A:THR:HA	7	0.13
(1,1189)	1:37:A:THR:H	1:10:A:VAL:HG11	16	0.13
(1,1189)	1:37:A:THR:H	1:10:A:VAL:HG12	16	0.13
(1,1189)	1:37:A:THR:H	1:10:A:VAL:HG13	16	0.13
(1,1174)	1:37:A:THR:HA	1:8:A:LEU:HA	11	0.13
(1,1134)	1:36:A:LEU:HD11	1:35:A:ILE:HA	1	0.13
(1,1134)	1:36:A:LEU:HD12	1:35:A:ILE:HA	1	0.13
(1,1134)	1:36:A:LEU:HD13	1:35:A:ILE:HA	1	0.13
(1,1134)	1:36:A:LEU:HD11	1:35:A:ILE:HA	11	0.13
(1,1134)	1:36:A:LEU:HD12	1:35:A:ILE:HA	11	0.13
(1,1134)	1:36:A:LEU:HD13	1:35:A:ILE:HA	11	0.13
(1,1134)	1:36:A:LEU:HD11	1:35:A:ILE:HA	18	0.13
(1,1134)	1:36:A:LEU:HD12	1:35:A:ILE:HA	18	0.13
(1,1134)	1:36:A:LEU:HD13	1:35:A:ILE:HA	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1080)	1:35:A:ILE:HG12	1:29:A:CYS:HA	4	0.13
(1,1080)	1:35:A:ILE:HG13	1:29:A:CYS:HA	4	0.13
(1,1052)	1:35:A:ILE:HA	1:11:A:ALA:HA	10	0.13
(1,1052)	1:35:A:ILE:HA	1:11:A:ALA:HA	18	0.13
(1,908)	1:31:A:GLY:H	1:20:A:GLU:H	20	0.13
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	8	0.13
(1,752)	1:24:A:THR:H	1:22:A:GLU:HB2	13	0.13
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA2	14	0.13
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA3	14	0.13
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA2	15	0.13
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA3	15	0.13
(1,712)	1:23:A:GLY:HA2	1:24:A:THR:HB	14	0.13
(1,712)	1:23:A:GLY:HA3	1:24:A:THR:HB	14	0.13
(1,712)	1:23:A:GLY:HA2	1:24:A:THR:HB	15	0.13
(1,712)	1:23:A:GLY:HA3	1:24:A:THR:HB	15	0.13
(1,622)	1:20:A:GLU:H	1:31:A:GLY:H	20	0.13
(1,498)	1:16:A:GLU:H	1:33:A:GLY:H	19	0.13
(1,444)	1:15:A:CYS:HA	1:14:A:LYS:HG2	1	0.13
(1,444)	1:15:A:CYS:HA	1:14:A:LYS:HG3	1	0.13
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG12	7	0.13
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG13	7	0.13
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG12	7	0.13
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG13	7	0.13
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG12	9	0.13
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG13	9	0.13
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG12	9	0.13
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG13	9	0.13
(1,369)	1:11:A:ALA:HA	1:35:A:ILE:HA	10	0.13
(1,369)	1:11:A:ALA:HA	1:35:A:ILE:HA	18	0.13
(1,338)	1:10:A:VAL:HG11	1:36:A:LEU:HA	9	0.13
(1,338)	1:10:A:VAL:HG12	1:36:A:LEU:HA	9	0.13
(1,338)	1:10:A:VAL:HG13	1:36:A:LEU:HA	9	0.13
(1,244)	1:8:A:LEU:HD11	1:39:A:GLN:HB2	3	0.13
(1,244)	1:8:A:LEU:HD12	1:39:A:GLN:HB2	3	0.13
(1,244)	1:8:A:LEU:HD13	1:39:A:GLN:HB2	3	0.13
(1,244)	1:8:A:LEU:HD11	1:39:A:GLN:HB2	12	0.13
(1,244)	1:8:A:LEU:HD12	1:39:A:GLN:HB2	12	0.13
(1,244)	1:8:A:LEU:HD13	1:39:A:GLN:HB2	12	0.13
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	18	0.13
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	18	0.13
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	18	0.13
(1,77)	1:3:A:ILE:HG21	1:39:B:GLN:HG2	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:3:A:ILE:HG21	1:39:B:GLN:HG3	10	0.13
(1,77)	1:3:A:ILE:HG22	1:39:B:GLN:HG2	10	0.13
(1,77)	1:3:A:ILE:HG22	1:39:B:GLN:HG3	10	0.13
(1,77)	1:3:A:ILE:HG23	1:39:B:GLN:HG2	10	0.13
(1,77)	1:3:A:ILE:HG23	1:39:B:GLN:HG3	10	0.13
(1,76)	1:3:A:ILE:HG21	1:39:B:GLN:HE21	20	0.13
(1,76)	1:3:A:ILE:HG21	1:39:B:GLN:HE22	20	0.13
(1,76)	1:3:A:ILE:HG22	1:39:B:GLN:HE21	20	0.13
(1,76)	1:3:A:ILE:HG22	1:39:B:GLN:HE22	20	0.13
(1,76)	1:3:A:ILE:HG23	1:39:B:GLN:HE21	20	0.13
(1,76)	1:3:A:ILE:HG23	1:39:B:GLN:HE22	20	0.13
(1,32)	1:2:A:VAL:HG11	1:1:A:FME:HG2	6	0.13
(1,32)	1:2:A:VAL:HG11	1:1:A:FME:HG3	6	0.13
(1,32)	1:2:A:VAL:HG12	1:1:A:FME:HG2	6	0.13
(1,32)	1:2:A:VAL:HG12	1:1:A:FME:HG3	6	0.13
(1,32)	1:2:A:VAL:HG13	1:1:A:FME:HG2	6	0.13
(1,32)	1:2:A:VAL:HG13	1:1:A:FME:HG3	6	0.13
(2,1556)	1:43:C:LEU:HD13	1:8:C:LEU:HD23	14	0.12
(2,1405)	1:15:B:CYS:HA	1:17:B:ARG:HD2	7	0.12
(2,1376)	1:24:C:THR:HG22	1:22:C:GLU:HB2	4	0.12
(2,1375)	1:24:B:THR:HG23	1:22:B:GLU:HB2	10	0.12
(2,1348)	1:8:B:LEU:HD22	1:43:B:LEU:HG	6	0.12
(2,1327)	1:30:B:SER:HB3	1:32:B:LYS:HD3	16	0.12
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	3	0.12
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	12	0.12
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	13	0.12
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	4	0.12
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	9	0.12
(2,873)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	1	0.12
(2,872)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	4	0.12
(2,871)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	18	0.12
(2,870)	1:31:C:GLY:HA2	1:26:C:CYS:HB3	1	0.12
(2,869)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	4	0.12
(2,868)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	18	0.12
(2,696)	1:15:B:CYS:HA	1:17:B:ARG:HD2	7	0.12
(2,569)	1:24:C:THR:HG22	1:22:C:GLU:HB2	4	0.12
(2,568)	1:24:B:THR:HG23	1:22:B:GLU:HB2	10	0.12
(2,485)	1:51:C:LEU:HD12	1:47:B:ILE:HB	14	0.12
(2,483)	1:51:A:LEU:HD12	1:47:C:ILE:HB	17	0.12
(2,470)	1:43:C:LEU:HD13	1:8:C:LEU:HD23	14	0.12
(2,356)	1:14:A:LYS:HD3	1:22:A:GLU:HA	7	0.12
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	12	0.12
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	13	0.12
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	4	0.12
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	9	0.12
(2,267)	1:51:B:LEU:HB2	1:52:B:ASN:HB2	9	0.12
(2,266)	1:51:A:LEU:HB2	1:52:A:ASN:HB2	6	0.12
(2,265)	1:49:C:LYS:HE2	1:53:C:LYS:HB3	13	0.12
(2,264)	1:49:B:LYS:HE2	1:53:B:LYS:HB3	3	0.12
(2,61)	1:3:C:ILE:H	1:2:C:VAL:HB	1	0.12
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD11	16	0.12
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD12	16	0.12
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD13	16	0.12
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	6	0.12
(1,5308)	1:53:C:LYS:HG2	1:48:C:GLN:HB2	7	0.12
(1,5308)	1:53:C:LYS:HG3	1:48:C:GLN:HB2	7	0.12
(1,5298)	1:53:C:LYS:HD2	1:49:C:LYS:HG2	1	0.12
(1,5298)	1:53:C:LYS:HD2	1:49:C:LYS:HG3	1	0.12
(1,5298)	1:53:C:LYS:HD3	1:49:C:LYS:HG2	1	0.12
(1,5298)	1:53:C:LYS:HD3	1:49:C:LYS:HG3	1	0.12
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	6	0.12
(1,5110)	1:48:C:GLN:HB2	1:51:A:LEU:HD11	15	0.12
(1,5110)	1:48:C:GLN:HB2	1:51:A:LEU:HD12	15	0.12
(1,5110)	1:48:C:GLN:HB2	1:51:A:LEU:HD13	15	0.12
(1,5100)	1:48:C:GLN:HB3	1:49:C:LYS:HB3	4	0.12
(1,5057)	1:46:C:PHE:H	1:48:C:GLN:HB3	16	0.12
(1,5057)	1:46:C:PHE:H	1:48:C:GLN:HB3	17	0.12
(1,5057)	1:46:C:PHE:H	1:48:C:GLN:HB3	19	0.12
(1,4894)	1:43:C:LEU:HA	1:3:B:ILE:HG12	15	0.12
(1,4894)	1:43:C:LEU:HA	1:3:B:ILE:HG13	15	0.12
(1,4797)	1:40:C:GLY:H	1:43:C:LEU:HB3	3	0.12
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB2	6	0.12
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB3	6	0.12
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB2	6	0.12
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB3	6	0.12
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB2	6	0.12
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB3	6	0.12
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB2	13	0.12
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB3	13	0.12
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB2	13	0.12
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB3	13	0.12
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB2	13	0.12
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB3	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB2	19	0.12
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB3	19	0.12
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB2	19	0.12
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB3	19	0.12
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB2	19	0.12
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB3	19	0.12
(1,4743)	1:38:C:ALA:HA	1:42:C:THR:HA	6	0.12
(1,4743)	1:38:C:ALA:HA	1:42:C:THR:HA	18	0.12
(1,4666)	1:36:C:LEU:HD11	1:35:C:ILE:HA	17	0.12
(1,4666)	1:36:C:LEU:HD12	1:35:C:ILE:HA	17	0.12
(1,4666)	1:36:C:LEU:HD13	1:35:C:ILE:HA	17	0.12
(1,4450)	1:31:C:GLY:H	1:20:C:GLU:H	14	0.12
(1,4297)	1:24:C:THR:H	1:22:C:GLU:HB2	19	0.12
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA2	9	0.12
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA3	9	0.12
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA2	18	0.12
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA3	18	0.12
(1,4258)	1:23:C:GLY:HA2	1:24:C:THR:HB	9	0.12
(1,4258)	1:23:C:GLY:HA3	1:24:C:THR:HB	9	0.12
(1,4258)	1:23:C:GLY:HA2	1:24:C:THR:HB	18	0.12
(1,4258)	1:23:C:GLY:HA3	1:24:C:THR:HB	18	0.12
(1,4193)	1:21:C:ILE:HD11	1:15:C:CYS:HA	1	0.12
(1,4193)	1:21:C:ILE:HD12	1:15:C:CYS:HA	1	0.12
(1,4193)	1:21:C:ILE:HD13	1:15:C:CYS:HA	1	0.12
(1,4193)	1:21:C:ILE:HD11	1:15:C:CYS:HA	4	0.12
(1,4193)	1:21:C:ILE:HD12	1:15:C:CYS:HA	4	0.12
(1,4193)	1:21:C:ILE:HD13	1:15:C:CYS:HA	4	0.12
(1,4193)	1:21:C:ILE:HD11	1:15:C:CYS:HA	9	0.12
(1,4193)	1:21:C:ILE:HD12	1:15:C:CYS:HA	9	0.12
(1,4193)	1:21:C:ILE:HD13	1:15:C:CYS:HA	9	0.12
(1,4172)	1:20:C:GLU:H	1:31:C:GLY:H	14	0.12
(1,4166)	1:20:C:GLU:H	1:18:C:ALA:H	17	0.12
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	15	0.12
(1,3949)	1:12:C:CYS:H	1:34:C:VAL:HB	2	0.12
(1,3949)	1:12:C:CYS:H	1:34:C:VAL:HB	7	0.12
(1,3801)	1:8:C:LEU:HD11	1:39:C:GLN:HB2	4	0.12
(1,3801)	1:8:C:LEU:HD12	1:39:C:GLN:HB2	4	0.12
(1,3801)	1:8:C:LEU:HD13	1:39:C:GLN:HB2	4	0.12
(1,3801)	1:8:C:LEU:HD11	1:39:C:GLN:HB2	11	0.12
(1,3801)	1:8:C:LEU:HD12	1:39:C:GLN:HB2	11	0.12
(1,3801)	1:8:C:LEU:HD13	1:39:C:GLN:HB2	11	0.12
(1,3801)	1:8:C:LEU:HD11	1:39:C:GLN:HB2	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3801)	1:8:C:LEU:HD12	1:39:C:GLN:HB2	19	0.12
(1,3801)	1:8:C:LEU:HD13	1:39:C:GLN:HB2	19	0.12
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	19	0.12
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	19	0.12
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	19	0.12
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG21	7	0.12
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG22	7	0.12
(1,3574)	1:1:C:FME:HE1	1:3:C:ILE:HG23	7	0.12
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD11	4	0.12
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD12	4	0.12
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD13	4	0.12
(1,3555)	1:53:B:LYS:H	1:49:B:LYS:H	1	0.12
(1,3555)	1:53:B:LYS:H	1:49:B:LYS:H	2	0.12
(1,3432)	1:49:B:LYS:H	1:53:B:LYS:H	1	0.12
(1,3432)	1:49:B:LYS:H	1:53:B:LYS:H	2	0.12
(1,3342)	1:48:B:GLN:HB3	1:49:B:LYS:HB3	5	0.12
(1,3299)	1:46:B:PHE:H	1:48:B:GLN:HB3	4	0.12
(1,3299)	1:46:B:PHE:H	1:48:B:GLN:HB3	5	0.12
(1,3299)	1:46:B:PHE:H	1:48:B:GLN:HB3	7	0.12
(1,3299)	1:46:B:PHE:H	1:48:B:GLN:HB3	11	0.12
(1,3299)	1:46:B:PHE:H	1:48:B:GLN:HB3	16	0.12
(1,3107)	1:42:B:THR:HB	1:3:A:ILE:HB	1	0.12
(1,3107)	1:42:B:THR:HB	1:3:A:ILE:HB	6	0.12
(1,3107)	1:42:B:THR:HB	1:3:A:ILE:HB	10	0.12
(1,3107)	1:42:B:THR:HB	1:3:A:ILE:HB	14	0.12
(1,3039)	1:40:B:GLY:H	1:43:B:LEU:HB3	16	0.12
(1,3039)	1:40:B:GLY:H	1:43:B:LEU:HB3	17	0.12
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB2	6	0.12
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB3	6	0.12
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB2	6	0.12
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB3	6	0.12
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB2	6	0.12
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB3	6	0.12
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB2	11	0.12
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB3	11	0.12
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB2	11	0.12
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB3	11	0.12
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB2	11	0.12
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB3	11	0.12
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB2	13	0.12
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB3	13	0.12
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB2	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB3	13	0.12
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB2	13	0.12
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB3	13	0.12
(1,2971)	1:37:B:THR:H	1:36:B:LEU:HG	6	0.12
(1,2971)	1:37:B:THR:H	1:36:B:LEU:HG	11	0.12
(1,2971)	1:37:B:THR:H	1:36:B:LEU:HG	14	0.12
(1,2908)	1:36:B:LEU:HD11	1:35:B:ILE:HA	4	0.12
(1,2908)	1:36:B:LEU:HD12	1:35:B:ILE:HA	4	0.12
(1,2908)	1:36:B:LEU:HD13	1:35:B:ILE:HA	4	0.12
(1,2831)	1:35:B:ILE:HA	1:11:B:ALA:HA	2	0.12
(1,2831)	1:35:B:ILE:HA	1:11:B:ALA:HA	8	0.12
(1,2831)	1:35:B:ILE:HA	1:11:B:ALA:HA	19	0.12
(1,2821)	1:34:B:VAL:H	1:32:B:LYS:HA	7	0.12
(1,2821)	1:34:B:VAL:H	1:32:B:LYS:HA	20	0.12
(1,2721)	1:32:B:LYS:HD2	1:29:B:CYS:HB2	6	0.12
(1,2721)	1:32:B:LYS:HD3	1:29:B:CYS:HB2	6	0.12
(1,2656)	1:29:B:CYS:HB2	1:32:B:LYS:HD2	6	0.12
(1,2656)	1:29:B:CYS:HB2	1:32:B:LYS:HD3	6	0.12
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG21	17	0.12
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	17	0.12
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG23	17	0.12
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG21	17	0.12
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG22	17	0.12
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG23	17	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA2	2	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA3	2	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA2	5	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA3	5	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA2	8	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA3	8	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA2	11	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA3	11	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA2	13	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA3	13	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA2	17	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA3	17	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA2	18	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA3	18	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA2	20	0.12
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA3	20	0.12
(1,2500)	1:23:B:GLY:HA2	1:24:B:THR:HB	2	0.12
(1,2500)	1:23:B:GLY:HA3	1:24:B:THR:HB	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2500)	1:23:B:GLY:HA2	1:24:B:THR:HB	5	0.12
(1,2500)	1:23:B:GLY:HA3	1:24:B:THR:HB	5	0.12
(1,2500)	1:23:B:GLY:HA2	1:24:B:THR:HB	8	0.12
(1,2500)	1:23:B:GLY:HA3	1:24:B:THR:HB	8	0.12
(1,2500)	1:23:B:GLY:HA2	1:24:B:THR:HB	11	0.12
(1,2500)	1:23:B:GLY:HA3	1:24:B:THR:HB	11	0.12
(1,2500)	1:23:B:GLY:HA2	1:24:B:THR:HB	13	0.12
(1,2500)	1:23:B:GLY:HA3	1:24:B:THR:HB	13	0.12
(1,2500)	1:23:B:GLY:HA2	1:24:B:THR:HB	17	0.12
(1,2500)	1:23:B:GLY:HA3	1:24:B:THR:HB	17	0.12
(1,2500)	1:23:B:GLY:HA2	1:24:B:THR:HB	18	0.12
(1,2500)	1:23:B:GLY:HA3	1:24:B:THR:HB	18	0.12
(1,2500)	1:23:B:GLY:HA2	1:24:B:THR:HB	20	0.12
(1,2500)	1:23:B:GLY:HA3	1:24:B:THR:HB	20	0.12
(1,2435)	1:21:B:ILE:HD11	1:15:B:CYS:HA	15	0.12
(1,2435)	1:21:B:ILE:HD12	1:15:B:CYS:HA	15	0.12
(1,2435)	1:21:B:ILE:HD13	1:15:B:CYS:HA	15	0.12
(1,2435)	1:21:B:ILE:HD11	1:15:B:CYS:HA	18	0.12
(1,2435)	1:21:B:ILE:HD12	1:15:B:CYS:HA	18	0.12
(1,2435)	1:21:B:ILE:HD13	1:15:B:CYS:HA	18	0.12
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD2	5	0.12
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD3	5	0.12
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD2	7	0.12
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD3	7	0.12
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD2	14	0.12
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD3	14	0.12
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD2	18	0.12
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD3	18	0.12
(1,2250)	1:15:B:CYS:HB2	1:21:B:ILE:HB	2	0.12
(1,2192)	1:12:B:CYS:H	1:34:B:VAL:HB	17	0.12
(1,2160)	1:11:B:ALA:HA	1:35:B:ILE:HA	2	0.12
(1,2160)	1:11:B:ALA:HA	1:35:B:ILE:HA	8	0.12
(1,2160)	1:11:B:ALA:HA	1:35:B:ILE:HA	19	0.12
(1,2152)	1:10:B:VAL:H	1:36:B:LEU:HA	13	0.12
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	16	0.12
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	16	0.12
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	16	0.12
(1,2131)	1:10:B:VAL:HG11	1:36:B:LEU:HA	17	0.12
(1,2131)	1:10:B:VAL:HG12	1:36:B:LEU:HA	17	0.12
(1,2131)	1:10:B:VAL:HG13	1:36:B:LEU:HA	17	0.12
(1,2054)	1:8:B:LEU:HD21	1:39:B:GLN:HG2	7	0.12
(1,2054)	1:8:B:LEU:HD21	1:39:B:GLN:HG3	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2054)	1:8:B:LEU:HD22	1:39:B:GLN:HG2	7	0.12
(1,2054)	1:8:B:LEU:HD22	1:39:B:GLN:HG3	7	0.12
(1,2054)	1:8:B:LEU:HD23	1:39:B:GLN:HG2	7	0.12
(1,2054)	1:8:B:LEU:HD23	1:39:B:GLN:HG3	7	0.12
(1,2044)	1:8:B:LEU:HD11	1:39:B:GLN:HB2	3	0.12
(1,2044)	1:8:B:LEU:HD12	1:39:B:GLN:HB2	3	0.12
(1,2044)	1:8:B:LEU:HD13	1:39:B:GLN:HB2	3	0.12
(1,2044)	1:8:B:LEU:HD11	1:39:B:GLN:HB2	12	0.12
(1,2044)	1:8:B:LEU:HD12	1:39:B:GLN:HB2	12	0.12
(1,2044)	1:8:B:LEU:HD13	1:39:B:GLN:HB2	12	0.12
(1,2044)	1:8:B:LEU:HD11	1:39:B:GLN:HB2	16	0.12
(1,2044)	1:8:B:LEU:HD12	1:39:B:GLN:HB2	16	0.12
(1,2044)	1:8:B:LEU:HD13	1:39:B:GLN:HB2	16	0.12
(1,1837)	1:2:B:VAL:HG11	1:1:B:FME:HG2	13	0.12
(1,1837)	1:2:B:VAL:HG11	1:1:B:FME:HG3	13	0.12
(1,1837)	1:2:B:VAL:HG12	1:1:B:FME:HG2	13	0.12
(1,1837)	1:2:B:VAL:HG12	1:1:B:FME:HG3	13	0.12
(1,1837)	1:2:B:VAL:HG13	1:1:B:FME:HG2	13	0.12
(1,1837)	1:2:B:VAL:HG13	1:1:B:FME:HG3	13	0.12
(1,1800)	1:53:A:LYS:H	1:49:A:LYS:H	1	0.12
(1,1672)	1:49:A:LYS:H	1:53:A:LYS:H	1	0.12
(1,1598)	1:48:A:GLN:HG2	1:45:A:ASP:HB2	13	0.12
(1,1598)	1:48:A:GLN:HG2	1:45:A:ASP:HB3	13	0.12
(1,1598)	1:48:A:GLN:HG3	1:45:A:ASP:HB2	13	0.12
(1,1598)	1:48:A:GLN:HG3	1:45:A:ASP:HB3	13	0.12
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD11	5	0.12
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD12	5	0.12
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD13	5	0.12
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD11	12	0.12
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD12	12	0.12
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD13	12	0.12
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	4	0.12
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	9	0.12
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	10	0.12
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	13	0.12
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	16	0.12
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	17	0.12
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	18	0.12
(1,1491)	1:45:A:ASP:H	1:44:A:LEU:HG	15	0.12
(1,1487)	1:45:A:ASP:HB2	1:48:A:GLN:HG2	13	0.12
(1,1487)	1:45:A:ASP:HB2	1:48:A:GLN:HG3	13	0.12
(1,1487)	1:45:A:ASP:HB3	1:48:A:GLN:HG2	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1487)	1:45:A:ASP:HB3	1:48:A:GLN:HG3	13	0.12
(1,1457)	1:44:A:LEU:HG	1:45:A:ASP:H	15	0.12
(1,1354)	1:42:A:THR:H	1:38:A:ALA:HA	17	0.12
(1,1325)	1:42:A:THR:HB	1:3:C:ILE:HB	11	0.12
(1,1325)	1:42:A:THR:HB	1:3:C:ILE:HB	17	0.12
(1,1263)	1:40:A:GLY:H	1:43:A:LEU:HB3	14	0.12
(1,1211)	1:38:A:ALA:HA	1:42:A:THR:HA	10	0.12
(1,1211)	1:38:A:ALA:HA	1:42:A:THR:HA	16	0.12
(1,1211)	1:38:A:ALA:HA	1:42:A:THR:HA	19	0.12
(1,1193)	1:37:A:THR:H	1:36:A:LEU:HG	6	0.12
(1,842)	1:28:A:ALA:H	1:30:A:SER:H	17	0.12
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA2	4	0.12
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA3	4	0.12
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA2	6	0.12
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA3	6	0.12
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA2	18	0.12
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA3	18	0.12
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA2	19	0.12
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA3	19	0.12
(1,712)	1:23:A:GLY:HA2	1:24:A:THR:HB	4	0.12
(1,712)	1:23:A:GLY:HA3	1:24:A:THR:HB	4	0.12
(1,712)	1:23:A:GLY:HA2	1:24:A:THR:HB	6	0.12
(1,712)	1:23:A:GLY:HA3	1:24:A:THR:HB	6	0.12
(1,712)	1:23:A:GLY:HA2	1:24:A:THR:HB	18	0.12
(1,712)	1:23:A:GLY:HA3	1:24:A:THR:HB	18	0.12
(1,712)	1:23:A:GLY:HA2	1:24:A:THR:HB	19	0.12
(1,712)	1:23:A:GLY:HA3	1:24:A:THR:HB	19	0.12
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD2	9	0.12
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD3	9	0.12
(1,377)	1:11:A:ALA:H	1:10:A:VAL:HB	8	0.12
(1,358)	1:10:A:VAL:H	1:36:A:LEU:HA	4	0.12
(1,338)	1:10:A:VAL:HG11	1:36:A:LEU:HA	14	0.12
(1,338)	1:10:A:VAL:HG12	1:36:A:LEU:HA	14	0.12
(1,338)	1:10:A:VAL:HG13	1:36:A:LEU:HA	14	0.12
(1,338)	1:10:A:VAL:HG11	1:36:A:LEU:HA	16	0.12
(1,338)	1:10:A:VAL:HG12	1:36:A:LEU:HA	16	0.12
(1,338)	1:10:A:VAL:HG13	1:36:A:LEU:HA	16	0.12
(1,331)	1:10:A:VAL:HB	1:11:A:ALA:H	8	0.12
(1,244)	1:8:A:LEU:HD11	1:39:A:GLN:HB2	11	0.12
(1,244)	1:8:A:LEU:HD12	1:39:A:GLN:HB2	11	0.12
(1,244)	1:8:A:LEU:HD13	1:39:A:GLN:HB2	11	0.12
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	15	0.12
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	15	0.12
(1,111)	1:4:A:ALA:HB1	1:1:A:FME:HE1	19	0.12
(1,111)	1:4:A:ALA:HB2	1:1:A:FME:HE1	19	0.12
(1,111)	1:4:A:ALA:HB3	1:1:A:FME:HE1	19	0.12
(1,77)	1:3:A:ILE:HG21	1:39:B:GLN:HG2	12	0.12
(1,77)	1:3:A:ILE:HG21	1:39:B:GLN:HG3	12	0.12
(1,77)	1:3:A:ILE:HG22	1:39:B:GLN:HG2	12	0.12
(1,77)	1:3:A:ILE:HG22	1:39:B:GLN:HG3	12	0.12
(1,77)	1:3:A:ILE:HG23	1:39:B:GLN:HG2	12	0.12
(1,77)	1:3:A:ILE:HG23	1:39:B:GLN:HG3	12	0.12
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	2	0.12
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	2	0.12
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	2	0.12
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG21	12	0.12
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG22	12	0.12
(1,15)	1:1:A:FME:HE1	1:3:A:ILE:HG23	12	0.12
(2,1556)	1:43:C:LEU:HD11	1:8:C:LEU:HD22	6	0.11
(2,1554)	1:43:A:LEU:HD13	1:8:A:LEU:HD21	6	0.11
(2,1475)	1:34:C:VAL:HG12	1:9:C:GLU:HB3	10	0.11
(2,1406)	1:15:C:CYS:HA	1:17:C:ARG:HD2	2	0.11
(2,1348)	1:8:B:LEU:HD23	1:43:B:LEU:HG	2	0.11
(2,1348)	1:8:B:LEU:HD21	1:43:B:LEU:HG	5	0.11
(2,1321)	1:43:B:LEU:HD21	1:43:C:LEU:HA	3	0.11
(2,1070)	1:29:A:CYS:HB3	1:32:A:LYS:HD2	8	0.11
(2,985)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	16	0.11
(2,984)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	19	0.11
(2,983)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	15	0.11
(2,961)	1:47:A:ILE:HB	1:47:B:ILE:HB	10	0.11
(2,872)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	7	0.11
(2,871)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	3	0.11
(2,869)	1:31:B:GLY:HA2	1:26:B:CYS:HB3	7	0.11
(2,868)	1:31:A:GLY:HA2	1:26:A:CYS:HB3	3	0.11
(2,697)	1:15:C:CYS:HA	1:17:C:ARG:HD2	2	0.11
(2,508)	1:43:B:LEU:HD21	1:43:C:LEU:HA	3	0.11
(2,484)	1:51:B:LEU:HD13	1:47:A:ILE:HB	13	0.11
(2,470)	1:43:C:LEU:HD11	1:8:C:LEU:HD22	6	0.11
(2,468)	1:43:A:LEU:HD13	1:8:A:LEU:HD21	6	0.11
(2,322)	1:53:C:LYS:HB3	1:49:C:LYS:HB2	16	0.11
(2,321)	1:53:B:LYS:HB3	1:49:B:LYS:HB2	19	0.11
(2,320)	1:53:A:LYS:HB3	1:49:A:LYS:HB2	15	0.11
(2,270)	1:14:B:LYS:HE2	1:15:B:CYS:HB2	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,270)	1:14:B:LYS:HE3	1:15:B:CYS:HB2	4	0.11
(2,267)	1:51:B:LEU:HB2	1:52:B:ASN:HB2	1	0.11
(2,266)	1:51:A:LEU:HB2	1:52:A:ASN:HB2	17	0.11
(2,266)	1:51:A:LEU:HB2	1:52:A:ASN:HB2	20	0.11
(2,265)	1:49:C:LYS:HE2	1:53:C:LYS:HB3	20	0.11
(2,264)	1:49:B:LYS:HE2	1:53:B:LYS:HB3	1	0.11
(2,264)	1:49:B:LYS:HE2	1:53:B:LYS:HB3	16	0.11
(2,263)	1:49:A:LYS:HE2	1:53:A:LYS:HB3	3	0.11
(2,154)	1:40:C:GLY:H	1:38:C:ALA:HA	11	0.11
(2,153)	1:40:B:GLY:H	1:38:B:ALA:HA	20	0.11
(2,69)	1:51:B:LEU:H	1:51:C:LEU:HD12	19	0.11
(2,61)	1:3:C:ILE:H	1:2:C:VAL:HB	2	0.11
(2,61)	1:3:C:ILE:H	1:2:C:VAL:HB	7	0.11
(2,61)	1:3:C:ILE:H	1:2:C:VAL:HB	8	0.11
(2,61)	1:3:C:ILE:H	1:2:C:VAL:HB	19	0.11
(2,61)	1:3:C:ILE:H	1:2:C:VAL:HB	20	0.11
(2,60)	1:3:B:ILE:H	1:2:B:VAL:HB	2	0.11
(2,60)	1:3:B:ILE:H	1:2:B:VAL:HB	4	0.11
(2,60)	1:3:B:ILE:H	1:2:B:VAL:HB	7	0.11
(2,60)	1:3:B:ILE:H	1:2:B:VAL:HB	8	0.11
(2,31)	1:18:A:ALA:H	1:17:A:ARG:HB3	13	0.11
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD11	6	0.11
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD12	6	0.11
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD13	6	0.11
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD11	12	0.11
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD12	12	0.11
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD13	12	0.11
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	5	0.11
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	15	0.11
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	20	0.11
(1,5308)	1:53:C:LYS:HG2	1:48:C:GLN:HB2	5	0.11
(1,5308)	1:53:C:LYS:HG3	1:48:C:GLN:HB2	5	0.11
(1,5308)	1:53:C:LYS:HG2	1:48:C:GLN:HB2	6	0.11
(1,5308)	1:53:C:LYS:HG3	1:48:C:GLN:HB2	6	0.11
(1,5299)	1:53:C:LYS:HE2	1:45:C:ASP:HA	3	0.11
(1,5299)	1:53:C:LYS:HE3	1:45:C:ASP:HA	3	0.11
(1,5298)	1:53:C:LYS:HD2	1:49:C:LYS:HG2	11	0.11
(1,5298)	1:53:C:LYS:HD2	1:49:C:LYS:HG3	11	0.11
(1,5298)	1:53:C:LYS:HD3	1:49:C:LYS:HG2	11	0.11
(1,5298)	1:53:C:LYS:HD3	1:49:C:LYS:HG3	11	0.11
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	5	0.11
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	20	0.11
(1,5110)	1:48:C:GLN:HB2	1:51:A:LEU:HD11	16	0.11
(1,5110)	1:48:C:GLN:HB2	1:51:A:LEU:HD12	16	0.11
(1,5110)	1:48:C:GLN:HB2	1:51:A:LEU:HD13	16	0.11
(1,5100)	1:48:C:GLN:HB3	1:49:C:LYS:HB3	11	0.11
(1,5015)	1:45:C:ASP:H	1:44:C:LEU:HG	1	0.11
(1,4983)	1:44:C:LEU:HG	1:45:C:ASP:H	1	0.11
(1,4854)	1:42:C:THR:HB	1:3:B:ILE:HB	1	0.11
(1,4854)	1:42:C:THR:HB	1:3:B:ILE:HB	8	0.11
(1,4854)	1:42:C:THR:HB	1:3:B:ILE:HB	12	0.11
(1,4797)	1:40:C:GLY:H	1:43:C:LEU:HB3	13	0.11
(1,4797)	1:40:C:GLY:H	1:43:C:LEU:HB3	15	0.11
(1,4797)	1:40:C:GLY:H	1:43:C:LEU:HB3	16	0.11
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB2	4	0.11
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB3	4	0.11
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB2	4	0.11
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB3	4	0.11
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB2	4	0.11
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB3	4	0.11
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB2	5	0.11
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB3	5	0.11
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB2	5	0.11
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB3	5	0.11
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB2	5	0.11
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB3	5	0.11
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB2	14	0.11
(1,4745)	1:38:C:ALA:HB1	1:1:B:FME:HB3	14	0.11
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB2	14	0.11
(1,4745)	1:38:C:ALA:HB2	1:1:B:FME:HB3	14	0.11
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB2	14	0.11
(1,4745)	1:38:C:ALA:HB3	1:1:B:FME:HB3	14	0.11
(1,4743)	1:38:C:ALA:HA	1:42:C:THR:HA	5	0.11
(1,4743)	1:38:C:ALA:HA	1:42:C:THR:HA	20	0.11
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	13	0.11
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	20	0.11
(1,4581)	1:34:C:VAL:H	1:32:C:LYS:HG2	7	0.11
(1,4581)	1:34:C:VAL:H	1:32:C:LYS:HG3	7	0.11
(1,4430)	1:30:C:SER:HA	1:32:C:LYS:HE2	15	0.11
(1,4430)	1:30:C:SER:HA	1:32:C:LYS:HE3	15	0.11
(1,4292)	1:24:C:THR:HG21	1:25:C:PRO:HG2	17	0.11
(1,4292)	1:24:C:THR:HG21	1:25:C:PRO:HG3	17	0.11
(1,4292)	1:24:C:THR:HG22	1:25:C:PRO:HG2	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4292)	1:24:C:THR:HG22	1:25:C:PRO:HG3	17	0.11
(1,4292)	1:24:C:THR:HG23	1:25:C:PRO:HG2	17	0.11
(1,4292)	1:24:C:THR:HG23	1:25:C:PRO:HG3	17	0.11
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA2	3	0.11
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA3	3	0.11
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA2	5	0.11
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA3	5	0.11
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA2	8	0.11
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA3	8	0.11
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA2	14	0.11
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA3	14	0.11
(1,4258)	1:23:C:GLY:HA2	1:24:C:THR:HB	3	0.11
(1,4258)	1:23:C:GLY:HA3	1:24:C:THR:HB	3	0.11
(1,4258)	1:23:C:GLY:HA2	1:24:C:THR:HB	5	0.11
(1,4258)	1:23:C:GLY:HA3	1:24:C:THR:HB	5	0.11
(1,4258)	1:23:C:GLY:HA2	1:24:C:THR:HB	8	0.11
(1,4258)	1:23:C:GLY:HA3	1:24:C:THR:HB	8	0.11
(1,4258)	1:23:C:GLY:HA2	1:24:C:THR:HB	14	0.11
(1,4258)	1:23:C:GLY:HA3	1:24:C:THR:HB	14	0.11
(1,4166)	1:20:C:GLU:H	1:18:C:ALA:H	16	0.11
(1,4140)	1:20:C:GLU:HA	1:27:C:PRO:HD2	20	0.11
(1,4140)	1:20:C:GLU:HA	1:27:C:PRO:HD3	20	0.11
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	2	0.11
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	6	0.11
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	13	0.11
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	2	0.11
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	2	0.11
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	2	0.11
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	2	0.11
(1,3949)	1:12:C:CYS:H	1:34:C:VAL:HB	1	0.11
(1,3949)	1:12:C:CYS:H	1:34:C:VAL:HB	13	0.11
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	13	0.11
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	20	0.11
(1,3909)	1:10:C:VAL:H	1:36:C:LEU:HA	2	0.11
(1,3888)	1:10:C:VAL:HG11	1:36:C:LEU:HA	2	0.11
(1,3888)	1:10:C:VAL:HG12	1:36:C:LEU:HA	2	0.11
(1,3888)	1:10:C:VAL:HG13	1:36:C:LEU:HA	2	0.11
(1,3888)	1:10:C:VAL:HG11	1:36:C:LEU:HA	9	0.11
(1,3888)	1:10:C:VAL:HG12	1:36:C:LEU:HA	9	0.11
(1,3888)	1:10:C:VAL:HG13	1:36:C:LEU:HA	9	0.11
(1,3801)	1:8:C:LEU:HD11	1:39:C:GLN:HB2	7	0.11
(1,3801)	1:8:C:LEU:HD12	1:39:C:GLN:HB2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3801)	1:8:C:LEU:HD13	1:39:C:GLN:HB2	7	0.11
(1,3801)	1:8:C:LEU:HD11	1:39:C:GLN:HB2	18	0.11
(1,3801)	1:8:C:LEU:HD12	1:39:C:GLN:HB2	18	0.11
(1,3801)	1:8:C:LEU:HD13	1:39:C:GLN:HB2	18	0.11
(1,3735)	1:6:C:ASP:HA	1:9:C:GLU:HG2	1	0.11
(1,3735)	1:6:C:ASP:HA	1:9:C:GLU:HG3	1	0.11
(1,3670)	1:4:C:ALA:HB1	1:1:C:FME:HE1	7	0.11
(1,3670)	1:4:C:ALA:HB2	1:1:C:FME:HE1	7	0.11
(1,3670)	1:4:C:ALA:HB3	1:1:C:FME:HE1	7	0.11
(1,3629)	1:3:C:ILE:HG12	1:1:C:FME:HG2	15	0.11
(1,3629)	1:3:C:ILE:HG12	1:1:C:FME:HG3	15	0.11
(1,3629)	1:3:C:ILE:HG13	1:1:C:FME:HG2	15	0.11
(1,3629)	1:3:C:ILE:HG13	1:1:C:FME:HG3	15	0.11
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD11	3	0.11
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD12	3	0.11
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD13	3	0.11
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD11	17	0.11
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD12	17	0.11
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD13	17	0.11
(1,3555)	1:53:B:LYS:H	1:49:B:LYS:H	3	0.11
(1,3555)	1:53:B:LYS:H	1:49:B:LYS:H	15	0.11
(1,3555)	1:53:B:LYS:H	1:49:B:LYS:H	16	0.11
(1,3549)	1:53:B:LYS:HG2	1:48:B:GLN:HB2	20	0.11
(1,3549)	1:53:B:LYS:HG3	1:48:B:GLN:HB2	20	0.11
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG2	13	0.11
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG3	13	0.11
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG2	13	0.11
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG3	13	0.11
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG2	14	0.11
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG3	14	0.11
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG2	14	0.11
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG3	14	0.11
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG2	18	0.11
(1,3539)	1:53:B:LYS:HD2	1:49:B:LYS:HG3	18	0.11
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG2	18	0.11
(1,3539)	1:53:B:LYS:HD3	1:49:B:LYS:HG3	18	0.11
(1,3480)	1:51:B:LEU:HD21	1:48:A:GLN:HE21	15	0.11
(1,3480)	1:51:B:LEU:HD21	1:48:A:GLN:HE22	15	0.11
(1,3480)	1:51:B:LEU:HD22	1:48:A:GLN:HE21	15	0.11
(1,3480)	1:51:B:LEU:HD22	1:48:A:GLN:HE22	15	0.11
(1,3480)	1:51:B:LEU:HD23	1:48:A:GLN:HE21	15	0.11
(1,3480)	1:51:B:LEU:HD23	1:48:A:GLN:HE22	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3432)	1:49:B:LYS:H	1:53:B:LYS:H	3	0.11
(1,3432)	1:49:B:LYS:H	1:53:B:LYS:H	15	0.11
(1,3432)	1:49:B:LYS:H	1:53:B:LYS:H	16	0.11
(1,3342)	1:48:B:GLN:HB3	1:49:B:LYS:HB3	9	0.11
(1,3342)	1:48:B:GLN:HB3	1:49:B:LYS:HB3	13	0.11
(1,3342)	1:48:B:GLN:HB3	1:49:B:LYS:HB3	20	0.11
(1,3299)	1:46:B:PHE:H	1:48:B:GLN:HB3	15	0.11
(1,3299)	1:46:B:PHE:H	1:48:B:GLN:HB3	18	0.11
(1,3257)	1:45:B:ASP:H	1:44:B:LEU:HG	15	0.11
(1,3257)	1:45:B:ASP:H	1:44:B:LEU:HG	16	0.11
(1,3257)	1:45:B:ASP:H	1:44:B:LEU:HG	19	0.11
(1,3225)	1:44:B:LEU:HG	1:45:B:ASP:H	15	0.11
(1,3225)	1:44:B:LEU:HG	1:45:B:ASP:H	16	0.11
(1,3225)	1:44:B:LEU:HG	1:45:B:ASP:H	19	0.11
(1,3145)	1:43:B:LEU:HA	1:3:A:ILE:HG12	20	0.11
(1,3145)	1:43:B:LEU:HA	1:3:A:ILE:HG13	20	0.11
(1,3122)	1:42:B:THR:HG21	1:8:A:LEU:HD11	13	0.11
(1,3122)	1:42:B:THR:HG21	1:8:A:LEU:HD12	13	0.11
(1,3122)	1:42:B:THR:HG21	1:8:A:LEU:HD13	13	0.11
(1,3122)	1:42:B:THR:HG22	1:8:A:LEU:HD11	13	0.11
(1,3122)	1:42:B:THR:HG22	1:8:A:LEU:HD12	13	0.11
(1,3122)	1:42:B:THR:HG22	1:8:A:LEU:HD13	13	0.11
(1,3122)	1:42:B:THR:HG23	1:8:A:LEU:HD11	13	0.11
(1,3122)	1:42:B:THR:HG23	1:8:A:LEU:HD12	13	0.11
(1,3122)	1:42:B:THR:HG23	1:8:A:LEU:HD13	13	0.11
(1,3107)	1:42:B:THR:HB	1:3:A:ILE:HB	11	0.11
(1,3107)	1:42:B:THR:HB	1:3:A:ILE:HB	12	0.11
(1,3039)	1:40:B:GLY:H	1:43:B:LEU:HB3	1	0.11
(1,3039)	1:40:B:GLY:H	1:43:B:LEU:HB3	4	0.11
(1,3039)	1:40:B:GLY:H	1:43:B:LEU:HB3	9	0.11
(1,3039)	1:40:B:GLY:H	1:43:B:LEU:HB3	11	0.11
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB2	1	0.11
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB3	1	0.11
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB2	1	0.11
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB3	1	0.11
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB2	1	0.11
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB3	1	0.11
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB2	3	0.11
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB3	3	0.11
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB2	3	0.11
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB3	3	0.11
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB2	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB3	3	0.11
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB2	4	0.11
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB3	4	0.11
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB2	4	0.11
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB3	4	0.11
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB2	4	0.11
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB3	4	0.11
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB2	12	0.11
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB3	12	0.11
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB2	12	0.11
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB3	12	0.11
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB2	12	0.11
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB3	12	0.11
(1,2927)	1:36:B:LEU:HD21	1:44:B:LEU:HD21	10	0.11
(1,2927)	1:36:B:LEU:HD21	1:44:B:LEU:HD22	10	0.11
(1,2927)	1:36:B:LEU:HD21	1:44:B:LEU:HD23	10	0.11
(1,2927)	1:36:B:LEU:HD22	1:44:B:LEU:HD21	10	0.11
(1,2927)	1:36:B:LEU:HD22	1:44:B:LEU:HD22	10	0.11
(1,2927)	1:36:B:LEU:HD22	1:44:B:LEU:HD23	10	0.11
(1,2927)	1:36:B:LEU:HD23	1:44:B:LEU:HD21	10	0.11
(1,2927)	1:36:B:LEU:HD23	1:44:B:LEU:HD22	10	0.11
(1,2927)	1:36:B:LEU:HD23	1:44:B:LEU:HD23	10	0.11
(1,2908)	1:36:B:LEU:HD11	1:35:B:ILE:HA	11	0.11
(1,2908)	1:36:B:LEU:HD12	1:35:B:ILE:HA	11	0.11
(1,2908)	1:36:B:LEU:HD13	1:35:B:ILE:HA	11	0.11
(1,2857)	1:35:B:ILE:HG12	1:29:B:CYS:HA	6	0.11
(1,2857)	1:35:B:ILE:HG13	1:29:B:CYS:HA	6	0.11
(1,2765)	1:33:B:GLY:H	1:29:B:CYS:HA	1	0.11
(1,2640)	1:29:B:CYS:HA	1:33:B:GLY:H	1	0.11
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG21	6	0.11
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	6	0.11
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG23	6	0.11
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG21	6	0.11
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG22	6	0.11
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG23	6	0.11
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG21	12	0.11
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	12	0.11
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG23	12	0.11
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG21	12	0.11
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG22	12	0.11
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG23	12	0.11
(1,2573)	1:26:B:CYS:HA	1:21:B:ILE:HG12	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2573)	1:26:B:CYS:HA	1:21:B:ILE:HG13	2	0.11
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	3	0.11
(1,2539)	1:24:B:THR:H	1:22:B:GLU:HB2	10	0.11
(1,2528)	1:24:B:THR:HG21	1:22:B:GLU:HG2	3	0.11
(1,2528)	1:24:B:THR:HG21	1:22:B:GLU:HG3	3	0.11
(1,2528)	1:24:B:THR:HG22	1:22:B:GLU:HG2	3	0.11
(1,2528)	1:24:B:THR:HG22	1:22:B:GLU:HG3	3	0.11
(1,2528)	1:24:B:THR:HG23	1:22:B:GLU:HG2	3	0.11
(1,2528)	1:24:B:THR:HG23	1:22:B:GLU:HG3	3	0.11
(1,2435)	1:21:B:ILE:HD11	1:15:B:CYS:HA	7	0.11
(1,2435)	1:21:B:ILE:HD12	1:15:B:CYS:HA	7	0.11
(1,2435)	1:21:B:ILE:HD13	1:15:B:CYS:HA	7	0.11
(1,2435)	1:21:B:ILE:HD11	1:15:B:CYS:HA	9	0.11
(1,2435)	1:21:B:ILE:HD12	1:15:B:CYS:HA	9	0.11
(1,2435)	1:21:B:ILE:HD13	1:15:B:CYS:HA	9	0.11
(1,2408)	1:20:B:GLU:H	1:18:B:ALA:H	1	0.11
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD2	15	0.11
(1,2382)	1:20:B:GLU:HA	1:27:B:PRO:HD3	15	0.11
(1,2222)	1:14:B:LYS:HE2	1:21:B:ILE:HD11	9	0.11
(1,2222)	1:14:B:LYS:HE2	1:21:B:ILE:HD12	9	0.11
(1,2222)	1:14:B:LYS:HE2	1:21:B:ILE:HD13	9	0.11
(1,2222)	1:14:B:LYS:HE3	1:21:B:ILE:HD11	9	0.11
(1,2222)	1:14:B:LYS:HE3	1:21:B:ILE:HD12	9	0.11
(1,2222)	1:14:B:LYS:HE3	1:21:B:ILE:HD13	9	0.11
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG12	4	0.11
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG13	4	0.11
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG12	4	0.11
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG13	4	0.11
(1,2044)	1:8:B:LEU:HD11	1:39:B:GLN:HB2	7	0.11
(1,2044)	1:8:B:LEU:HD12	1:39:B:GLN:HB2	7	0.11
(1,2044)	1:8:B:LEU:HD13	1:39:B:GLN:HB2	7	0.11
(1,2044)	1:8:B:LEU:HD11	1:39:B:GLN:HB2	11	0.11
(1,2044)	1:8:B:LEU:HD12	1:39:B:GLN:HB2	11	0.11
(1,2044)	1:8:B:LEU:HD13	1:39:B:GLN:HB2	11	0.11
(1,1913)	1:4:B:ALA:HB1	1:1:B:FME:HE1	11	0.11
(1,1913)	1:4:B:ALA:HB2	1:1:B:FME:HE1	11	0.11
(1,1913)	1:4:B:ALA:HB3	1:1:B:FME:HE1	11	0.11
(1,1886)	1:3:B:ILE:HG21	1:39:C:GLN:HG2	4	0.11
(1,1886)	1:3:B:ILE:HG21	1:39:C:GLN:HG3	4	0.11
(1,1886)	1:3:B:ILE:HG22	1:39:C:GLN:HG2	4	0.11
(1,1886)	1:3:B:ILE:HG22	1:39:C:GLN:HG3	4	0.11
(1,1886)	1:3:B:ILE:HG23	1:39:C:GLN:HG2	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1886)	1:3:B:ILE:HG23	1:39:C:GLN:HG3	4	0.11
(1,1886)	1:3:B:ILE:HG21	1:39:C:GLN:HG2	5	0.11
(1,1886)	1:3:B:ILE:HG21	1:39:C:GLN:HG3	5	0.11
(1,1886)	1:3:B:ILE:HG22	1:39:C:GLN:HG2	5	0.11
(1,1886)	1:3:B:ILE:HG22	1:39:C:GLN:HG3	5	0.11
(1,1886)	1:3:B:ILE:HG23	1:39:C:GLN:HG2	5	0.11
(1,1886)	1:3:B:ILE:HG23	1:39:C:GLN:HG3	5	0.11
(1,1886)	1:3:B:ILE:HG21	1:39:C:GLN:HG2	11	0.11
(1,1886)	1:3:B:ILE:HG21	1:39:C:GLN:HG3	11	0.11
(1,1886)	1:3:B:ILE:HG22	1:39:C:GLN:HG2	11	0.11
(1,1886)	1:3:B:ILE:HG22	1:39:C:GLN:HG3	11	0.11
(1,1886)	1:3:B:ILE:HG23	1:39:C:GLN:HG2	11	0.11
(1,1886)	1:3:B:ILE:HG23	1:39:C:GLN:HG3	11	0.11
(1,1841)	1:2:B:VAL:HG11	1:3:B:ILE:HG21	12	0.11
(1,1841)	1:2:B:VAL:HG11	1:3:B:ILE:HG22	12	0.11
(1,1841)	1:2:B:VAL:HG11	1:3:B:ILE:HG23	12	0.11
(1,1841)	1:2:B:VAL:HG12	1:3:B:ILE:HG21	12	0.11
(1,1841)	1:2:B:VAL:HG12	1:3:B:ILE:HG22	12	0.11
(1,1841)	1:2:B:VAL:HG12	1:3:B:ILE:HG23	12	0.11
(1,1841)	1:2:B:VAL:HG13	1:3:B:ILE:HG21	12	0.11
(1,1841)	1:2:B:VAL:HG13	1:3:B:ILE:HG22	12	0.11
(1,1841)	1:2:B:VAL:HG13	1:3:B:ILE:HG23	12	0.11
(1,1800)	1:53:A:LYS:H	1:49:A:LYS:H	3	0.11
(1,1800)	1:53:A:LYS:H	1:49:A:LYS:H	10	0.11
(1,1800)	1:53:A:LYS:H	1:49:A:LYS:H	19	0.11
(1,1742)	1:52:A:ASN:HB2	1:51:B:LEU:HD11	18	0.11
(1,1742)	1:52:A:ASN:HB2	1:51:B:LEU:HD12	18	0.11
(1,1742)	1:52:A:ASN:HB2	1:51:B:LEU:HD13	18	0.11
(1,1672)	1:49:A:LYS:H	1:53:A:LYS:H	3	0.11
(1,1672)	1:49:A:LYS:H	1:53:A:LYS:H	10	0.11
(1,1672)	1:49:A:LYS:H	1:53:A:LYS:H	19	0.11
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD11	2	0.11
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD12	2	0.11
(1,1583)	1:48:A:GLN:HB2	1:51:B:LEU:HD13	2	0.11
(1,1581)	1:48:A:GLN:HB3	1:49:A:LYS:HB3	12	0.11
(1,1581)	1:48:A:GLN:HB3	1:49:A:LYS:HB3	20	0.11
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	12	0.11
(1,1499)	1:45:A:ASP:H	1:48:A:GLN:HB3	11	0.11
(1,1499)	1:45:A:ASP:H	1:48:A:GLN:HB3	18	0.11
(1,1491)	1:45:A:ASP:H	1:44:A:LEU:HG	1	0.11
(1,1491)	1:45:A:ASP:H	1:44:A:LEU:HG	6	0.11
(1,1491)	1:45:A:ASP:H	1:44:A:LEU:HG	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1491)	1:45:A:ASP:H	1:44:A:LEU:HG	14	0.11
(1,1491)	1:45:A:ASP:H	1:44:A:LEU:HG	16	0.11
(1,1457)	1:44:A:LEU:HG	1:45:A:ASP:H	1	0.11
(1,1457)	1:44:A:LEU:HG	1:45:A:ASP:H	6	0.11
(1,1457)	1:44:A:LEU:HG	1:45:A:ASP:H	11	0.11
(1,1457)	1:44:A:LEU:HG	1:45:A:ASP:H	14	0.11
(1,1457)	1:44:A:LEU:HG	1:45:A:ASP:H	16	0.11
(1,1325)	1:42:A:THR:HB	1:3:C:ILE:HB	13	0.11
(1,1211)	1:38:A:ALA:HA	1:42:A:THR:HA	3	0.11
(1,1211)	1:38:A:ALA:HA	1:42:A:THR:HA	9	0.11
(1,1211)	1:38:A:ALA:HA	1:42:A:THR:HA	17	0.11
(1,1193)	1:37:A:THR:H	1:36:A:LEU:HG	19	0.11
(1,1152)	1:36:A:LEU:HD21	1:44:A:LEU:HD21	16	0.11
(1,1152)	1:36:A:LEU:HD21	1:44:A:LEU:HD22	16	0.11
(1,1152)	1:36:A:LEU:HD21	1:44:A:LEU:HD23	16	0.11
(1,1152)	1:36:A:LEU:HD22	1:44:A:LEU:HD21	16	0.11
(1,1152)	1:36:A:LEU:HD22	1:44:A:LEU:HD22	16	0.11
(1,1152)	1:36:A:LEU:HD22	1:44:A:LEU:HD23	16	0.11
(1,1152)	1:36:A:LEU:HD23	1:44:A:LEU:HD21	16	0.11
(1,1152)	1:36:A:LEU:HD23	1:44:A:LEU:HD22	16	0.11
(1,1152)	1:36:A:LEU:HD23	1:44:A:LEU:HD23	16	0.11
(1,1134)	1:36:A:LEU:HD11	1:35:A:ILE:HA	17	0.11
(1,1134)	1:36:A:LEU:HD12	1:35:A:ILE:HA	17	0.11
(1,1134)	1:36:A:LEU:HD13	1:35:A:ILE:HA	17	0.11
(1,1080)	1:35:A:ILE:HG12	1:29:A:CYS:HA	13	0.11
(1,1080)	1:35:A:ILE:HG13	1:29:A:CYS:HA	13	0.11
(1,1052)	1:35:A:ILE:HA	1:11:A:ALA:HA	5	0.11
(1,1052)	1:35:A:ILE:HA	1:11:A:ALA:HA	19	0.11
(1,945)	1:32:A:LYS:HE2	1:29:A:CYS:HB3	14	0.11
(1,945)	1:32:A:LYS:HE3	1:29:A:CYS:HB3	14	0.11
(1,900)	1:31:A:GLY:HA2	1:19:A:GLY:HA2	20	0.11
(1,900)	1:31:A:GLY:HA2	1:19:A:GLY:HA3	20	0.11
(1,900)	1:31:A:GLY:HA3	1:19:A:GLY:HA2	20	0.11
(1,900)	1:31:A:GLY:HA3	1:19:A:GLY:HA3	20	0.11
(1,793)	1:26:A:CYS:HB2	1:15:A:CYS:HB2	13	0.11
(1,793)	1:26:A:CYS:HB3	1:15:A:CYS:HB2	13	0.11
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA2	2	0.11
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA3	2	0.11
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA2	5	0.11
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA3	5	0.11
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA2	7	0.11
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA3	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA2	11	0.11
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA3	11	0.11
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA2	12	0.11
(1,733)	1:24:A:THR:HB	1:23:A:GLY:HA3	12	0.11
(1,712)	1:23:A:GLY:HA2	1:24:A:THR:HB	2	0.11
(1,712)	1:23:A:GLY:HA3	1:24:A:THR:HB	2	0.11
(1,712)	1:23:A:GLY:HA2	1:24:A:THR:HB	5	0.11
(1,712)	1:23:A:GLY:HA3	1:24:A:THR:HB	5	0.11
(1,712)	1:23:A:GLY:HA2	1:24:A:THR:HB	7	0.11
(1,712)	1:23:A:GLY:HA3	1:24:A:THR:HB	7	0.11
(1,712)	1:23:A:GLY:HA2	1:24:A:THR:HB	11	0.11
(1,712)	1:23:A:GLY:HA3	1:24:A:THR:HB	11	0.11
(1,712)	1:23:A:GLY:HA2	1:24:A:THR:HB	12	0.11
(1,712)	1:23:A:GLY:HA3	1:24:A:THR:HB	12	0.11
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD2	13	0.11
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD3	13	0.11
(1,566)	1:19:A:GLY:HA2	1:31:A:GLY:HA2	20	0.11
(1,566)	1:19:A:GLY:HA2	1:31:A:GLY:HA3	20	0.11
(1,566)	1:19:A:GLY:HA3	1:31:A:GLY:HA2	20	0.11
(1,566)	1:19:A:GLY:HA3	1:31:A:GLY:HA3	20	0.11
(1,498)	1:16:A:GLU:H	1:33:A:GLY:H	11	0.11
(1,460)	1:15:A:CYS:HB2	1:26:A:CYS:HB2	13	0.11
(1,460)	1:15:A:CYS:HB2	1:26:A:CYS:HB3	13	0.11
(1,444)	1:15:A:CYS:HA	1:14:A:LYS:HG2	11	0.11
(1,444)	1:15:A:CYS:HA	1:14:A:LYS:HG3	11	0.11
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG12	3	0.11
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG13	3	0.11
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG12	3	0.11
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG13	3	0.11
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG12	15	0.11
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG13	15	0.11
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG12	15	0.11
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG13	15	0.11
(1,369)	1:11:A:ALA:HA	1:35:A:ILE:HA	5	0.11
(1,369)	1:11:A:ALA:HA	1:35:A:ILE:HA	19	0.11
(1,358)	1:10:A:VAL:H	1:36:A:LEU:HA	1	0.11
(1,352)	1:10:A:VAL:H	1:10:A:VAL:HG11	1	0.11
(1,352)	1:10:A:VAL:H	1:10:A:VAL:HG12	1	0.11
(1,352)	1:10:A:VAL:H	1:10:A:VAL:HG13	1	0.11
(1,336)	1:10:A:VAL:HG11	1:10:A:VAL:H	1	0.11
(1,336)	1:10:A:VAL:HG12	1:10:A:VAL:H	1	0.11
(1,336)	1:10:A:VAL:HG13	1:10:A:VAL:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:8:A:LEU:HD11	1:39:A:GLN:HB2	4	0.11
(1,244)	1:8:A:LEU:HD12	1:39:A:GLN:HB2	4	0.11
(1,244)	1:8:A:LEU:HD13	1:39:A:GLN:HB2	4	0.11
(1,244)	1:8:A:LEU:HD11	1:39:A:GLN:HB2	9	0.11
(1,244)	1:8:A:LEU:HD12	1:39:A:GLN:HB2	9	0.11
(1,244)	1:8:A:LEU:HD13	1:39:A:GLN:HB2	9	0.11
(1,205)	1:7:A:ASP:HA	1:4:A:ALA:H	9	0.11
(1,77)	1:3:A:ILE:HG21	1:39:B:GLN:HG2	8	0.11
(1,77)	1:3:A:ILE:HG21	1:39:B:GLN:HG3	8	0.11
(1,77)	1:3:A:ILE:HG22	1:39:B:GLN:HG2	8	0.11
(1,77)	1:3:A:ILE:HG22	1:39:B:GLN:HG3	8	0.11
(1,77)	1:3:A:ILE:HG23	1:39:B:GLN:HG2	8	0.11
(1,77)	1:3:A:ILE:HG23	1:39:B:GLN:HG3	8	0.11
(1,32)	1:2:A:VAL:HG11	1:1:A:FME:HG2	4	0.11
(1,32)	1:2:A:VAL:HG11	1:1:A:FME:HG3	4	0.11
(1,32)	1:2:A:VAL:HG12	1:1:A:FME:HG2	4	0.11
(1,32)	1:2:A:VAL:HG12	1:1:A:FME:HG3	4	0.11
(1,32)	1:2:A:VAL:HG13	1:1:A:FME:HG2	4	0.11
(1,32)	1:2:A:VAL:HG13	1:1:A:FME:HG3	4	0.11
(2,1405)	1:15:B:CYS:HA	1:17:B:ARG:HD2	20	0.1
(2,1375)	1:24:B:THR:HG22	1:22:B:GLU:HB2	8	0.1
(2,1189)	1:13:B:PRO:HG2	1:28:B:ALA:HB2	10	0.1
(2,1017)	1:13:B:PRO:HB2	1:21:B:ILE:HG22	6	0.1
(2,696)	1:15:B:CYS:HA	1:17:B:ARG:HD2	20	0.1
(2,572)	1:2:C:VAL:HG11	1:1:C:FME:HA	16	0.1
(2,568)	1:24:B:THR:HG22	1:22:B:GLU:HB2	8	0.1
(2,485)	1:51:C:LEU:HD11	1:47:B:ILE:HB	16	0.1
(2,483)	1:51:A:LEU:HD13	1:47:C:ILE:HB	9	0.1
(2,268)	1:51:C:LEU:HB2	1:52:C:ASN:HB2	9	0.1
(2,263)	1:49:A:LYS:HE2	1:53:A:LYS:HB3	5	0.1
(2,263)	1:49:A:LYS:HE2	1:53:A:LYS:HB3	7	0.1
(2,250)	1:14:C:LYS:HE2	1:22:C:GLU:HB2	13	0.1
(2,60)	1:3:B:ILE:H	1:2:B:VAL:HB	15	0.1
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD11	4	0.1
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD12	4	0.1
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD13	4	0.1
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD11	9	0.1
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD12	9	0.1
(1,5321)	1:53:C:LYS:H	1:51:A:LEU:HD13	9	0.1
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	2	0.1
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	9	0.1
(1,5314)	1:53:C:LYS:H	1:49:C:LYS:H	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	2	0.1
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	9	0.1
(1,5191)	1:49:C:LYS:H	1:53:C:LYS:H	10	0.1
(1,5110)	1:48:C:GLN:HB2	1:51:A:LEU:HD11	9	0.1
(1,5110)	1:48:C:GLN:HB2	1:51:A:LEU:HD12	9	0.1
(1,5110)	1:48:C:GLN:HB2	1:51:A:LEU:HD13	9	0.1
(1,5100)	1:48:C:GLN:HB3	1:49:C:LYS:HB3	6	0.1
(1,5057)	1:46:C:PHE:H	1:48:C:GLN:HB3	3	0.1
(1,5057)	1:46:C:PHE:H	1:48:C:GLN:HB3	5	0.1
(1,5015)	1:45:C:ASP:H	1:44:C:LEU:HG	12	0.1
(1,5015)	1:45:C:ASP:H	1:44:C:LEU:HG	13	0.1
(1,4983)	1:44:C:LEU:HG	1:45:C:ASP:H	12	0.1
(1,4983)	1:44:C:LEU:HG	1:45:C:ASP:H	13	0.1
(1,4883)	1:42:C:THR:H	1:38:C:ALA:HA	3	0.1
(1,4743)	1:38:C:ALA:HA	1:42:C:THR:HA	19	0.1
(1,4685)	1:36:C:LEU:HD21	1:44:C:LEU:HD21	10	0.1
(1,4685)	1:36:C:LEU:HD21	1:44:C:LEU:HD22	10	0.1
(1,4685)	1:36:C:LEU:HD21	1:44:C:LEU:HD23	10	0.1
(1,4685)	1:36:C:LEU:HD22	1:44:C:LEU:HD21	10	0.1
(1,4685)	1:36:C:LEU:HD22	1:44:C:LEU:HD22	10	0.1
(1,4685)	1:36:C:LEU:HD22	1:44:C:LEU:HD23	10	0.1
(1,4685)	1:36:C:LEU:HD23	1:44:C:LEU:HD21	10	0.1
(1,4685)	1:36:C:LEU:HD23	1:44:C:LEU:HD22	10	0.1
(1,4685)	1:36:C:LEU:HD23	1:44:C:LEU:HD23	10	0.1
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	3	0.1
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	10	0.1
(1,4589)	1:35:C:ILE:HA	1:11:C:ALA:HA	16	0.1
(1,4559)	1:34:C:VAL:HG11	1:11:C:ALA:HA	19	0.1
(1,4559)	1:34:C:VAL:HG12	1:11:C:ALA:HA	19	0.1
(1,4559)	1:34:C:VAL:HG13	1:11:C:ALA:HA	19	0.1
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA2	2	0.1
(1,4278)	1:24:C:THR:HB	1:23:C:GLY:HA3	2	0.1
(1,4258)	1:23:C:GLY:HA2	1:24:C:THR:HB	2	0.1
(1,4258)	1:23:C:GLY:HA3	1:24:C:THR:HB	2	0.1
(1,4193)	1:21:C:ILE:HD11	1:15:C:CYS:HA	12	0.1
(1,4193)	1:21:C:ILE:HD12	1:15:C:CYS:HA	12	0.1
(1,4193)	1:21:C:ILE:HD13	1:15:C:CYS:HA	12	0.1
(1,4048)	1:16:C:GLU:H	1:33:C:GLY:H	4	0.1
(1,4034)	1:16:C:GLU:HG2	1:11:C:ALA:HB1	15	0.1
(1,4034)	1:16:C:GLU:HG2	1:11:C:ALA:HB2	15	0.1
(1,4034)	1:16:C:GLU:HG2	1:11:C:ALA:HB3	15	0.1
(1,4034)	1:16:C:GLU:HG3	1:11:C:ALA:HB1	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4034)	1:16:C:GLU:HG3	1:11:C:ALA:HB2	15	0.1
(1,4034)	1:16:C:GLU:HG3	1:11:C:ALA:HB3	15	0.1
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG12	10	0.1
(1,3961)	1:13:C:PRO:HG2	1:21:C:ILE:HG13	10	0.1
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG12	10	0.1
(1,3961)	1:13:C:PRO:HG3	1:21:C:ILE:HG13	10	0.1
(1,3949)	1:12:C:CYS:H	1:34:C:VAL:HB	14	0.1
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	3	0.1
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	10	0.1
(1,3917)	1:11:C:ALA:HA	1:35:C:ILE:HA	16	0.1
(1,3801)	1:8:C:LEU:HD11	1:39:C:GLN:HB2	17	0.1
(1,3801)	1:8:C:LEU:HD12	1:39:C:GLN:HB2	17	0.1
(1,3801)	1:8:C:LEU:HD13	1:39:C:GLN:HB2	17	0.1
(1,3643)	1:3:C:ILE:HG21	1:39:A:GLN:HG2	2	0.1
(1,3643)	1:3:C:ILE:HG21	1:39:A:GLN:HG3	2	0.1
(1,3643)	1:3:C:ILE:HG22	1:39:A:GLN:HG2	2	0.1
(1,3643)	1:3:C:ILE:HG22	1:39:A:GLN:HG3	2	0.1
(1,3643)	1:3:C:ILE:HG23	1:39:A:GLN:HG2	2	0.1
(1,3643)	1:3:C:ILE:HG23	1:39:A:GLN:HG3	2	0.1
(1,3643)	1:3:C:ILE:HG21	1:39:A:GLN:HG2	7	0.1
(1,3643)	1:3:C:ILE:HG21	1:39:A:GLN:HG3	7	0.1
(1,3643)	1:3:C:ILE:HG22	1:39:A:GLN:HG2	7	0.1
(1,3643)	1:3:C:ILE:HG22	1:39:A:GLN:HG3	7	0.1
(1,3643)	1:3:C:ILE:HG23	1:39:A:GLN:HG2	7	0.1
(1,3643)	1:3:C:ILE:HG23	1:39:A:GLN:HG3	7	0.1
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD11	10	0.1
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD12	10	0.1
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD13	10	0.1
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD11	20	0.1
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD12	20	0.1
(1,3562)	1:53:B:LYS:H	1:51:C:LEU:HD13	20	0.1
(1,3555)	1:53:B:LYS:H	1:49:B:LYS:H	8	0.1
(1,3555)	1:53:B:LYS:H	1:49:B:LYS:H	20	0.1
(1,3432)	1:49:B:LYS:H	1:53:B:LYS:H	8	0.1
(1,3432)	1:49:B:LYS:H	1:53:B:LYS:H	20	0.1
(1,3299)	1:46:B:PHE:H	1:48:B:GLN:HB3	3	0.1
(1,3257)	1:45:B:ASP:H	1:44:B:LEU:HG	1	0.1
(1,3225)	1:44:B:LEU:HG	1:45:B:ASP:H	1	0.1
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB2	8	0.1
(1,2987)	1:38:B:ALA:HB1	1:1:A:FME:HB3	8	0.1
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB2	8	0.1
(1,2987)	1:38:B:ALA:HB2	1:1:A:FME:HB3	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB2	8	0.1
(1,2987)	1:38:B:ALA:HB3	1:1:A:FME:HB3	8	0.1
(1,2985)	1:38:B:ALA:HA	1:42:B:THR:HA	19	0.1
(1,2927)	1:36:B:LEU:HD21	1:44:B:LEU:HD21	15	0.1
(1,2927)	1:36:B:LEU:HD21	1:44:B:LEU:HD22	15	0.1
(1,2927)	1:36:B:LEU:HD21	1:44:B:LEU:HD23	15	0.1
(1,2927)	1:36:B:LEU:HD22	1:44:B:LEU:HD21	15	0.1
(1,2927)	1:36:B:LEU:HD22	1:44:B:LEU:HD22	15	0.1
(1,2927)	1:36:B:LEU:HD22	1:44:B:LEU:HD23	15	0.1
(1,2927)	1:36:B:LEU:HD23	1:44:B:LEU:HD21	15	0.1
(1,2927)	1:36:B:LEU:HD23	1:44:B:LEU:HD22	15	0.1
(1,2927)	1:36:B:LEU:HD23	1:44:B:LEU:HD23	15	0.1
(1,2831)	1:35:B:ILE:HA	1:11:B:ALA:HA	6	0.1
(1,2672)	1:30:B:SER:HA	1:32:B:LYS:HE2	7	0.1
(1,2672)	1:30:B:SER:HA	1:32:B:LYS:HE3	7	0.1
(1,2672)	1:30:B:SER:HA	1:32:B:LYS:HE2	8	0.1
(1,2672)	1:30:B:SER:HA	1:32:B:LYS:HE3	8	0.1
(1,2629)	1:28:B:ALA:H	1:30:B:SER:H	20	0.1
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG21	11	0.1
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG22	11	0.1
(1,2608)	1:27:B:PRO:HG2	1:21:B:ILE:HG23	11	0.1
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG21	11	0.1
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG22	11	0.1
(1,2608)	1:27:B:PRO:HG3	1:21:B:ILE:HG23	11	0.1
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA2	10	0.1
(1,2520)	1:24:B:THR:HB	1:23:B:GLY:HA3	10	0.1
(1,2500)	1:23:B:GLY:HA2	1:24:B:THR:HB	10	0.1
(1,2500)	1:23:B:GLY:HA3	1:24:B:THR:HB	10	0.1
(1,2408)	1:20:B:GLU:H	1:18:B:ALA:H	5	0.1
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG12	19	0.1
(1,2204)	1:13:B:PRO:HG2	1:21:B:ILE:HG13	19	0.1
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG12	19	0.1
(1,2204)	1:13:B:PRO:HG3	1:21:B:ILE:HG13	19	0.1
(1,2192)	1:12:B:CYS:H	1:34:B:VAL:HB	15	0.1
(1,2160)	1:11:B:ALA:HA	1:35:B:ILE:HA	6	0.1
(1,2044)	1:8:B:LEU:HD11	1:39:B:GLN:HB2	6	0.1
(1,2044)	1:8:B:LEU:HD12	1:39:B:GLN:HB2	6	0.1
(1,2044)	1:8:B:LEU:HD13	1:39:B:GLN:HB2	6	0.1
(1,1953)	1:5:B:THR:HG21	1:9:B:GLU:HB2	4	0.1
(1,1953)	1:5:B:THR:HG22	1:9:B:GLU:HB2	4	0.1
(1,1953)	1:5:B:THR:HG23	1:9:B:GLU:HB2	4	0.1
(1,1841)	1:2:B:VAL:HG11	1:3:B:ILE:HG21	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1841)	1:2:B:VAL:HG11	1:3:B:ILE:HG22	1	0.1
(1,1841)	1:2:B:VAL:HG11	1:3:B:ILE:HG23	1	0.1
(1,1841)	1:2:B:VAL:HG12	1:3:B:ILE:HG21	1	0.1
(1,1841)	1:2:B:VAL:HG12	1:3:B:ILE:HG22	1	0.1
(1,1841)	1:2:B:VAL:HG12	1:3:B:ILE:HG23	1	0.1
(1,1841)	1:2:B:VAL:HG13	1:3:B:ILE:HG21	1	0.1
(1,1841)	1:2:B:VAL:HG13	1:3:B:ILE:HG22	1	0.1
(1,1841)	1:2:B:VAL:HG13	1:3:B:ILE:HG23	1	0.1
(1,1800)	1:53:A:LYS:H	1:49:A:LYS:H	4	0.1
(1,1672)	1:49:A:LYS:H	1:53:A:LYS:H	4	0.1
(1,1557)	1:47:A:ILE:HG21	1:47:A:ILE:H	12	0.1
(1,1557)	1:47:A:ILE:HG22	1:47:A:ILE:H	12	0.1
(1,1557)	1:47:A:ILE:HG23	1:47:A:ILE:H	12	0.1
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	2	0.1
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	3	0.1
(1,1536)	1:46:A:PHE:H	1:48:A:GLN:HB3	5	0.1
(1,1491)	1:45:A:ASP:H	1:44:A:LEU:HG	13	0.1
(1,1457)	1:44:A:LEU:HG	1:45:A:ASP:H	13	0.1
(1,1263)	1:40:A:GLY:H	1:43:A:LEU:HB3	8	0.1
(1,1263)	1:40:A:GLY:H	1:43:A:LEU:HB3	16	0.1
(1,1263)	1:40:A:GLY:H	1:43:A:LEU:HB3	20	0.1
(1,1211)	1:38:A:ALA:HA	1:42:A:THR:HA	4	0.1
(1,1211)	1:38:A:ALA:HA	1:42:A:THR:HA	14	0.1
(1,1193)	1:37:A:THR:H	1:36:A:LEU:HG	17	0.1
(1,1043)	1:34:A:VAL:H	1:32:A:LYS:HA	1	0.1
(1,1043)	1:34:A:VAL:H	1:32:A:LYS:HA	13	0.1
(1,741)	1:24:A:THR:HG21	1:22:A:GLU:HG2	1	0.1
(1,741)	1:24:A:THR:HG21	1:22:A:GLU:HG3	1	0.1
(1,741)	1:24:A:THR:HG22	1:22:A:GLU:HG2	1	0.1
(1,741)	1:24:A:THR:HG22	1:22:A:GLU:HG3	1	0.1
(1,741)	1:24:A:THR:HG23	1:22:A:GLU:HG2	1	0.1
(1,741)	1:24:A:THR:HG23	1:22:A:GLU:HG3	1	0.1
(1,641)	1:21:A:ILE:HD11	1:13:A:PRO:HD2	8	0.1
(1,641)	1:21:A:ILE:HD11	1:13:A:PRO:HD3	8	0.1
(1,641)	1:21:A:ILE:HD12	1:13:A:PRO:HD2	8	0.1
(1,641)	1:21:A:ILE:HD12	1:13:A:PRO:HD3	8	0.1
(1,641)	1:21:A:ILE:HD13	1:13:A:PRO:HD2	8	0.1
(1,641)	1:21:A:ILE:HD13	1:13:A:PRO:HD3	8	0.1
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD2	5	0.1
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD3	5	0.1
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD2	12	0.1
(1,590)	1:20:A:GLU:HA	1:27:A:PRO:HD3	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,444)	1:15:A:CYS:HA	1:14:A:LYS:HG2	15	0.1
(1,444)	1:15:A:CYS:HA	1:14:A:LYS:HG3	15	0.1
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG12	16	0.1
(1,412)	1:13:A:PRO:HG2	1:21:A:ILE:HG13	16	0.1
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG12	16	0.1
(1,412)	1:13:A:PRO:HG3	1:21:A:ILE:HG13	16	0.1
(1,358)	1:10:A:VAL:H	1:36:A:LEU:HA	13	0.1
(1,244)	1:8:A:LEU:HD11	1:39:A:GLN:HB2	6	0.1
(1,244)	1:8:A:LEU:HD12	1:39:A:GLN:HB2	6	0.1
(1,244)	1:8:A:LEU:HD13	1:39:A:GLN:HB2	6	0.1
(1,77)	1:3:A:ILE:HG21	1:39:B:GLN:HG2	2	0.1
(1,77)	1:3:A:ILE:HG21	1:39:B:GLN:HG3	2	0.1
(1,77)	1:3:A:ILE:HG22	1:39:B:GLN:HG2	2	0.1
(1,77)	1:3:A:ILE:HG22	1:39:B:GLN:HG3	2	0.1
(1,77)	1:3:A:ILE:HG23	1:39:B:GLN:HG2	2	0.1
(1,77)	1:3:A:ILE:HG23	1:39:B:GLN:HG3	2	0.1
(1,77)	1:3:A:ILE:HG21	1:39:B:GLN:HG2	17	0.1
(1,77)	1:3:A:ILE:HG21	1:39:B:GLN:HG3	17	0.1
(1,77)	1:3:A:ILE:HG22	1:39:B:GLN:HG2	17	0.1
(1,77)	1:3:A:ILE:HG22	1:39:B:GLN:HG3	17	0.1
(1,77)	1:3:A:ILE:HG23	1:39:B:GLN:HG2	17	0.1
(1,77)	1:3:A:ILE:HG23	1:39:B:GLN:HG3	17	0.1

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

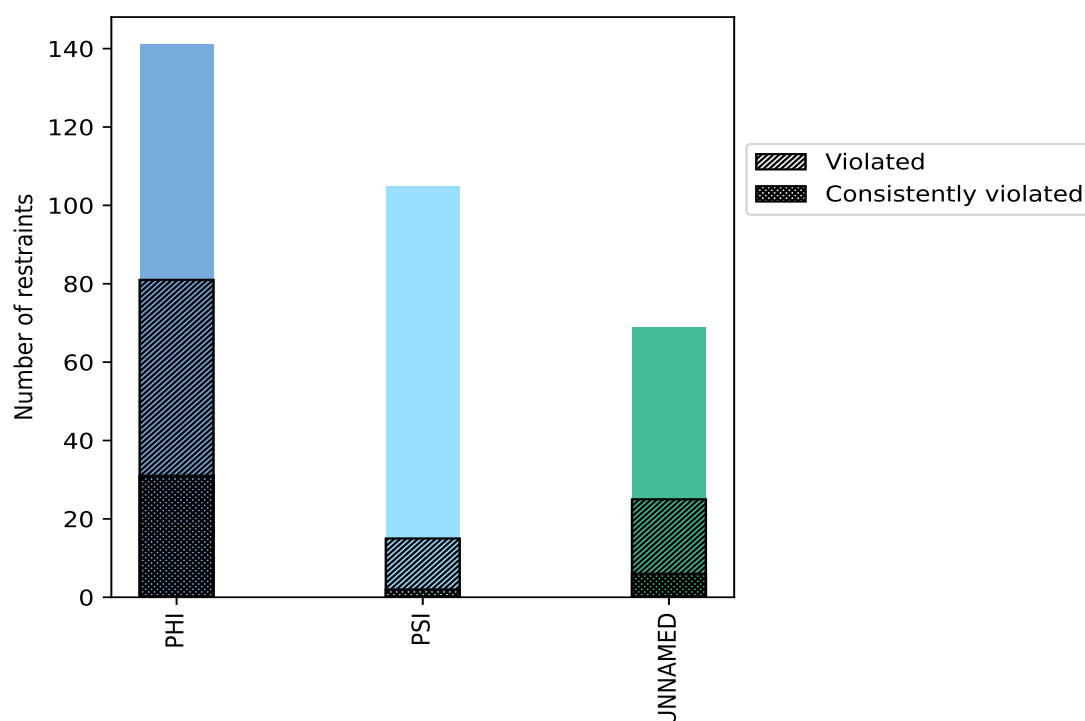
10.1 Summary of dihedral-angle violations [i](#)

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	141	44.8	81	57.4	25.7	31	22.0	9.8
PSI	105	33.3	15	14.3	4.8	2	1.9	0.6
UNNAMED	69	21.9	25	36.2	7.9	6	8.7	1.9
Total	315	100.0	121	38.4	38.4	39	12.4	12.4

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](#)



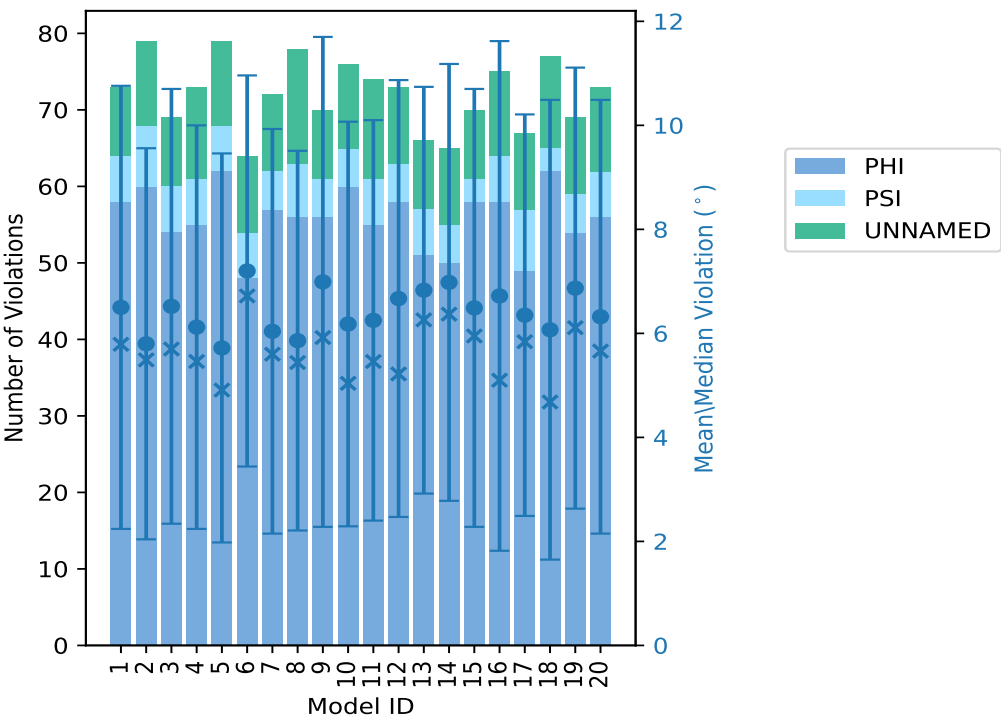
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	UNNAMED	Total				
1	58	6	9	73	6.5	18.88	4.26	5.79
2	60	8	11	79	5.8	15.66	3.76	5.49
3	54	6	9	69	6.52	16.99	4.18	5.7
4	55	6	12	73	6.12	15.25	3.88	5.46
5	62	6	11	79	5.72	16.37	3.74	4.91
6	48	6	10	64	7.2	17.04	3.76	6.72
7	57	5	10	72	6.04	16.28	3.89	5.6
8	56	7	15	78	5.86	14.88	3.65	5.44
9	56	5	9	70	6.99	18.23	4.71	5.92
10	60	5	11	76	6.18	15.08	3.89	5.04
11	55	6	13	74	6.25	15.34	3.85	5.46
12	58	5	10	73	6.67	17.1	4.2	5.22
13	51	6	9	66	6.83	17.25	3.91	6.26
14	50	5	10	65	6.98	17.62	4.2	6.37
15	58	3	9	70	6.49	15.8	4.21	5.95
16	58	6	11	75	6.72	20.56	4.9	5.1
17	49	8	10	67	6.35	16.68	3.86	5.84
18	62	3	12	77	6.07	17.0	4.42	4.68
19	54	5	10	69	6.87	18.53	4.24	6.11
20	56	6	11	73	6.32	18.35	4.17	5.66

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

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

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints				Fraction of the ensemble	
PHI	PSI	UNNAMED	Total	Count ¹	%
6	6	6	18	1	5.0
7	1	1	9	2	10.0
2	1	8	11	3	15.0
1	0	0	1	4	20.0
2	1	1	4	5	25.0
1	0	0	1	6	30.0
3	0	0	3	7	35.0
1	0	0	1	8	40.0
1	0	0	1	9	45.0
1	0	0	1	10	50.0
0	1	0	1	11	55.0

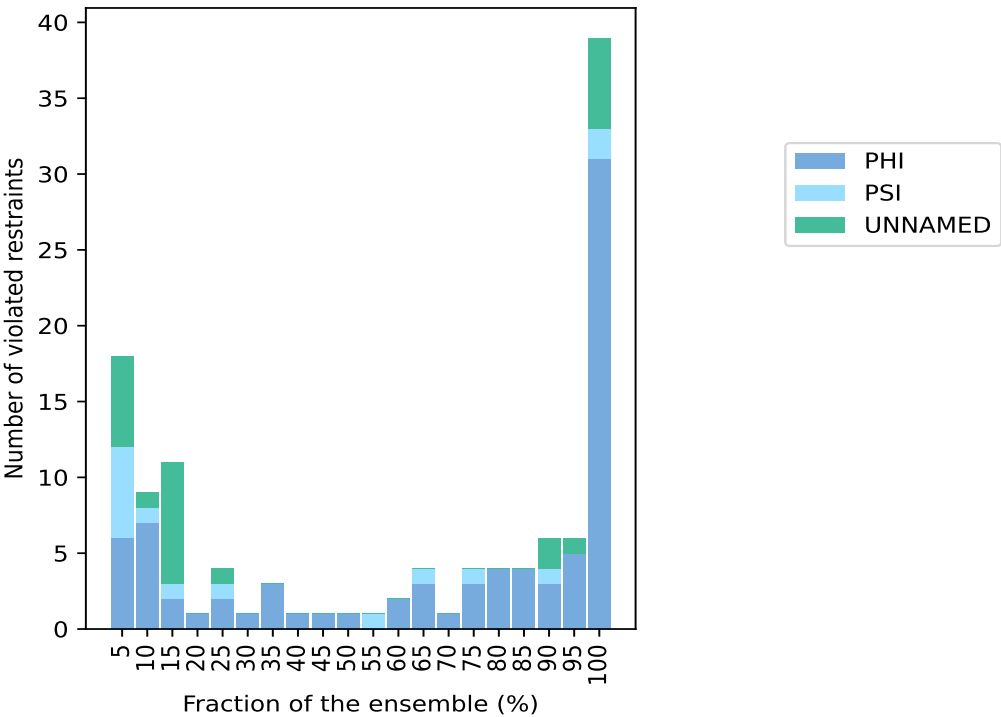
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Number of violated restraints				Fraction of the ensemble	
PHI	PSI	UNNAMED	Total	Count ¹	%
2	0	0	2	12	60.0
3	1	0	4	13	65.0
1	0	0	1	14	70.0
3	1	0	4	15	75.0
4	0	0	4	16	80.0
4	0	0	4	17	85.0
3	1	2	6	18	90.0
5	0	1	6	19	95.0
31	2	6	39	20	100.0

¹ Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

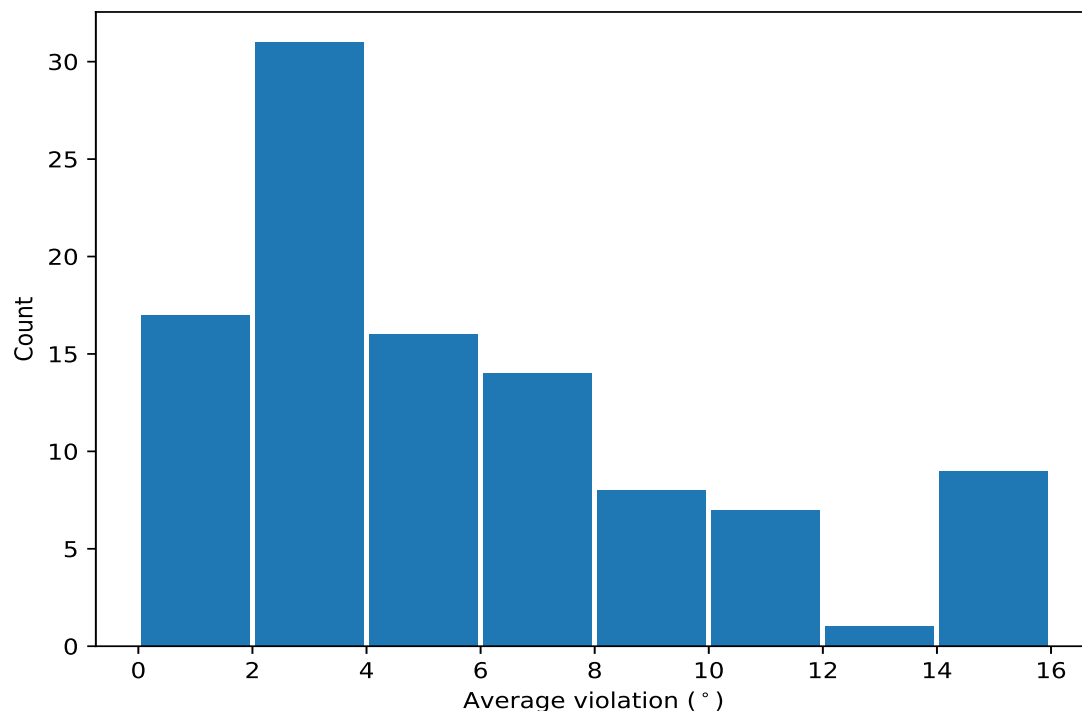


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	20	15.61	1.8	15.4
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	20	15.31	2.36	15.7
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	20	14.9	2.19	15.4
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	20	14.59	0.86	14.66
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	20	14.49	1.27	14.76
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	20	14.48	0.96	14.33
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	20	11.11	0.71	11.0
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	20	10.99	0.66	11.08
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	20	10.93	0.77	10.84
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	20	10.92	1.3	10.75
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	20	10.75	1.26	10.33
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	20	10.61	1.26	10.32
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	20	10.14	1.38	10.04
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	20	9.96	0.72	10.0
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	20	9.96	0.81	10.05
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	20	9.79	0.73	9.92
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	20	9.79	0.91	9.69
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	20	9.57	1.16	9.45
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	20	8.69	0.75	8.86
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	20	8.53	0.76	8.56

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	20	8.32	0.57	8.23
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	20	7.88	0.51	7.8
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	20	7.78	0.63	7.6
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	20	7.67	0.52	7.48
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	20	6.23	1.27	6.46
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	20	6.19	0.6	6.36
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	20	6.08	0.64	6.14
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	20	5.77	0.67	5.92
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	20	5.75	0.57	5.56
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	20	5.56	0.43	5.68
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	20	5.44	0.64	5.54
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	20	4.21	1.0	4.03
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	20	4.18	0.67	4.16
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	20	4.1	0.61	3.99
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	20	3.46	0.8	3.36
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	20	3.44	0.71	3.4
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	20	3.2	0.54	3.22
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	20	3.18	0.51	3.26
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	20	3.15	0.63	3.26
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	19	6.7	0.69	6.8
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	19	6.33	1.31	6.48
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	19	6.31	0.83	6.33
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	19	3.54	1.21	3.29
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	19	2.95	1.35	2.54
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	19	1.99	0.58	1.92
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	18	4.22	0.97	4.32
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	18	4.04	0.96	4.26
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	18	3.2	0.9	3.18
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	18	2.45	0.63	2.52
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	18	1.82	0.47	1.83
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	18	1.6	0.42	1.52
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	17	6.64	0.74	6.73
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	17	2.84	0.92	2.58
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	17	2.6	0.8	2.58
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	17	2.47	1.02	2.43
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	16	6.55	0.77	6.44
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	16	4.14	0.72	4.16
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	16	4.04	0.88	4.22
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	16	2.75	0.83	2.38
(1,200)	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1:35:B:ILE:N	15	5.78	1.27	6.25
(1,2)	1:1:B:FME:C	1:2:B:VAL:N	1:2:B:VAL:CA	1:2:B:VAL:C	15	2.77	1.16	2.62
(1,52)	1:25:A:PRO:C	1:26:A:CYS:N	1:26:A:CYS:CA	1:26:A:CYS:C	15	2.47	0.41	2.37
(1,38)	1:16:B:GLU:C	1:17:B:ARG:N	1:17:B:ARG:CA	1:17:B:ARG:C	15	2.34	1.1	2.17
(1,72)	1:35:C:ILE:C	1:36:C:LEU:N	1:36:C:LEU:CA	1:36:C:LEU:C	14	4.28	0.86	4.36
(1,201)	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	1:35:C:ILE:N	13	6.51	0.84	6.63
(1,70)	1:35:A:ILE:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	13	3.79	1.34	4.16
(1,41)	1:17:B:ARG:C	1:18:B:ALA:N	1:18:B:ALA:CA	1:18:B:ALA:C	13	2.08	0.77	1.79
(1,37)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	13	1.93	0.72	1.81
(1,40)	1:17:A:ARG:C	1:18:A:ALA:N	1:18:A:ALA:CA	1:18:A:ALA:C	12	2.34	1.11	2.0
(1,39)	1:16:C:GLU:C	1:17:C:ARG:N	1:17:C:ARG:CA	1:17:C:ARG:C	12	1.68	0.6	1.42
(1,199)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:ILE:N	11	6.61	1.1	6.81

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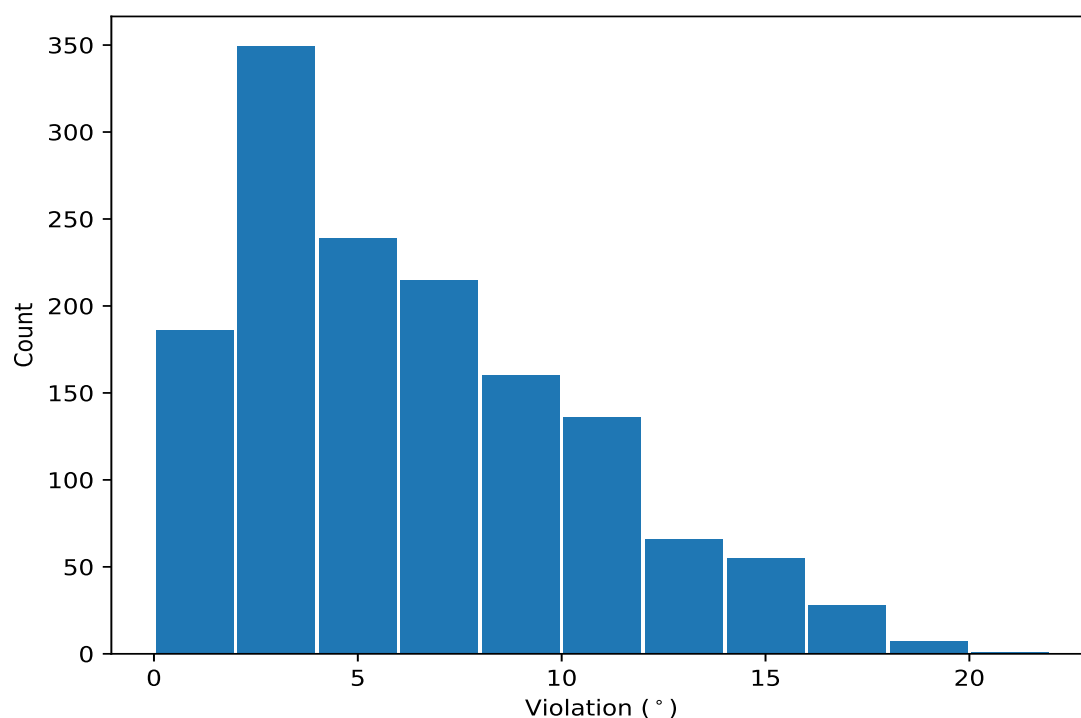
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,42)	1:17:C:ARG:C	1:18:C:ALA:N	1:18:C:ALA:CA	1:18:C:ALA:C	10	2.15	0.91	1.81
(1,67)	1:34:A:VAL:C	1:35:A:ILE:N	1:35:A:ILE:CA	1:35:A:ILE:C	9	14.21	3.38	16.28
(1,66)	1:33:C:GLY:C	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	8	1.62	0.5	1.42
(1,69)	1:34:C:VAL:C	1:35:C:ILE:N	1:35:C:ILE:CA	1:35:C:ILE:C	7	14.2	1.94	13.92
(1,22)	1:9:A:GLU:C	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	7	5.05	3.12	6.17
(1,34)	1:15:A:CYS:C	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	7	2.54	1.02	2.51
(1,35)	1:15:B:CYS:C	1:16:B:GLU:N	1:16:B:GLU:CA	1:16:B:GLU:C	6	3.48	2.18	2.99
(1,68)	1:34:B:VAL:C	1:35:B:ILE:N	1:35:B:ILE:CA	1:35:B:ILE:C	5	14.84	1.81	14.53
(1,160)	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	1:11:A:ALA:N	5	3.37	0.75	2.94
(1,36)	1:15:C:CYS:C	1:16:C:GLU:N	1:16:C:GLU:CA	1:16:C:GLU:C	5	2.49	0.89	2.37
(1,297)	1:43:C:LEU:HA	1:43:C:LEU:CA	1:43:C:LEU:CB	1:43:C:LEU:HB3	5	1.59	0.43	1.61
(1,23)	1:9:B:GLU:C	1:10:B:VAL:N	1:10:B:VAL:CA	1:10:B:VAL:C	4	6.42	2.14	6.91
(1,161)	1:10:B:VAL:N	1:10:B:VAL:CA	1:10:B:VAL:C	1:11:B:ALA:N	3	3.18	0.45	3.38
(1,16)	1:7:A:ASP:C	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	3	2.21	0.41	2.01
(1,18)	1:7:C:ASP:C	1:8:C:LEU:N	1:8:C:LEU:CA	1:8:C:LEU:C	3	2.1	0.64	2.47
(1,273)	1:22:C:GLU:HA	1:22:C:GLU:CA	1:22:C:GLU:CB	1:22:C:GLU:HB3	3	1.5	0.35	1.6
(1,292)	1:41:A:TYR:HA	1:41:A:TYR:CA	1:41:A:TYR:CB	1:41:A:TYR:HB3	3	1.48	0.25	1.39
(1,282)	1:29:C:CYS:HA	1:29:C:CYS:CA	1:29:C:CYS:CB	1:29:C:CYS:HB3	3	1.42	0.24	1.43
(1,272)	1:22:B:GLU:HA	1:22:B:GLU:CA	1:22:B:GLU:CB	1:22:B:GLU:HB3	3	1.37	0.26	1.48
(1,296)	1:43:B:LEU:HA	1:43:B:LEU:CA	1:43:B:LEU:CB	1:43:B:LEU:HB3	3	1.35	0.23	1.2
(1,293)	1:41:B:TYR:HA	1:41:B:TYR:CA	1:41:B:TYR:CB	1:41:B:TYR:HB3	3	1.19	0.13	1.12
(1,294)	1:41:C:TYR:HA	1:41:C:TYR:CA	1:41:C:TYR:CB	1:41:C:TYR:HB3	3	1.17	0.04	1.18
(1,295)	1:43:A:LEU:HA	1:43:A:LEU:CA	1:43:A:LEU:CB	1:43:A:LEU:HB3	3	1.12	0.04	1.14
(1,97)	1:48:A:GLN:C	1:49:A:LYS:N	1:49:A:LYS:CA	1:49:A:LYS:C	2	12.16	0.02	12.16
(1,24)	1:9:C:GLU:C	1:10:C:VAL:N	1:10:C:VAL:CA	1:10:C:VAL:C	2	4.62	3.51	4.62
(1,157)	1:9:A:GLU:N	1:9:A:GLU:CA	1:9:A:GLU:C	1:10:A:VAL:N	2	4.5	0.16	4.5
(1,313)	1:53:A:LYS:HA	1:53:A:LYS:CA	1:53:A:LYS:CB	1:53:A:LYS:HB3	2	3.69	0.12	3.69
(1,64)	1:33:A:GLY:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	2	2.49	0.43	2.49
(1,106)	1:51:A:LEU:C	1:52:A:ASN:N	1:52:A:ASN:CA	1:52:A:ASN:C	2	2.12	0.08	2.12
(1,17)	1:7:B:ASP:C	1:8:B:LEU:N	1:8:B:LEU:CA	1:8:B:LEU:C	2	2.08	0.39	2.08
(1,19)	1:8:A:LEU:C	1:9:A:GLU:N	1:9:A:GLU:CA	1:9:A:GLU:C	2	1.98	0.38	1.98
(1,87)	1:43:C:LEU:C	1:44:C:LEU:N	1:44:C:LEU:CA	1:44:C:LEU:C	2	1.63	0.07	1.63

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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 (°)
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	16	20.56
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	1	18.88
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	19	18.53
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	20	18.35
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	9	18.23
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	16	18.2
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	19	18.11
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	16	18.02
(1,67)	1:34:A:VAL:C	1:35:A:ILE:N	1:35:A:ILE:CA	1:35:A:ILE:C	9	17.94
(1,69)	1:34:C:VAL:C	1:35:C:ILE:N	1:35:C:ILE:CA	1:35:C:ILE:C	9	17.85
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	14	17.62
(1,68)	1:34:B:VAL:C	1:35:B:ILE:N	1:35:B:ILE:CA	1:35:B:ILE:C	16	17.53
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	9	17.51
(1,67)	1:34:A:VAL:C	1:35:A:ILE:N	1:35:A:ILE:CA	1:35:A:ILE:C	14	17.43
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	13	17.25
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	14	17.15
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	12	17.1
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	6	17.04
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	18	17.0
(1,67)	1:34:A:VAL:C	1:35:A:ILE:N	1:35:A:ILE:CA	1:35:A:ILE:C	3	16.99
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	12	16.79

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	17	16.68
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	13	16.58
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	20	16.52
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	1	16.43
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1	16.38
(1,67)	1:34:A:VAL:C	1:35:A:ILE:N	1:35:A:ILE:CA	1:35:A:ILE:C	5	16.37
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	9	16.32
(1,67)	1:34:A:VAL:C	1:35:A:ILE:N	1:35:A:ILE:CA	1:35:A:ILE:C	7	16.28
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	12	16.2
(1,68)	1:34:B:VAL:C	1:35:B:ILE:N	1:35:B:ILE:CA	1:35:B:ILE:C	12	16.2
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	3	16.15
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	18	16.12
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	20	16.12
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	18	16.11
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	9	16.09
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	6	15.99
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	17	15.96
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	20	15.94
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1	15.94
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	17	15.87
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	15	15.8
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	6	15.74
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	19	15.67
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	2	15.66
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1	15.66
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	20	15.59
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	19	15.59
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	14	15.57
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	12	15.56
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	2	15.54
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	15	15.49
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	3	15.45
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	14	15.4
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	11	15.34
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	14	15.3
(1,69)	1:34:C:VAL:C	1:35:C:ILE:N	1:35:C:ILE:CA	1:35:C:ILE:C	4	15.25
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	16	15.21
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	19	15.19
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	11	15.19
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	7	15.17
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	20	15.09
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	4	15.09
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	6	15.08
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	10	15.08
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	2	14.99
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	3	14.98
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	13	14.92
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1	14.91
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	8	14.88
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	19	14.77
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	6	14.75

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	10	14.75
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	7	14.74
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	11	14.67
(1,69)	1:34:C:VAL:C	1:35:C:ILE:N	1:35:C:ILE:CA	1:35:C:ILE:C	12	14.56
(1,68)	1:34:B:VAL:C	1:35:B:ILE:N	1:35:B:ILE:CA	1:35:B:ILE:C	18	14.53
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	15	14.51
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	8	14.45
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	13	14.43
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	13	14.42
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	3	14.38
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	10	14.38
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	4	14.28
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	4	14.28
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	3	14.25
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	15	14.17
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	7	14.15
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	13	14.07
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	5	14.06
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	6	14.06
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	9	13.98
(1,69)	1:34:C:VAL:C	1:35:C:ILE:N	1:35:C:ILE:CA	1:35:C:ILE:C	18	13.92
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	11	13.88
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	11	13.88
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	18	13.88
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	5	13.86
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	8	13.79
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	16	13.77
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	5	13.77
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	15	13.73
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	14	13.69
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	18	13.69
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	10	13.69
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	5	13.63
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	16	13.62
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	16	13.61
(1,69)	1:34:C:VAL:C	1:35:C:ILE:N	1:35:C:ILE:CA	1:35:C:ILE:C	15	13.58
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	7	13.55
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	9	13.54
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	17	13.54
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	8	13.49
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	4	13.47
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	11	13.44
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	4	13.43
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	16	13.35
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	18	13.31
(1,69)	1:34:C:VAL:C	1:35:C:ILE:N	1:35:C:ILE:CA	1:35:C:ILE:C	10	13.29
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	8	13.24
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	9	13.23
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	15	13.21
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	10	13.18
(1,100)	1:49:A:LYS:C	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	12	13.17

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,68)	1:34:B:VAL:C	1:35:B:ILE:N	1:35:B:ILE:CA	1:35:B:ILE:C	10	13.17
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	10	13.13
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	3	13.08
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	9	13.06
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	3	12.98
(1,67)	1:34:A:VAL:C	1:35:A:ILE:N	1:35:A:ILE:CA	1:35:A:ILE:C	16	12.97
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	8	12.96
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	4	12.87
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	2	12.86
(1,101)	1:49:B:LYS:C	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	18	12.83
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	7	12.81
(1,33)	1:14:C:LYS:C	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	2	12.78
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	7	12.78
(1,68)	1:34:B:VAL:C	1:35:B:ILE:N	1:35:B:ILE:CA	1:35:B:ILE:C	15	12.76
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	5	12.71
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	17	12.67
(1,179)	1:21:B:ILE:N	1:21:B:ILE:CA	1:21:B:ILE:C	1:22:B:GLU:N	2	12.66
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	2	12.66
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	16	12.63
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	10	12.44
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	18	12.41
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	3	12.32
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	9	12.32
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	19	12.32
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	5	12.23
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	16	12.21
(1,97)	1:48:A:GLN:C	1:49:A:LYS:N	1:49:A:LYS:CA	1:49:A:LYS:C	11	12.18
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	16	12.18
(1,97)	1:48:A:GLN:C	1:49:A:LYS:N	1:49:A:LYS:CA	1:49:A:LYS:C	18	12.13
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	3	12.11
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	17	12.1
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	16	12.06
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	16	12.06
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	19	12.02
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	11	11.87
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	2	11.87
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	15	11.83
(1,102)	1:49:C:LYS:C	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	12	11.82
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	19	11.75
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	8	11.75
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	12	11.74
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	6	11.69
(1,67)	1:34:A:VAL:C	1:35:A:ILE:N	1:35:A:ILE:CA	1:35:A:ILE:C	15	11.66
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	13	11.59
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	12	11.58
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	9	11.58
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	17	11.52
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	1	11.51
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	11	11.51
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	16	11.48
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	4	11.46

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	15	11.46
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	20	11.46
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	10	11.42
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	15	11.39
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	6	11.39
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	1	11.38
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	11	11.32
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	13	11.31
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	12	11.29
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	15	11.29
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	9	11.26
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	12	11.25
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	6	11.24
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	10	11.24
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	17	11.19
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	1	11.18
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	18	11.17
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	4	11.16
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	8	11.12
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	15	11.1
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	13	11.09
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	19	11.07
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	16	11.07
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	11	11.05
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	9	11.05
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	13	11.04
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	18	11.03
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	5	11.01
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	14	11.01
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	2	11.0
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	9	11.0
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	18	10.99
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	10	10.99
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	12	10.99
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	12	10.98
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	17	10.98
(1,69)	1:34:C:VAL:C	1:35:C:ILE:N	1:35:C:ILE:CA	1:35:C:ILE:C	19	10.98
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	19	10.93
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	5	10.92
(1,31)	1:14:A:LYS:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	5	10.9
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	2	10.87
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	1	10.87
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	11	10.85
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	20	10.84
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	4	10.83
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	1	10.81
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	9	10.8
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	16	10.78
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	1	10.77
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	8	10.77
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	4	10.77

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	19	10.77
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	8	10.73
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	3	10.71
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	3	10.71
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	20	10.7
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	12	10.68
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	16	10.65
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	12	10.64
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	18	10.63
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	7	10.6
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	7	10.58
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	8	10.57
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	1	10.56
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	19	10.56
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	13	10.54
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	12	10.54
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	18	10.54
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	14	10.53
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	13	10.5
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	19	10.49
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	15	10.49
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	20	10.47
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	17	10.47
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	17	10.45
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	19	10.44
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	7	10.43
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	7	10.42
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	16	10.42
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	3	10.41
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	13	10.4
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	3	10.39
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	6	10.38
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	14	10.37
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	6	10.35
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	1	10.35
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	19	10.34
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	10	10.33
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	18	10.33
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	15	10.32
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	5	10.31
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	6	10.29
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	2	10.27
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	20	10.25
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	14	10.24
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	15	10.24
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	14	10.23
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	1	10.23
(1,67)	1:34:A:VAL:C	1:35:A:ILE:N	1:35:A:ILE:CA	1:35:A:ILE:C	8	10.23
(1,32)	1:14:B:LYS:C	1:15:B:CYS:N	1:15:B:CYS:CA	1:15:B:CYS:C	5	10.21
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	9	10.2
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	1	10.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	8	10.18
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	6	10.18
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	20	10.17
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	20	10.17
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	13	10.16
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	6	10.15
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	7	10.12
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	12	10.12
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	8	10.1
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	4	10.08
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	17	10.06
(1,259)	1:13:A:PRO:HA	1:13:A:PRO:CA	1:13:A:PRO:CB	1:13:A:PRO:HB3	9	10.04
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	14	10.04
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	14	10.04
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	4	10.03
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	14	10.0
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	9	10.0
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	10	9.99
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	7	9.99
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	16	9.98
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	3	9.98
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	11	9.97
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	4	9.97
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	11	9.97
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	7	9.96
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	3	9.96
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	13	9.95
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	20	9.95
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	6	9.94
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	1	9.94
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	14	9.93
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	14	9.91
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	16	9.9
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	10	9.89
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	20	9.89
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	11	9.87
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	4	9.87
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	18	9.84
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	13	9.84
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	17	9.82
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	6	9.82
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	19	9.81
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	15	9.8
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	9	9.79
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	19	9.76
(1,260)	1:13:B:PRO:HA	1:13:B:PRO:CA	1:13:B:PRO:CB	1:13:B:PRO:HB3	14	9.75
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	5	9.72
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	12	9.71
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	11	9.7
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	7	9.69
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	9	9.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	16	9.69
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	20	9.69
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	10	9.68
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	14	9.66
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	15	9.66
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	10	9.64
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	6	9.63
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	9	9.61
(1,261)	1:13:C:PRO:HA	1:13:C:PRO:CA	1:13:C:PRO:CB	1:13:C:PRO:HB3	2	9.59
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	5	9.56
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	15	9.5
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	5	9.48
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	14	9.42
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	17	9.4
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	6	9.4
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	13	9.34
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	10	9.33
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	3	9.3
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	1	9.29
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	3	9.29
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	3	9.29
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	11	9.27
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	18	9.25
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	1	9.24
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	4	9.23
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	17	9.2
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	7	9.2
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	20	9.19
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	4	9.16
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	1	9.15
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	1	9.15
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	18	9.14
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	15	9.13
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	18	9.13
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	3	9.13
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	17	9.12
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	11	9.11
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	2	9.11
(1,22)	1:9:A:GLU:C	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	15	9.1
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	4	9.09
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	20	9.08
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	13	9.06
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	9	9.06
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	20	9.06
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	2	9.05
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	17	9.05
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	20	9.03
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	13	9.01
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	6	8.99
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	7	8.99
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	13	8.98

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	10	8.98
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	2	8.97
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	4	8.97
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	2	8.95
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	8	8.93
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	11	8.9
(1,84)	1:42:C:THR:C	1:43:C:LEU:N	1:43:C:LEU:CA	1:43:C:LEU:C	12	8.9
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	8	8.9
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	6	8.89
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	19	8.89
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	7	8.84
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	3	8.83
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	20	8.83
(1,82)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	5	8.81
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	8	8.81
(1,23)	1:9:B:GLU:C	1:10:B:VAL:N	1:10:B:VAL:CA	1:10:B:VAL:C	4	8.76
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	7	8.75
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	12	8.73
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1	8.73
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	8	8.71
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	6	8.7
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	5	8.7
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	2	8.68
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	10	8.67
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	4	8.65
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	8	8.64
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	5	8.62
(1,78)	1:40:C:GLY:C	1:41:C:TYR:N	1:41:C:TYR:CA	1:41:C:TYR:C	5	8.62
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	19	8.61
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	16	8.6
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	16	8.59
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	7	8.59
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	16	8.58
(1,199)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:ILE:N	6	8.58
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	11	8.57
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	2	8.57
(1,77)	1:40:B:GLY:C	1:41:B:TYR:N	1:41:B:TYR:CA	1:41:B:TYR:C	17	8.54
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	10	8.51
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	3	8.51
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	2	8.46
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	5	8.45
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	15	8.45
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	11	8.42
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	19	8.42
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	14	8.4
(1,22)	1:9:A:GLU:C	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	12	8.37
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	1	8.35
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	14	8.35
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	5	8.31
(1,83)	1:42:B:THR:C	1:43:B:LEU:N	1:43:B:LEU:CA	1:43:B:LEU:C	18	8.28
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	17	8.27

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	10	8.27
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	19	8.26
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	15	8.22
(1,92)	1:45:B:ASP:C	1:46:B:PHE:N	1:46:B:PHE:CA	1:46:B:PHE:C	7	8.21
(1,76)	1:40:A:GLY:C	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:C	2	8.2
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	2	8.19
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	9	8.17
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	15	8.17
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	12	8.16
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	1	8.14
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	20	8.14
(1,24)	1:9:C:GLU:C	1:10:C:VAL:N	1:10:C:VAL:CA	1:10:C:VAL:C	17	8.13
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	13	8.12
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	18	8.1
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	12	8.09
(1,67)	1:34:A:VAL:C	1:35:A:ILE:N	1:35:A:ILE:CA	1:35:A:ILE:C	10	8.06
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	4	8.05
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	13	8.05
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	8	8.04
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	2	8.03
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	18	8.02
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	17	8.02
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	9	8.01
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	8	8.01
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	1	7.99
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	11	7.98
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	19	7.98
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	10	7.96
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	17	7.95
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	12	7.92
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	1	7.92
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	6	7.9
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	10	7.9
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	15	7.89
(1,201)	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	1:35:C:ILE:N	6	7.88
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	15	7.87
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	18	7.87
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	3	7.86
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	11	7.85
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	6	7.85
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	18	7.82
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	11	7.82
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	13	7.8
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	13	7.77
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	11	7.77
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	3	7.76
(1,23)	1:9:B:GLU:C	1:10:B:VAL:N	1:10:B:VAL:CA	1:10:B:VAL:C	11	7.76
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	12	7.72
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	10	7.71
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	16	7.71
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	13	7.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	4	7.69
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	5	7.69
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	12	7.66
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	7	7.65
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	19	7.63
(1,93)	1:45:C:ASP:C	1:46:C:PHE:N	1:46:C:PHE:CA	1:46:C:PHE:C	8	7.59
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	17	7.58
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	4	7.56
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	2	7.56
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	5	7.56
(1,199)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:ILE:N	20	7.55
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	2	7.54
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	10	7.53
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	1	7.53
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	10	7.51
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	18	7.5
(1,91)	1:45:A:ASP:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	17	7.5
(1,200)	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1:35:B:ILE:N	6	7.49
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	5	7.48
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	7	7.47
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	16	7.47
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	9	7.46
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	7	7.44
(1,201)	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	1:35:C:ILE:N	20	7.41
(1,89)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	15	7.4
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	6	7.39
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	8	7.38
(1,199)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:ILE:N	18	7.37
(1,199)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:ILE:N	4	7.36
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	5	7.35
(1,199)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:ILE:N	11	7.35
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	7	7.34
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	6	7.34
(1,201)	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	1:35:C:ILE:N	8	7.34
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	19	7.32
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	14	7.32
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	12	7.31
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	8	7.29
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	6	7.29
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	19	7.28
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	20	7.27
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	6	7.27
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	14	7.26
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	14	7.26
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	14	7.25
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	9	7.25
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	13	7.24
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	16	7.24
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	4	7.23
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	13	7.22
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	14	7.22

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	6	7.22
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	13	7.22
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	8	7.2
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	1	7.2
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	17	7.17
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	19	7.17
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	3	7.17
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	2	7.16
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	19	7.14
(1,278)	1:27:B:PRO:HA	1:27:B:PRO:CA	1:27:B:PRO:CB	1:27:B:PRO:HB3	20	7.13
(1,201)	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	1:35:C:ILE:N	17	7.12
(1,35)	1:15:B:CYS:C	1:16:B:GLU:N	1:16:B:GLU:CA	1:16:B:GLU:C	19	7.12
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	9	7.12
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	9	7.07
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	9	7.07
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	20	7.04
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	4	7.02
(1,200)	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1:35:B:ILE:N	13	7.0
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	15	7.0
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	14	6.99
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	12	6.99
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	1	6.98
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	7	6.96
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	20	6.92
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	3	6.92
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	17	6.91
(1,277)	1:27:A:PRO:HA	1:27:A:PRO:CA	1:27:A:PRO:CB	1:27:A:PRO:HB3	4	6.9
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	16	6.9
(1,201)	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	1:35:C:ILE:N	2	6.89
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	3	6.89
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	17	6.87
(1,22)	1:9:A:GLU:C	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	17	6.87
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	4	6.86
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	15	6.85
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	4	6.85
(1,90)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	8	6.84
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	2	6.83
(1,200)	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1:35:B:ILE:N	7	6.82
(1,279)	1:27:C:PRO:HA	1:27:C:PRO:CA	1:27:C:PRO:CB	1:27:C:PRO:HB3	3	6.81
(1,199)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:ILE:N	19	6.81
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	1	6.8
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	15	6.8
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	6	6.79
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	14	6.79
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	10	6.77
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	5	6.75
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	18	6.74
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	11	6.74
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	8	6.73
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	10	6.73
(1,88)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	17	6.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	2	6.68
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	13	6.67
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	14	6.67
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	6	6.65
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	11	6.65
(1,201)	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	1:35:C:ILE:N	11	6.64
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	16	6.64
(1,201)	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	1:35:C:ILE:N	7	6.63
(1,200)	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1:35:B:ILE:N	1	6.62
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	9	6.62
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	12	6.62
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	2	6.61
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	3	6.6
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	13	6.59
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	19	6.58
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	6	6.55
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	14	6.53
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	6	6.53
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	20	6.53
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	2	6.53
(1,200)	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1:35:B:ILE:N	9	6.51
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	8	6.51
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	8	6.48
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	7	6.48
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	20	6.47
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	10	6.46
(1,200)	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1:35:B:ILE:N	20	6.45
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	2	6.45
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	17	6.45
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	9	6.45
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	16	6.45
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	18	6.45
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	11	6.43
(1,201)	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	1:35:C:ILE:N	13	6.41
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	5	6.41
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	10	6.41
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	3	6.4
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	10	6.39
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	20	6.39
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	10	6.38
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	5	6.38
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	14	6.38
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	14	6.37
(1,200)	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1:35:B:ILE:N	19	6.33
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	8	6.33
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	9	6.32
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	18	6.31
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	8	6.3
(1,199)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:ILE:N	13	6.29
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	20	6.27
(1,200)	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1:35:B:ILE:N	8	6.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	13	6.23
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	20	6.22
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	1	6.2
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	15	6.2
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	4	6.19
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	11	6.19
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	6	6.19
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	7	6.18
(1,201)	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	1:35:C:ILE:N	14	6.17
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	3	6.17
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	17	6.17
(1,22)	1:9:A:GLU:C	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	2	6.17
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	10	6.16
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	2	6.15
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	1	6.14
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	19	6.13
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	4	6.13
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	16	6.12
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	5	6.11
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	19	6.11
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	18	6.08
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	19	6.08
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	15	6.08
(1,200)	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1:35:B:ILE:N	17	6.07
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	11	6.07
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	13	6.07
(1,200)	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1:35:B:ILE:N	2	6.06
(1,23)	1:9:B:GLU:C	1:10:B:VAL:N	1:10:B:VAL:CA	1:10:B:VAL:C	5	6.06
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	1	6.04
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	14	6.03
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	2	6.03
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	11	6.02
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	4	6.01
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	12	6.0
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	15	6.0
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	3	5.99
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	9	5.98
(1,200)	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1:35:B:ILE:N	14	5.97
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	12	5.97
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	5	5.97
(1,201)	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	1:35:C:ILE:N	3	5.96
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	7	5.96
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	18	5.96
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	15	5.96
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	15	5.94
(1,72)	1:35:C:ILE:C	1:36:C:LEU:N	1:36:C:LEU:CA	1:36:C:LEU:C	13	5.93
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	20	5.92
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	13	5.91
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	8	5.89
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	11	5.88
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	1	5.88

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	8	5.87
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	9	5.85
(1,47)	1:20:B:GLU:C	1:21:B:ILE:N	1:21:B:ILE:CA	1:21:B:ILE:C	2	5.84
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	17	5.84
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	1	5.83
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	3	5.82
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	12	5.82
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	2	5.81
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	16	5.81
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	18	5.81
(1,201)	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	1:35:C:ILE:N	5	5.8
(1,199)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:ILE:N	17	5.8
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	20	5.8
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	7	5.8
(1,201)	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	1:35:C:ILE:N	1	5.79
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	16	5.79
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	5	5.77
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	8	5.77
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	15	5.75
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	4	5.75
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	8	5.75
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	5	5.74
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	2	5.72
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	3	5.7
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	16	5.69
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	14	5.69
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	8	5.68
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	5	5.68
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	10	5.68
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	9	5.68
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	13	5.68
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	12	5.67
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	20	5.66
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	14	5.65
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	9	5.65
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	17	5.64
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	11	5.63
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	7	5.63
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	7	5.62
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	7	5.62
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	6	5.62
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	5	5.61
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	7	5.61
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	3	5.61
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	2	5.6
(1,70)	1:35:A:ILE:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	19	5.59
(1,27)	1:10:C:VAL:C	1:11:C:ALA:N	1:11:C:ALA:CA	1:11:C:ALA:C	7	5.59
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	7	5.58
(1,26)	1:10:B:VAL:C	1:11:B:ALA:N	1:11:B:ALA:CA	1:11:B:ALA:C	8	5.58
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	11	5.58
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	12	5.55

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,199)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:ILE:N	1	5.54
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	15	5.53
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	18	5.53
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	10	5.52
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	18	5.52
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	4	5.5
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	13	5.5
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	17	5.49
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	2	5.49
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	4	5.47
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	4	5.46
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	18	5.44
(1,35)	1:15:B:CYS:C	1:16:B:GLU:N	1:16:B:GLU:CA	1:16:B:GLU:C	12	5.44
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	17	5.44
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	14	5.43
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	1	5.41
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	6	5.37
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	14	5.36
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	6	5.36
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	2	5.35
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	17	5.35
(1,199)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:ILE:N	2	5.33
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	11	5.33
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	5	5.32
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	1	5.31
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	13	5.31
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	16	5.3
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	8	5.3
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	7	5.3
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	11	5.28
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	11	5.28
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	14	5.27
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	5	5.27
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	7	5.26
(1,72)	1:35:C:ILE:C	1:36:C:LEU:N	1:36:C:LEU:CA	1:36:C:LEU:C	20	5.25
(1,25)	1:10:A:VAL:C	1:11:A:ALA:N	1:11:A:ALA:CA	1:11:A:ALA:C	8	5.25
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	15	5.23
(1,72)	1:35:C:ILE:C	1:36:C:LEU:N	1:36:C:LEU:CA	1:36:C:LEU:C	6	5.22
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	9	5.22
(1,38)	1:16:B:GLU:C	1:17:B:ARG:N	1:17:B:ARG:CA	1:17:B:ARG:C	12	5.22
(1,40)	1:17:A:ARG:C	1:18:A:ALA:N	1:18:A:ALA:CA	1:18:A:ALA:C	19	5.19
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	6	5.19
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	5	5.15
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	11	5.15
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	19	5.15
(1,2)	1:1:B:FME:C	1:2:B:VAL:N	1:2:B:VAL:CA	1:2:B:VAL:C	14	5.15
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	4	5.14
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	10	5.13
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	20	5.12
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	16	5.1
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	17	5.09

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	13	5.09
(1,70)	1:35:A:ILE:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	12	5.09
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	2	5.06
(1,70)	1:35:A:ILE:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	20	5.05
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	9	5.05
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	19	5.05
(1,70)	1:35:A:ILE:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	13	5.04
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	4	5.04
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	12	5.04
(1,10)	1:5:A:THR:C	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	20	5.03
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	12	5.02
(1,96)	1:46:C:PHE:C	1:47:C:ILE:N	1:47:C:ILE:CA	1:47:C:ILE:C	18	5.02
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	19	5.01
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	19	5.0
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	16	4.97
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	19	4.96
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	20	4.96
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	13	4.94
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	10	4.94
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	12	4.93
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	4	4.93
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	11	4.93
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	5	4.91
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	12	4.91
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	13	4.88
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	19	4.87
(1,70)	1:35:A:ILE:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	4	4.86
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	11	4.85
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	7	4.83
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	1	4.81
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	12	4.8
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	6	4.79
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	20	4.79
(1,199)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:ILE:N	12	4.78
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	11	4.77
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	10	4.76
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	6	4.75
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	14	4.71
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	14	4.71
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	6	4.71
(1,94)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	18	4.68
(1,72)	1:35:C:ILE:C	1:36:C:LEU:N	1:36:C:LEU:CA	1:36:C:LEU:C	16	4.68
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	12	4.67
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	10	4.67
(1,157)	1:9:A:GLU:N	1:9:A:GLU:CA	1:9:A:GLU:C	1:10:A:VAL:N	8	4.66
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	1	4.66
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	17	4.66
(1,95)	1:46:B:PHE:C	1:47:B:ILE:N	1:47:B:ILE:CA	1:47:B:ILE:C	3	4.63
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	2	4.63
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	20	4.61
(1,160)	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	1:11:A:ALA:N	10	4.57

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,72)	1:35:C:ILE:C	1:36:C:LEU:N	1:36:C:LEU:CA	1:36:C:LEU:C	8	4.57
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	1	4.57
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	17	4.56
(1,201)	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	1:35:C:ILE:N	16	4.55
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	17	4.55
(1,2)	1:1:B:FME:C	1:2:B:VAL:N	1:2:B:VAL:CA	1:2:B:VAL:C	10	4.54
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	3	4.53
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	18	4.52
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	19	4.51
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	5	4.51
(1,70)	1:35:A:ILE:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	2	4.51
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	6	4.5
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	16	4.49
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	14	4.49
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	3	4.47
(1,72)	1:35:C:ILE:C	1:36:C:LEU:N	1:36:C:LEU:CA	1:36:C:LEU:C	17	4.46
(1,72)	1:35:C:ILE:C	1:36:C:LEU:N	1:36:C:LEU:CA	1:36:C:LEU:C	3	4.45
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	2	4.45
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	5	4.42
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	11	4.42
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	8	4.41
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	13	4.4
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	9	4.39
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	11	4.36
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	1	4.36
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	19	4.36
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	2	4.36
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	16	4.36
(1,157)	1:9:A:GLU:N	1:9:A:GLU:CA	1:9:A:GLU:C	1:10:A:VAL:N	10	4.35
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	10	4.32
(1,42)	1:17:C:ARG:C	1:18:C:ALA:N	1:18:C:ALA:CA	1:18:C:ALA:C	20	4.32
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	12	4.31
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	4	4.31
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	12	4.3
(1,72)	1:35:C:ILE:C	1:36:C:LEU:N	1:36:C:LEU:CA	1:36:C:LEU:C	11	4.28
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	6	4.28
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	4	4.28
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	3	4.27
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	20	4.26
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	6	4.24
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	14	4.24
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	5	4.23
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	9	4.22
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	6	4.22
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	10	4.22
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	13	4.22
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	18	4.21
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	11	4.21
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	12	4.19
(1,11)	1:5:B:THR:C	1:6:B:ASP:N	1:6:B:ASP:CA	1:6:B:ASP:C	16	4.18
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	11	4.17

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,2)	1:1:B:FME:C	1:2:B:VAL:N	1:2:B:VAL:CA	1:2:B:VAL:C	12	4.17
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	15	4.16
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	6	4.16
(1,70)	1:35:A:ILE:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	6	4.16
(1,72)	1:35:C:ILE:C	1:36:C:LEU:N	1:36:C:LEU:CA	1:36:C:LEU:C	5	4.15
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	16	4.13
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	9	4.13
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	18	4.13
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	6	4.12
(1,72)	1:35:C:ILE:C	1:36:C:LEU:N	1:36:C:LEU:CA	1:36:C:LEU:C	7	4.12
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	13	4.11
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	7	4.1
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	17	4.09
(1,200)	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1:35:B:ILE:N	3	4.08
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	19	4.08
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	3	4.06
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	8	4.05
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	3	4.04
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	4	4.0
(1,200)	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1:35:B:ILE:N	5	3.99
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	3	3.99
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	8	3.99
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	18	3.98
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	15	3.96
(1,56)	1:27:B:PRO:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	3	3.95
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	4	3.95
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	7	3.94
(1,40)	1:17:A:ARG:C	1:18:A:ALA:N	1:18:A:ALA:CA	1:18:A:ALA:C	1	3.94
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	8	3.94
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	12	3.94
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	1	3.93
(1,160)	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	1:11:A:ALA:N	8	3.92
(1,38)	1:16:B:GLU:C	1:17:B:ARG:N	1:17:B:ARG:CA	1:17:B:ARG:C	19	3.91
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	14	3.89
(1,41)	1:17:B:ARG:C	1:18:B:ALA:N	1:18:B:ALA:CA	1:18:B:ALA:C	1	3.89
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	18	3.88
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	16	3.88
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	19	3.87
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	12	3.86
(1,36)	1:15:C:CYS:C	1:16:C:GLU:N	1:16:C:GLU:CA	1:16:C:GLU:C	8	3.85
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	15	3.84
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	20	3.84
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	14	3.83
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	5	3.82
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	4	3.82
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	2	3.82
(1,2)	1:1:B:FME:C	1:2:B:VAL:N	1:2:B:VAL:CA	1:2:B:VAL:C	9	3.82
(1,313)	1:53:A:LYS:HA	1:53:A:LYS:CA	1:53:A:LYS:CB	1:53:A:LYS:HB3	11	3.81
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	13	3.81
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	6	3.79
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	20	3.79

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	12	3.79
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	4	3.77
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	14	3.76
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	9	3.75
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	1	3.74
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	4	3.74
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	5	3.74
(1,37)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	5	3.74
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	7	3.73
(1,200)	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1:35:B:ILE:N	4	3.72
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	1	3.71
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	2	3.71
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	9	3.7
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	5	3.7
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	6	3.69
(1,72)	1:35:C:ILE:C	1:36:C:LEU:N	1:36:C:LEU:CA	1:36:C:LEU:C	14	3.69
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	5	3.68
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	12	3.67
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	19	3.67
(1,72)	1:35:C:ILE:C	1:36:C:LEU:N	1:36:C:LEU:CA	1:36:C:LEU:C	2	3.67
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	7	3.67
(1,34)	1:15:A:CYS:C	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	5	3.66
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	20	3.66
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	6	3.65
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	16	3.65
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	14	3.63
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	8	3.63
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	6	3.63
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	19	3.63
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	2	3.61
(1,161)	1:10:B:VAL:N	1:10:B:VAL:CA	1:10:B:VAL:C	1:11:B:ALA:N	11	3.6
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	13	3.59
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	12	3.59
(1,34)	1:15:A:CYS:C	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	8	3.59
(1,313)	1:53:A:LYS:HA	1:53:A:LYS:CA	1:53:A:LYS:CB	1:53:A:LYS:HB3	18	3.57
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	5	3.57
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	13	3.56
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	15	3.55
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	3	3.55
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	9	3.53
(1,12)	1:5:C:THR:C	1:6:C:ASP:N	1:6:C:ASP:CA	1:6:C:ASP:C	18	3.53
(1,2)	1:1:B:FME:C	1:2:B:VAL:N	1:2:B:VAL:CA	1:2:B:VAL:C	5	3.53
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	13	3.52
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	12	3.52
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	10	3.52
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	10	3.51
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	9	3.51
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	9	3.51
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	14	3.51
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	4	3.5
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	20	3.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	4	3.5
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	15	3.5
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	1	3.49
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	20	3.49
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	3	3.49
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	19	3.47
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	13	3.47
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	6	3.47
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	3	3.47
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	13	3.46
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	11	3.46
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	8	3.46
(1,34)	1:15:A:CYS:C	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	15	3.46
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	16	3.45
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	19	3.44
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	4	3.43
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	7	3.43
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	12	3.43
(1,35)	1:15:B:CYS:C	1:16:B:GLU:N	1:16:B:GLU:CA	1:16:B:GLU:C	3	3.43
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	12	3.42
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	9	3.41
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	10	3.41
(1,70)	1:35:A:ILE:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	18	3.41
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	1	3.4
(1,52)	1:25:A:PRO:C	1:26:A:CYS:N	1:26:A:CYS:CA	1:26:A:CYS:C	6	3.4
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	11	3.39
(1,161)	1:10:B:VAL:N	1:10:B:VAL:CA	1:10:B:VAL:C	1:11:B:ALA:N	5	3.38
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	16	3.38
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	15	3.37
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	9	3.37
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	3	3.37
(1,70)	1:35:A:ILE:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	1	3.36
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	5	3.36
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	10	3.36
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	5	3.36
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	2	3.35
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	15	3.35
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	15	3.35
(1,200)	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1:35:B:ILE:N	11	3.32
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	20	3.31
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	10	3.31
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	11	3.31
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	3	3.29
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	2	3.29
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	19	3.29
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	3	3.27
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	10	3.27
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	14	3.26
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	19	3.26
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	18	3.25
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	6	3.24

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	10	3.23
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	13	3.23
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	8	3.2
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	16	3.2
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	2	3.2
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	9	3.19
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	17	3.18
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	16	3.18
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	15	3.18
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	17	3.17
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	9	3.17
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	15	3.15
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	13	3.15
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	7	3.13
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	14	3.13
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	4	3.12
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	17	3.11
(1,23)	1:9:B:GLU:C	1:10:B:VAL:N	1:10:B:VAL:CA	1:10:B:VAL:C	3	3.11
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	8	3.1
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	14	3.09
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	8	3.09
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	4	3.08
(1,41)	1:17:B:ARG:C	1:18:B:ALA:N	1:18:B:ALA:CA	1:18:B:ALA:C	7	3.07
(1,42)	1:17:C:ARG:C	1:18:C:ALA:N	1:18:C:ALA:CA	1:18:C:ALA:C	12	3.06
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	12	3.03
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	2	3.03
(1,13)	1:6:A:ASP:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	9	3.03
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	1	3.02
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	17	3.02
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	1	3.0
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	17	3.0
(1,38)	1:16:B:GLU:C	1:17:B:ARG:N	1:17:B:ARG:CA	1:17:B:ARG:C	16	3.0
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	3	2.99
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	10	2.98
(1,36)	1:15:C:CYS:C	1:16:C:GLU:N	1:16:C:GLU:CA	1:16:C:GLU:C	14	2.97
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	18	2.97
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	10	2.96
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	7	2.96
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	10	2.96
(1,38)	1:16:B:GLU:C	1:17:B:ARG:N	1:17:B:ARG:CA	1:17:B:ARG:C	8	2.95
(1,160)	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	1:11:A:ALA:N	12	2.94
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	18	2.94
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	1	2.94
(1,52)	1:25:A:PRO:C	1:26:A:CYS:N	1:26:A:CYS:CA	1:26:A:CYS:C	1	2.92
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	5	2.91
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	7	2.91
(1,64)	1:33:A:GLY:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	20	2.91
(1,52)	1:25:A:PRO:C	1:26:A:CYS:N	1:26:A:CYS:CA	1:26:A:CYS:C	12	2.9
(1,14)	1:6:B:ASP:C	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	15	2.9
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	4	2.89
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	9	2.89

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	10	2.88
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	10	2.88
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	15	2.88
(1,160)	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	1:11:A:ALA:N	17	2.87
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	8	2.87
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	18	2.87
(1,39)	1:16:C:GLU:C	1:17:C:ARG:N	1:17:C:ARG:CA	1:17:C:ARG:C	7	2.87
(1,72)	1:35:C:ILE:C	1:36:C:LEU:N	1:36:C:LEU:CA	1:36:C:LEU:C	1	2.86
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	3	2.86
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	12	2.86
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	19	2.85
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	20	2.85
(1,70)	1:35:A:ILE:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	17	2.85
(1,52)	1:25:A:PRO:C	1:26:A:CYS:N	1:26:A:CYS:CA	1:26:A:CYS:C	16	2.85
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	8	2.82
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	11	2.82
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	10	2.81
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	1	2.81
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	17	2.8
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	9	2.8
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	4	2.79
(1,38)	1:16:B:GLU:C	1:17:B:ARG:N	1:17:B:ARG:CA	1:17:B:ARG:C	9	2.79
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	20	2.78
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	8	2.78
(1,16)	1:7:A:ASP:C	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	7	2.78
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	18	2.77
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	16	2.77
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	7	2.73
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	13	2.73
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	6	2.73
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	20	2.72
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	15	2.72
(1,2)	1:1:B:FME:C	1:2:B:VAL:N	1:2:B:VAL:CA	1:2:B:VAL:C	15	2.72
(1,52)	1:25:A:PRO:C	1:26:A:CYS:N	1:26:A:CYS:CA	1:26:A:CYS:C	2	2.71
(1,39)	1:16:C:GLU:C	1:17:C:ARG:N	1:17:C:ARG:CA	1:17:C:ARG:C	16	2.71
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	1	2.7
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	6	2.7
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	12	2.69
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	5	2.69
(1,52)	1:25:A:PRO:C	1:26:A:CYS:N	1:26:A:CYS:CA	1:26:A:CYS:C	11	2.69
(1,38)	1:16:B:GLU:C	1:17:B:ARG:N	1:17:B:ARG:CA	1:17:B:ARG:C	7	2.69
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	2	2.68
(1,61)	1:31:A:GLY:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	16	2.68
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	12	2.68
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	17	2.67
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	19	2.67
(1,2)	1:1:B:FME:C	1:2:B:VAL:N	1:2:B:VAL:CA	1:2:B:VAL:C	7	2.67
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	3	2.66
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	16	2.66
(1,72)	1:35:C:ILE:C	1:36:C:LEU:N	1:36:C:LEU:CA	1:36:C:LEU:C	9	2.65
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	15	2.65

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,41)	1:17:B:ARG:C	1:18:B:ALA:N	1:18:B:ALA:CA	1:18:B:ALA:C	2	2.65
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	17	2.65
(1,37)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1	2.64
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	14	2.63
(1,41)	1:17:B:ARG:C	1:18:B:ALA:N	1:18:B:ALA:CA	1:18:B:ALA:C	8	2.63
(1,40)	1:17:A:ARG:C	1:18:A:ALA:N	1:18:A:ALA:CA	1:18:A:ALA:C	5	2.63
(1,18)	1:7:C:ASP:C	1:8:C:LEU:N	1:8:C:LEU:CA	1:8:C:LEU:C	18	2.62
(1,2)	1:1:B:FME:C	1:2:B:VAL:N	1:2:B:VAL:CA	1:2:B:VAL:C	8	2.62
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	4	2.6
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	5	2.59
(1,42)	1:17:C:ARG:C	1:18:C:ALA:N	1:18:C:ALA:CA	1:18:C:ALA:C	17	2.59
(1,15)	1:6:C:ASP:C	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	19	2.59
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	8	2.58
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	1	2.58
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	11	2.58
(1,37)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	19	2.58
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	16	2.58
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	3	2.57
(1,161)	1:10:B:VAL:N	1:10:B:VAL:CA	1:10:B:VAL:C	1:11:B:ALA:N	4	2.56
(1,160)	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	1:11:A:ALA:N	2	2.55
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	5	2.55
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	10	2.55
(1,40)	1:17:A:ARG:C	1:18:A:ALA:N	1:18:A:ALA:CA	1:18:A:ALA:C	10	2.55
(1,35)	1:15:B:CYS:C	1:16:B:GLU:N	1:16:B:GLU:CA	1:16:B:GLU:C	5	2.55
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	5	2.54
(1,66)	1:33:C:GLY:C	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	20	2.53
(1,34)	1:15:A:CYS:C	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	13	2.51
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	15	2.5
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	18	2.5
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	8	2.48
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	8	2.47
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	11	2.47
(1,18)	1:7:C:ASP:C	1:8:C:LEU:N	1:8:C:LEU:CA	1:8:C:LEU:C	10	2.47
(1,17)	1:7:B:ASP:C	1:8:B:LEU:N	1:8:B:LEU:CA	1:8:B:LEU:C	10	2.47
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	4	2.45
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	18	2.45
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	7	2.44
(1,185)	1:24:B:THR:N	1:24:B:THR:CA	1:24:B:THR:C	1:25:B:PRO:N	3	2.43
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	8	2.43
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	18	2.4
(1,280)	1:29:A:CYS:HA	1:29:A:CYS:CA	1:29:A:CYS:CB	1:29:A:CYS:HB3	20	2.39
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	17	2.39
(1,37)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	12	2.39
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	9	2.38
(1,52)	1:25:A:PRO:C	1:26:A:CYS:N	1:26:A:CYS:CA	1:26:A:CYS:C	20	2.38
(1,52)	1:25:A:PRO:C	1:26:A:CYS:N	1:26:A:CYS:CA	1:26:A:CYS:C	7	2.37
(1,36)	1:15:C:CYS:C	1:16:C:GLU:N	1:16:C:GLU:CA	1:16:C:GLU:C	20	2.37
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	12	2.36
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	8	2.36
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	15	2.35
(1,19)	1:8:A:LEU:C	1:9:A:GLU:N	1:9:A:GLU:CA	1:9:A:GLU:C	10	2.35

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,2)	1:1:B:FME:C	1:2:B:VAL:N	1:2:B:VAL:CA	1:2:B:VAL:C	2	2.35
(1,38)	1:16:B:GLU:C	1:17:B:ARG:N	1:17:B:ARG:CA	1:17:B:ARG:C	5	2.34
(1,65)	1:33:B:GLY:C	1:34:B:VAL:N	1:34:B:VAL:CA	1:34:B:VAL:C	1	2.32
(1,297)	1:43:C:LEU:HA	1:43:C:LEU:CA	1:43:C:LEU:CB	1:43:C:LEU:HB3	11	2.31
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	11	2.31
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	9	2.3
(1,41)	1:17:B:ARG:C	1:18:B:ALA:N	1:18:B:ALA:CA	1:18:B:ALA:C	10	2.3
(1,40)	1:17:A:ARG:C	1:18:A:ALA:N	1:18:A:ALA:CA	1:18:A:ALA:C	2	2.3
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	19	2.29
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	2	2.29
(1,52)	1:25:A:PRO:C	1:26:A:CYS:N	1:26:A:CYS:CA	1:26:A:CYS:C	15	2.29
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	8	2.28
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	17	2.28
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	20	2.27
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	11	2.26
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	2	2.26
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	8	2.25
(1,42)	1:17:C:ARG:C	1:18:C:ALA:N	1:18:C:ALA:CA	1:18:C:ALA:C	18	2.25
(1,34)	1:15:A:CYS:C	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	2	2.25
(1,40)	1:17:A:ARG:C	1:18:A:ALA:N	1:18:A:ALA:CA	1:18:A:ALA:C	7	2.24
(1,39)	1:16:C:GLU:C	1:17:C:ARG:N	1:17:C:ARG:CA	1:17:C:ARG:C	20	2.24
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	13	2.23
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	2	2.23
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	7	2.22
(1,52)	1:25:A:PRO:C	1:26:A:CYS:N	1:26:A:CYS:CA	1:26:A:CYS:C	18	2.22
(1,106)	1:51:A:LEU:C	1:52:A:ASN:N	1:52:A:ASN:CA	1:52:A:ASN:C	5	2.2
(1,52)	1:25:A:PRO:C	1:26:A:CYS:N	1:26:A:CYS:CA	1:26:A:CYS:C	5	2.2
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	6	2.19
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	18	2.18
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	16	2.17
(1,52)	1:25:A:PRO:C	1:26:A:CYS:N	1:26:A:CYS:CA	1:26:A:CYS:C	10	2.17
(1,38)	1:16:B:GLU:C	1:17:B:ARG:N	1:17:B:ARG:CA	1:17:B:ARG:C	10	2.17
(1,256)	1:9:A:GLU:HA	1:9:A:GLU:CA	1:9:A:GLU:CB	1:9:A:GLU:HB3	8	2.15
(1,66)	1:33:C:GLY:C	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	1	2.15
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	16	2.15
(1,22)	1:9:A:GLU:C	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	1	2.15
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	7	2.15
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	19	2.14
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	7	2.13
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	13	2.13
(1,155)	1:7:B:ASP:N	1:7:B:ASP:CA	1:7:B:ASP:C	1:8:B:LEU:N	16	2.11
(1,148)	1:5:A:THR:N	1:5:A:THR:CA	1:5:A:THR:C	1:6:A:ASP:N	9	2.11
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	13	2.11
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	16	2.1
(1,36)	1:15:C:CYS:C	1:16:C:GLU:N	1:16:C:GLU:CA	1:16:C:GLU:C	16	2.1
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	10	2.09
(1,246)	1:50:C:HIS:N	1:50:C:HIS:CA	1:50:C:HIS:C	1:51:C:LEU:N	2	2.08
(1,70)	1:35:A:ILE:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	11	2.08
(1,42)	1:17:C:ARG:C	1:18:C:ALA:N	1:18:C:ALA:CA	1:18:C:ALA:C	2	2.07
(1,41)	1:17:B:ARG:C	1:18:B:ALA:N	1:18:B:ALA:CA	1:18:B:ALA:C	16	2.07
(1,64)	1:33:A:GLY:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	19	2.06

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	18	2.06
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	7	2.06
(1,52)	1:25:A:PRO:C	1:26:A:CYS:N	1:26:A:CYS:CA	1:26:A:CYS:C	17	2.06
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	4	2.05
(1,106)	1:51:A:LEU:C	1:52:A:ASN:N	1:52:A:ASN:CA	1:52:A:ASN:C	15	2.05
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	4	2.05
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	9	2.04
(1,16)	1:7:A:ASP:C	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	9	2.01
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	3	2.01
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	9	2.01
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	10	2.01
(1,2)	1:1:B:FME:C	1:2:B:VAL:N	1:2:B:VAL:CA	1:2:B:VAL:C	4	1.98
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	19	1.97
(1,37)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	20	1.97
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	18	1.97
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	6	1.96
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	18	1.96
(1,52)	1:25:A:PRO:C	1:26:A:CYS:N	1:26:A:CYS:CA	1:26:A:CYS:C	4	1.96
(1,118)	1:22:A:GLU:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	10	1.95
(1,66)	1:33:C:GLY:C	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	11	1.95
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	1	1.95
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	20	1.94
(1,271)	1:22:A:GLU:HA	1:22:A:GLU:CA	1:22:A:GLU:CB	1:22:A:GLU:HB3	8	1.94
(1,80)	1:41:B:TYR:C	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	18	1.94
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	16	1.93
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	3	1.92
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	2	1.92
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	19	1.92
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	9	1.9
(1,37)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	10	1.9
(1,273)	1:22:C:GLU:HA	1:22:C:GLU:CA	1:22:C:GLU:CB	1:22:C:GLU:HB3	19	1.88
(1,38)	1:16:B:GLU:C	1:17:B:ARG:N	1:17:B:ARG:CA	1:17:B:ARG:C	11	1.88
(1,55)	1:27:A:PRO:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	13	1.87
(1,52)	1:25:A:PRO:C	1:26:A:CYS:N	1:26:A:CYS:CA	1:26:A:CYS:C	3	1.87
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	15	1.87
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	14	1.85
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	18	1.85
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	6	1.83
(1,39)	1:16:C:GLU:C	1:17:C:ARG:N	1:17:C:ARG:CA	1:17:C:ARG:C	12	1.83
(1,16)	1:7:A:ASP:C	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	15	1.83
(1,292)	1:41:A:TYR:HA	1:41:A:TYR:CA	1:41:A:TYR:CB	1:41:A:TYR:HB3	17	1.82
(1,245)	1:50:B:HIS:N	1:50:B:HIS:CA	1:50:B:HIS:C	1:51:B:LEU:N	11	1.82
(1,81)	1:41:C:TYR:C	1:42:C:THR:N	1:42:C:THR:CA	1:42:C:THR:C	2	1.82
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	15	1.82
(1,37)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	18	1.81
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	11	1.8
(1,58)	1:28:A:ALA:C	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	10	1.8
(1,39)	1:16:C:GLU:C	1:17:C:ARG:N	1:17:C:ARG:CA	1:17:C:ARG:C	1	1.8
(1,41)	1:17:B:ARG:C	1:18:B:ALA:N	1:18:B:ALA:CA	1:18:B:ALA:C	15	1.79
(1,2)	1:1:B:FME:C	1:2:B:VAL:N	1:2:B:VAL:CA	1:2:B:VAL:C	18	1.77
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	4	1.75

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	14	1.75
(1,40)	1:17:A:ARG:C	1:18:A:ALA:N	1:18:A:ALA:CA	1:18:A:ALA:C	20	1.75
(1,2)	1:1:B:FME:C	1:2:B:VAL:N	1:2:B:VAL:CA	1:2:B:VAL:C	20	1.75
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	7	1.74
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	18	1.73
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	3	1.73
(1,119)	1:22:B:GLU:C	1:23:B:GLY:N	1:23:B:GLY:CA	1:23:B:GLY:C	4	1.73
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	13	1.72
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	11	1.72
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	14	1.72
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	7	1.72
(1,71)	1:35:B:ILE:C	1:36:B:LEU:N	1:36:B:LEU:CA	1:36:B:LEU:C	18	1.71
(1,282)	1:29:C:CYS:HA	1:29:C:CYS:CA	1:29:C:CYS:CB	1:29:C:CYS:HB3	4	1.7
(1,87)	1:43:C:LEU:C	1:44:C:LEU:N	1:44:C:LEU:CA	1:44:C:LEU:C	16	1.7
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	17	1.7
(1,41)	1:17:B:ARG:C	1:18:B:ALA:N	1:18:B:ALA:CA	1:18:B:ALA:C	20	1.7
(1,17)	1:7:B:ASP:C	1:8:B:LEU:N	1:8:B:LEU:CA	1:8:B:LEU:C	18	1.7
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	5	1.7
(1,3)	1:1:C:FME:C	1:2:C:VAL:N	1:2:C:VAL:CA	1:2:C:VAL:C	19	1.69
(1,57)	1:27:C:PRO:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	20	1.68
(1,40)	1:17:A:ARG:C	1:18:A:ALA:N	1:18:A:ALA:CA	1:18:A:ALA:C	12	1.68
(1,296)	1:43:B:LEU:HA	1:43:B:LEU:CA	1:43:B:LEU:CB	1:43:B:LEU:HB3	20	1.67
(1,70)	1:35:A:ILE:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	5	1.67
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	15	1.66
(1,297)	1:43:C:LEU:HA	1:43:C:LEU:CA	1:43:C:LEU:CB	1:43:C:LEU:HB3	17	1.65
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	11	1.65
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	13	1.65
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	13	1.64
(1,63)	1:31:C:GLY:C	1:32:C:LYS:N	1:32:C:LYS:CA	1:32:C:LYS:C	20	1.64
(1,60)	1:28:C:ALA:C	1:29:C:CYS:N	1:29:C:CYS:CA	1:29:C:CYS:C	5	1.64
(1,272)	1:22:B:GLU:HA	1:22:B:GLU:CA	1:22:B:GLU:CB	1:22:B:GLU:HB3	5	1.62
(1,297)	1:43:C:LEU:HA	1:43:C:LEU:CA	1:43:C:LEU:CB	1:43:C:LEU:HB3	2	1.61
(1,273)	1:22:C:GLU:HA	1:22:C:GLU:CA	1:22:C:GLU:CB	1:22:C:GLU:HB3	16	1.6
(1,70)	1:35:A:ILE:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	9	1.6
(1,41)	1:17:B:ARG:C	1:18:B:ALA:N	1:18:B:ALA:CA	1:18:B:ALA:C	13	1.6
(1,37)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	11	1.6
(1,19)	1:8:A:LEU:C	1:9:A:GLU:N	1:9:A:GLU:CA	1:9:A:GLU:C	8	1.6
(1,2)	1:1:B:FME:C	1:2:B:VAL:N	1:2:B:VAL:CA	1:2:B:VAL:C	16	1.6
(1,66)	1:33:C:GLY:C	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	7	1.59
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	15	1.56
(1,87)	1:43:C:LEU:C	1:44:C:LEU:N	1:44:C:LEU:CA	1:44:C:LEU:C	5	1.56
(1,40)	1:17:A:ARG:C	1:18:A:ALA:N	1:18:A:ALA:CA	1:18:A:ALA:C	18	1.56
(1,38)	1:16:B:GLU:C	1:17:B:ARG:N	1:17:B:ARG:CA	1:17:B:ARG:C	1	1.56
(1,38)	1:16:B:GLU:C	1:17:B:ARG:N	1:17:B:ARG:CA	1:17:B:ARG:C	3	1.56
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	10	1.55
(1,42)	1:17:C:ARG:C	1:18:C:ALA:N	1:18:C:ALA:CA	1:18:C:ALA:C	1	1.55
(1,22)	1:9:A:GLU:C	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	10	1.55
(1,42)	1:17:C:ARG:C	1:18:C:ALA:N	1:18:C:ALA:CA	1:18:C:ALA:C	19	1.54
(1,41)	1:17:B:ARG:C	1:18:B:ALA:N	1:18:B:ALA:CA	1:18:B:ALA:C	11	1.52
(1,40)	1:17:A:ARG:C	1:18:A:ALA:N	1:18:A:ALA:CA	1:18:A:ALA:C	14	1.52
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	8	1.49

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,2)	1:1:B:FME:C	1:2:B:VAL:N	1:2:B:VAL:CA	1:2:B:VAL:C	3	1.49
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	3	1.48
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	17	1.48
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	16	1.48
(1,272)	1:22:B:GLU:HA	1:22:B:GLU:CA	1:22:B:GLU:CB	1:22:B:GLU:HB3	2	1.48
(1,40)	1:17:A:ARG:C	1:18:A:ALA:N	1:18:A:ALA:CA	1:18:A:ALA:C	3	1.48
(1,38)	1:16:B:GLU:C	1:17:B:ARG:N	1:17:B:ARG:CA	1:17:B:ARG:C	15	1.48
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	15	1.46
(1,162)	1:10:C:VAL:N	1:10:C:VAL:CA	1:10:C:VAL:C	1:11:C:ALA:N	17	1.46
(1,39)	1:16:C:GLU:C	1:17:C:ARG:N	1:17:C:ARG:CA	1:17:C:ARG:C	11	1.45
(1,37)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	4	1.45
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	9	1.44
(1,282)	1:29:C:CYS:HA	1:29:C:CYS:CA	1:29:C:CYS:CB	1:29:C:CYS:HB3	7	1.43
(1,156)	1:7:C:ASP:N	1:7:C:ASP:CA	1:7:C:ASP:C	1:8:C:LEU:N	16	1.43
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	1	1.42
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	7	1.42
(1,42)	1:17:C:ARG:C	1:18:C:ALA:N	1:18:C:ALA:CA	1:18:C:ALA:C	7	1.42
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	5	1.41
(1,62)	1:31:B:GLY:C	1:32:B:LYS:N	1:32:B:LYS:CA	1:32:B:LYS:C	1	1.4
(1,53)	1:25:B:PRO:C	1:26:B:CYS:N	1:26:B:CYS:CA	1:26:B:CYS:C	4	1.4
(1,37)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	2	1.4
(1,292)	1:41:A:TYR:HA	1:41:A:TYR:CA	1:41:A:TYR:CB	1:41:A:TYR:HB3	12	1.39
(1,42)	1:17:C:ARG:C	1:18:C:ALA:N	1:18:C:ALA:CA	1:18:C:ALA:C	9	1.39
(1,39)	1:16:C:GLU:C	1:17:C:ARG:N	1:17:C:ARG:CA	1:17:C:ARG:C	2	1.39
(1,38)	1:16:B:GLU:C	1:17:B:ARG:N	1:17:B:ARG:CA	1:17:B:ARG:C	4	1.38
(1,293)	1:41:B:TYR:HA	1:41:B:TYR:CA	1:41:B:TYR:CB	1:41:B:TYR:HB3	4	1.37
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	16	1.37
(1,28)	1:13:A:PRO:C	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1	1.37
(1,244)	1:50:A:HIS:N	1:50:A:HIS:CA	1:50:A:HIS:C	1:51:A:LEU:N	5	1.36
(1,297)	1:43:C:LEU:HA	1:43:C:LEU:CA	1:43:C:LEU:CB	1:43:C:LEU:HB3	8	1.35
(1,37)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	15	1.35
(1,2)	1:1:B:FME:C	1:2:B:VAL:N	1:2:B:VAL:CA	1:2:B:VAL:C	19	1.35
(1,42)	1:17:C:ARG:C	1:18:C:ALA:N	1:18:C:ALA:CA	1:18:C:ALA:C	5	1.34
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	19	1.32
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	14	1.32
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	2	1.31
(1,35)	1:15:B:CYS:C	1:16:B:GLU:N	1:16:B:GLU:CA	1:16:B:GLU:C	8	1.31
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	4	1.31
(1,79)	1:41:A:TYR:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	7	1.29
(1,41)	1:17:B:ARG:C	1:18:B:ALA:N	1:18:B:ALA:CA	1:18:B:ALA:C	14	1.28
(1,281)	1:29:B:CYS:HA	1:29:B:CYS:CA	1:29:B:CYS:CB	1:29:B:CYS:HB3	16	1.27
(1,37)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	3	1.27
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	5	1.26
(1,66)	1:33:C:GLY:C	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	16	1.26
(1,39)	1:16:C:GLU:C	1:17:C:ARG:N	1:17:C:ARG:CA	1:17:C:ARG:C	9	1.26
(1,305)	1:49:B:LYS:HA	1:49:B:LYS:CA	1:49:B:LYS:CB	1:49:B:LYS:HB3	8	1.25
(1,41)	1:17:B:ARG:C	1:18:B:ALA:N	1:18:B:ALA:CA	1:18:B:ALA:C	18	1.25
(1,39)	1:16:C:GLU:C	1:17:C:ARG:N	1:17:C:ARG:CA	1:17:C:ARG:C	5	1.25
(1,41)	1:17:B:ARG:C	1:18:B:ALA:N	1:18:B:ALA:CA	1:18:B:ALA:C	9	1.24
(1,292)	1:41:A:TYR:HA	1:41:A:TYR:CA	1:41:A:TYR:CB	1:41:A:TYR:HB3	4	1.23
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	1	1.23

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,294)	1:41:C:TYR:HA	1:41:C:TYR:CA	1:41:C:TYR:CB	1:41:C:TYR:HB3	18	1.22
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	20	1.21
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	12	1.21
(1,40)	1:17:A:ARG:C	1:18:A:ALA:N	1:18:A:ALA:CA	1:18:A:ALA:C	16	1.21
(1,39)	1:16:C:GLU:C	1:17:C:ARG:N	1:17:C:ARG:CA	1:17:C:ARG:C	4	1.21
(1,296)	1:43:B:LEU:HA	1:43:B:LEU:CA	1:43:B:LEU:CB	1:43:B:LEU:HB3	5	1.2
(1,34)	1:15:A:CYS:C	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	17	1.2
(1,18)	1:7:C:ASP:C	1:8:C:LEU:N	1:8:C:LEU:CA	1:8:C:LEU:C	12	1.2
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	5	1.19
(1,296)	1:43:B:LEU:HA	1:43:B:LEU:CA	1:43:B:LEU:CB	1:43:B:LEU:HB3	7	1.18
(1,294)	1:41:C:TYR:HA	1:41:C:TYR:CA	1:41:C:TYR:CB	1:41:C:TYR:HB3	11	1.18
(1,66)	1:33:C:GLY:C	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	17	1.18
(1,36)	1:15:C:CYS:C	1:16:C:GLU:N	1:16:C:GLU:CA	1:16:C:GLU:C	7	1.18
(1,66)	1:33:C:GLY:C	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	2	1.17
(1,274)	1:25:A:PRO:HA	1:25:A:PRO:CA	1:25:A:PRO:CB	1:25:A:PRO:HB3	17	1.16
(1,59)	1:28:B:ALA:C	1:29:B:CYS:N	1:29:B:CYS:CA	1:29:B:CYS:C	12	1.16
(1,295)	1:43:A:LEU:HA	1:43:A:LEU:CA	1:43:A:LEU:CB	1:43:A:LEU:HB3	10	1.15
(1,295)	1:43:A:LEU:HA	1:43:A:LEU:CA	1:43:A:LEU:CB	1:43:A:LEU:HB3	8	1.14
(1,66)	1:33:C:GLY:C	1:34:C:VAL:N	1:34:C:VAL:CA	1:34:C:VAL:C	5	1.13
(1,294)	1:41:C:TYR:HA	1:41:C:TYR:CA	1:41:C:TYR:CB	1:41:C:TYR:HB3	10	1.12
(1,293)	1:41:B:TYR:HA	1:41:B:TYR:CA	1:41:B:TYR:CB	1:41:B:TYR:HB3	2	1.12
(1,282)	1:29:C:CYS:HA	1:29:C:CYS:CA	1:29:C:CYS:CB	1:29:C:CYS:HB3	18	1.12
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	20	1.12
(1,54)	1:25:C:PRO:C	1:26:C:CYS:N	1:26:C:CYS:CA	1:26:C:CYS:C	3	1.12
(1,39)	1:16:C:GLU:C	1:17:C:ARG:N	1:17:C:ARG:CA	1:17:C:ARG:C	15	1.12
(1,24)	1:9:C:GLU:C	1:10:C:VAL:N	1:10:C:VAL:CA	1:10:C:VAL:C	18	1.12
(1,22)	1:9:A:GLU:C	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	8	1.12
(1,293)	1:41:B:TYR:HA	1:41:B:TYR:CA	1:41:B:TYR:CB	1:41:B:TYR:HB3	14	1.08
(1,34)	1:15:A:CYS:C	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	18	1.08
(1,1)	1:1:A:FME:C	1:2:A:VAL:N	1:2:A:VAL:CA	1:2:A:VAL:C	1	1.07
(1,295)	1:43:A:LEU:HA	1:43:A:LEU:CA	1:43:A:LEU:CB	1:43:A:LEU:HB3	18	1.06
(1,38)	1:16:B:GLU:C	1:17:B:ARG:N	1:17:B:ARG:CA	1:17:B:ARG:C	13	1.06
(1,38)	1:16:B:GLU:C	1:17:B:ARG:N	1:17:B:ARG:CA	1:17:B:ARG:C	20	1.06
(1,275)	1:25:B:PRO:HA	1:25:B:PRO:CA	1:25:B:PRO:CB	1:25:B:PRO:HB3	2	1.05
(1,35)	1:15:B:CYS:C	1:16:B:GLU:N	1:16:B:GLU:CA	1:16:B:GLU:C	14	1.05
(1,85)	1:43:A:LEU:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	2	1.04
(1,273)	1:22:C:GLU:HA	1:22:C:GLU:CA	1:22:C:GLU:CB	1:22:C:GLU:HB3	11	1.03
(1,266)	1:16:B:GLU:HA	1:16:B:GLU:CA	1:16:B:GLU:CB	1:16:B:GLU:HB3	6	1.03
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	15	1.02
(1,297)	1:43:C:LEU:HA	1:43:C:LEU:CA	1:43:C:LEU:CB	1:43:C:LEU:HB3	12	1.01
(1,272)	1:22:B:GLU:HA	1:22:B:GLU:CA	1:22:B:GLU:CB	1:22:B:GLU:HB3	8	1.01
(1,39)	1:16:C:GLU:C	1:17:C:ARG:N	1:17:C:ARG:CA	1:17:C:ARG:C	18	1.01
(1,37)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	16	1.01
(1,276)	1:25:C:PRO:HA	1:25:C:PRO:CA	1:25:C:PRO:CB	1:25:C:PRO:HB3	2	1.0