



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 05:47 AM UTC

PDB ID : 9F4C / pdb_00009f4c
BMRB ID : 34916
Title : Structure of the C-terminal domain of CKAP5/chTOG
Authors : Pfuhl, M.
Deposited on : 2024-04-27

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

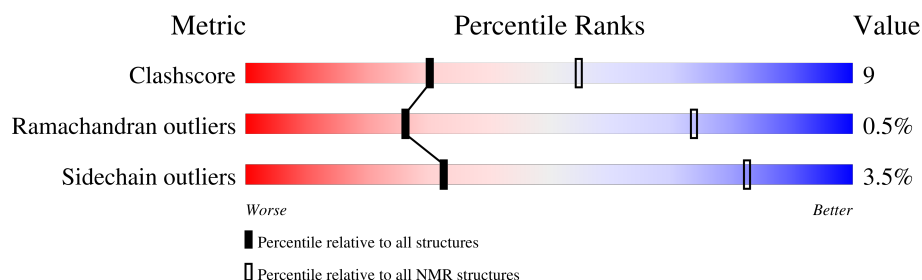
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	141	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 18 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:1829-A:1861, A:1865-A:1888 (57)	0.12	18
2	A:1905-A:1912 (8)	0.37	14

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 6 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2231 atoms, of which 1118 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cytoskeleton-associated protein 5.

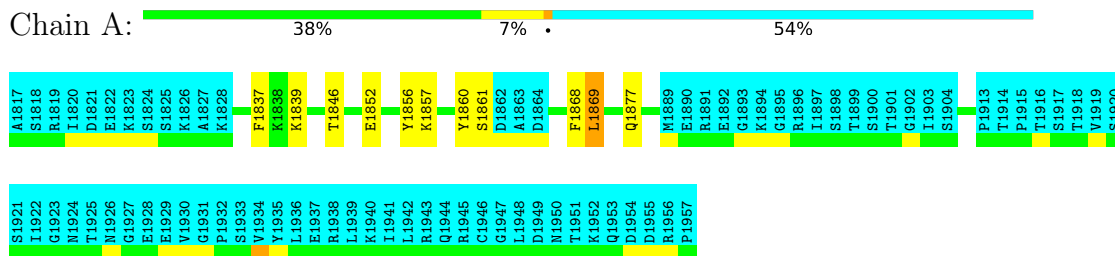
Mol	Chain	Residues	Atoms						Trace
1	A	141	Total	C	H	N	O	S	0
			2231	690	1118	193	226	4	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Cytoskeleton-associated protein 5

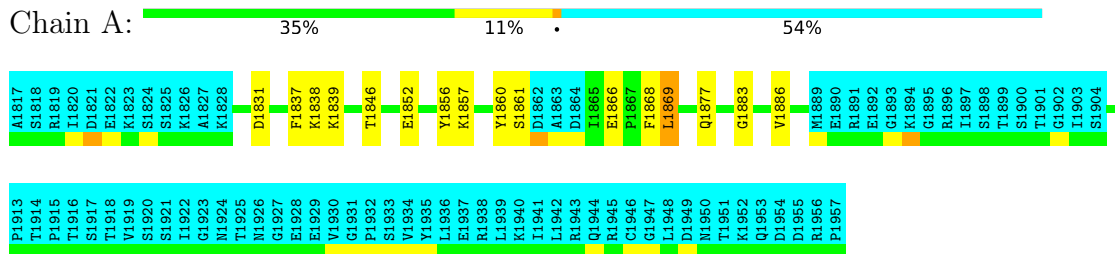


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

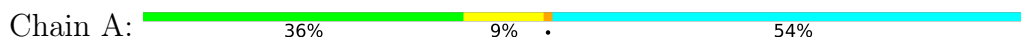
4.2.1 Score per residue for model 1

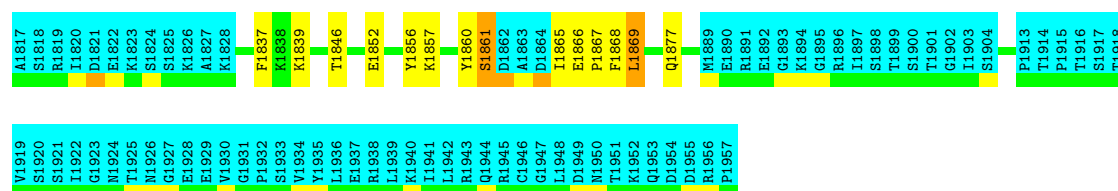
- Molecule 1: Cytoskeleton-associated protein 5



4.2.2 Score per residue for model 2

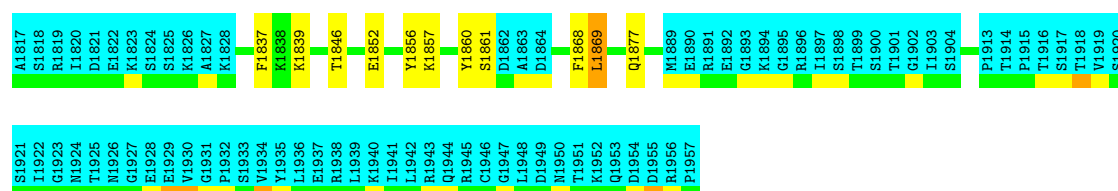
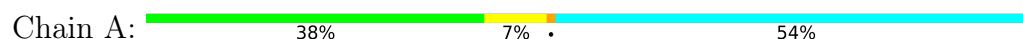
- Molecule 1: Cytoskeleton-associated protein 5





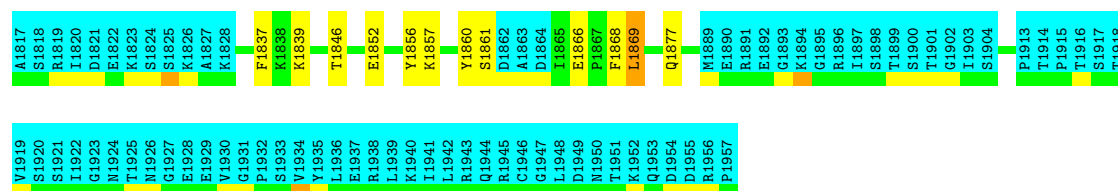
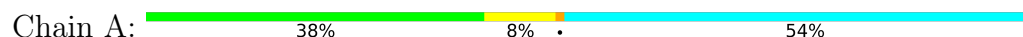
4.2.3 Score per residue for model 3

- Molecule 1: Cytoskeleton-associated protein 5



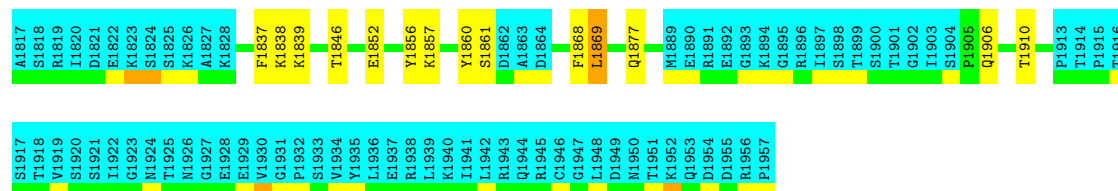
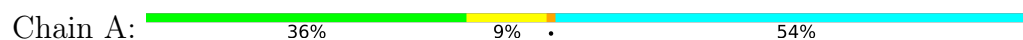
4.2.4 Score per residue for model 4

- Molecule 1: Cytoskeleton-associated protein 5



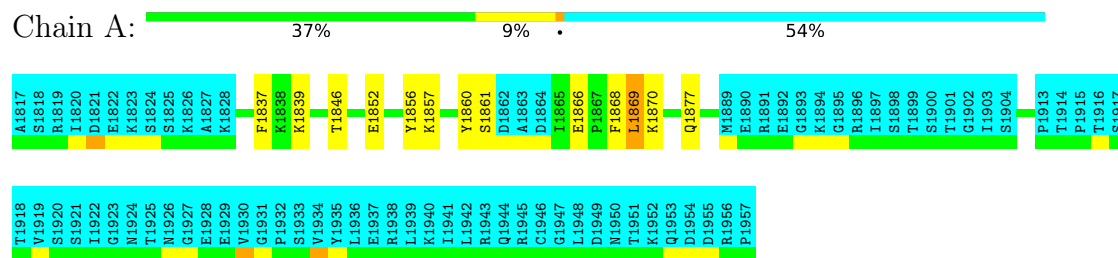
4.2.5 Score per residue for model 5

- Molecule 1: Cytoskeleton-associated protein 5



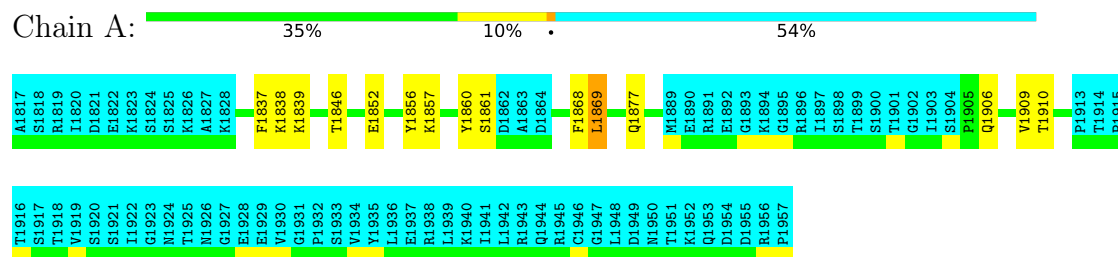
4.2.6 Score per residue for model 6

- Molecule 1: Cytoskeleton-associated protein 5



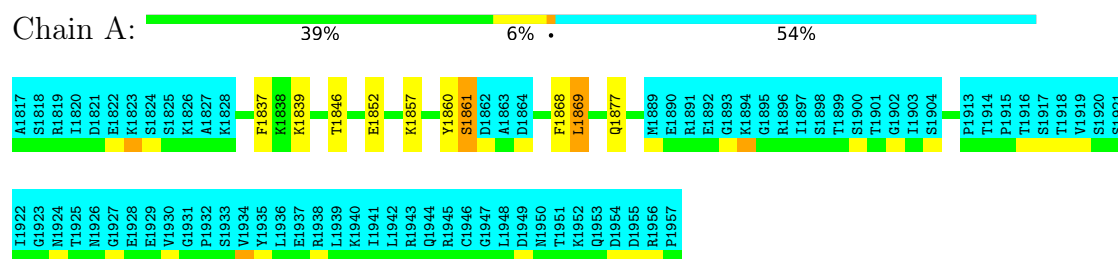
4.2.7 Score per residue for model 7

- Molecule 1: Cytoskeleton-associated protein 5



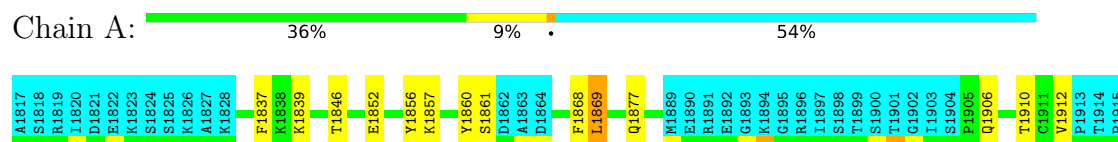
4.2.8 Score per residue for model 8

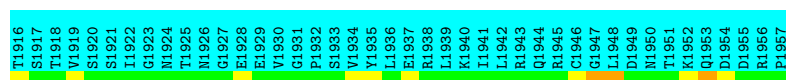
- Molecule 1: Cytoskeleton-associated protein 5



4.2.9 Score per residue for model 9

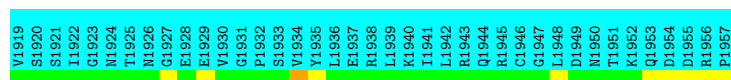
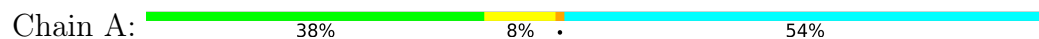
- Molecule 1: Cytoskeleton-associated protein 5





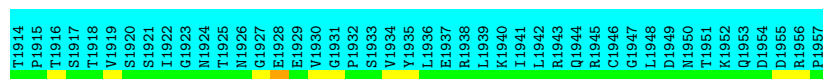
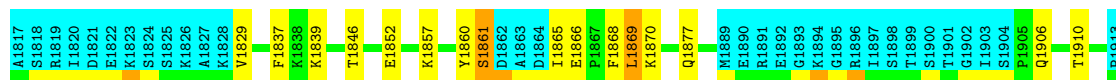
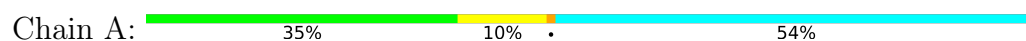
4.2.10 Score per residue for model 10

- Molecule 1: Cytoskeleton-associated protein 5



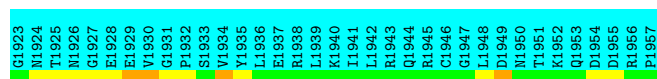
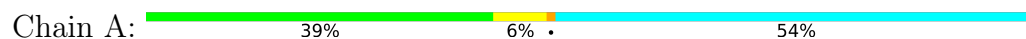
4.2.11 Score per residue for model 11

- Molecule 1: Cytoskeleton-associated protein 5



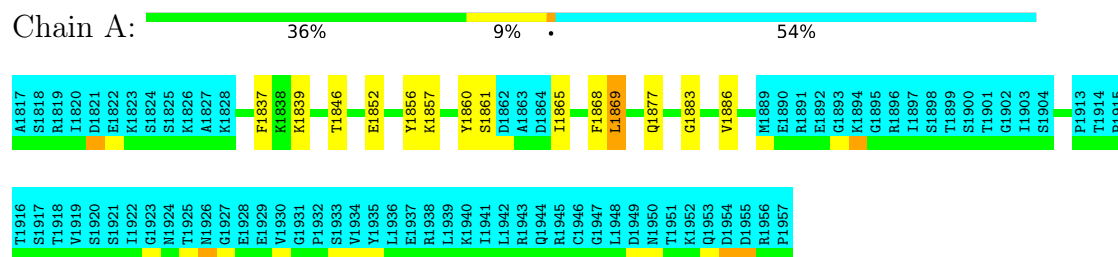
4.2.12 Score per residue for model 12

- Molecule 1: Cytoskeleton-associated protein 5



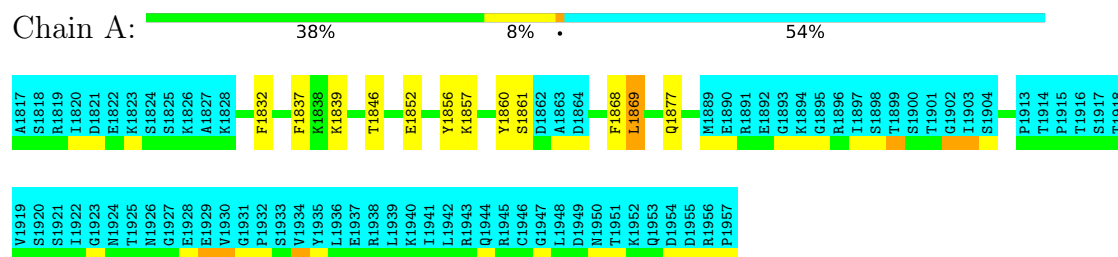
4.2.13 Score per residue for model 13

- Molecule 1: Cytoskeleton-associated protein 5



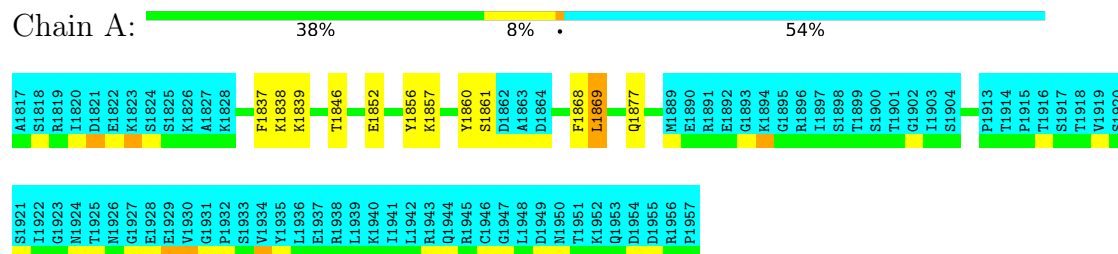
4.2.14 Score per residue for model 14

- Molecule 1: Cytoskeleton-associated protein 5



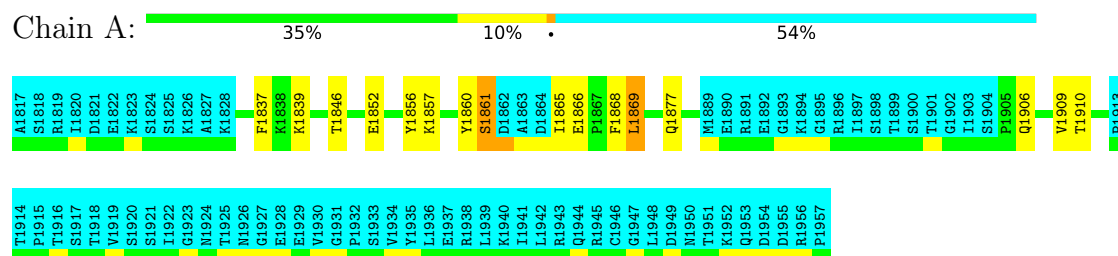
4.2.15 Score per residue for model 15

- Molecule 1: Cytoskeleton-associated protein 5



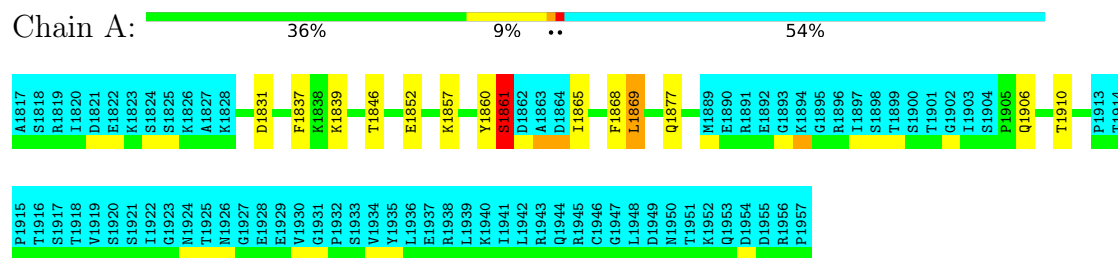
4.2.16 Score per residue for model 16

- Molecule 1: Cytoskeleton-associated protein 5



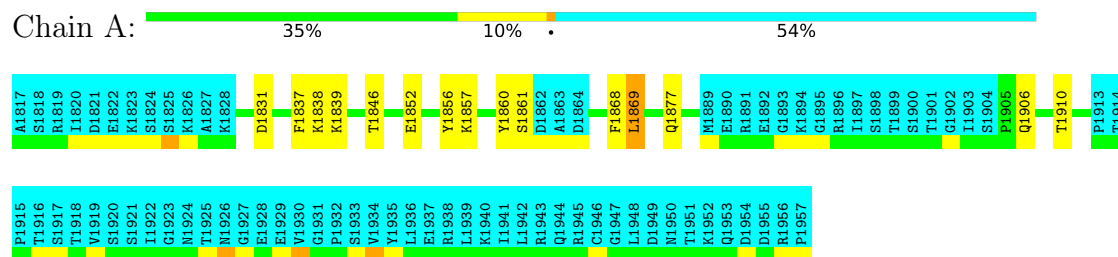
4.2.17 Score per residue for model 17

- Molecule 1: Cytoskeleton-associated protein 5



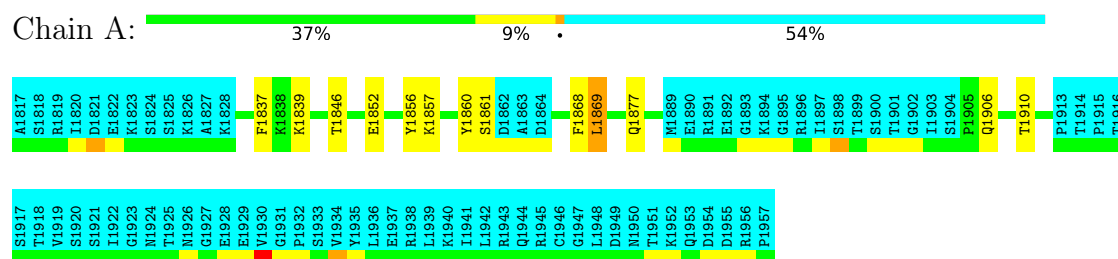
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Cytoskeleton-associated protein 5



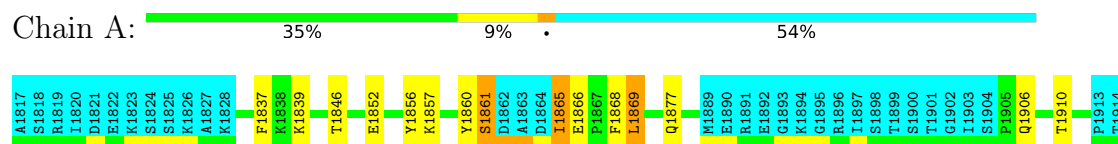
4.2.19 Score per residue for model 19

- Molecule 1: Cytoskeleton-associated protein 5



4.2.20 Score per residue for model 20

- Molecule 1: Cytoskeleton-associated protein 5



P1915	T1916	S1917	T1918	V1919	S1920	S1921	T1922	G1923	N1924	T1925	M1926	G1927	E1928	E1929	V1930	G1931	P1932	S1933	V1934	Y1935	L1936	E1937	R1938	L1939	K1940	T1941	L1942	R1943	Q1944	R1945	C1946	G1947	L1948	D1949	N1950	T1951	K1952	Q1953	D1954	D1955	R1956	P1957
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5 Refinement protocol and experimental data overview

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

Of the 200 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
ARIA	structure calculation	
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	1738
Number of shifts mapped to atoms	1737
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.72±0.03	0±0/549 (0.0± 0.0%)	1.06±0.01	0±0/736 (0.0± 0.1%)
All	All	0.72	0/10980 (0.0%)	1.06	4/14720 (0.0%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	1845	ASN	CA-CB-CG	-5.55	107.05	112.60	10	1
1	A	1865	ILE	N-CA-C	5.23	115.44	110.42	16	2
1	A	1832	PHE	CA-CB-CG	-5.09	108.71	113.80	14	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	538	541	541	10±2
All	All	10760	10820	10820	194

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1837:PHE:CE1	1:A:1868:PHE:CE2	0.70	2.79	9	4
1:A:1837:PHE:CE2	1:A:1868:PHE:CE2	0.68	2.82	10	3
1:A:1837:PHE:CE1	1:A:1868:PHE:CE1	0.66	2.84	17	9
1:A:1837:PHE:CE2	1:A:1868:PHE:CE1	0.64	2.85	6	4
1:A:1906:GLN:HE22	1:A:1910:THR:H	0.63	1.34	5	2
1:A:1869:LEU:HD13	1:A:1877:GLN:OE1	0.62	1.94	20	20
1:A:1857:LYS:O	1:A:1861:SER:N	0.61	2.33	17	20
1:A:1860:TYR:O	1:A:1861:SER:O	0.61	2.18	16	4
1:A:1839:LYS:NZ	1:A:1852:GLU:OE2	0.60	2.34	13	8
1:A:1839:LYS:NZ	1:A:1852:GLU:OE1	0.59	2.35	17	12
1:A:1906:GLN:NE2	1:A:1910:THR:H	0.58	1.96	5	1
1:A:1906:GLN:NE2	1:A:1910:THR:N	0.58	2.51	5	1
1:A:1866:GLU:CD	1:A:1870:LYS:NZ	0.55	2.65	6	2
1:A:1906:GLN:NE2	1:A:1910:THR:OG1	0.51	2.43	11	4
1:A:1906:GLN:CD	1:A:1910:THR:H	0.50	2.14	7	1
1:A:1839:LYS:NZ	1:A:1852:GLU:CD	0.50	2.70	7	2
1:A:1866:GLU:CG	1:A:1870:LYS:NZ	0.47	2.78	6	2
1:A:1906:GLN:NE2	1:A:1910:THR:O	0.47	2.46	16	1
1:A:1856:TYR:CE1	1:A:1860:TYR:CE2	0.47	3.02	13	4
1:A:1856:TYR:CE1	1:A:1860:TYR:CE1	0.46	3.03	19	4
1:A:1860:TYR:O	1:A:1861:SER:C	0.46	2.59	1	19
1:A:1869:LEU:CB	1:A:1877:GLN:OE1	0.46	2.64	20	20
1:A:1837:PHE:CE1	1:A:1868:PHE:CD1	0.46	3.04	16	2
1:A:1837:PHE:CD1	1:A:1868:PHE:CE1	0.46	3.04	16	5
1:A:1866:GLU:O	1:A:1866:GLU:OE1	0.45	2.33	20	3
1:A:1906:GLN:CD	1:A:1910:THR:OG1	0.45	2.60	9	6
1:A:1837:PHE:CD2	1:A:1868:PHE:CE2	0.45	3.04	10	2
1:A:1860:TYR:C	1:A:1861:SER:O	0.45	2.60	16	1
1:A:1856:TYR:CE2	1:A:1860:TYR:CE1	0.44	3.05	18	3
1:A:1856:TYR:CE2	1:A:1860:TYR:CE2	0.44	3.05	6	4
1:A:1909:VAL:O	1:A:1909:VAL:HG23	0.44	2.12	16	1
1:A:1906:GLN:HE22	1:A:1910:THR:N	0.44	2.06	5	1
1:A:1866:GLU:O	1:A:1866:GLU:OE2	0.42	2.37	16	2
1:A:1831:ASP:C	1:A:1831:ASP:OD1	0.42	2.62	17	2
1:A:1906:GLN:OE1	1:A:1910:THR:N	0.42	2.48	7	2
1:A:1837:PHE:CE2	1:A:1868:PHE:CD2	0.42	3.07	10	2
1:A:1837:PHE:CE1	1:A:1868:PHE:CD2	0.42	3.08	9	1
1:A:1837:PHE:CD1	1:A:1868:PHE:CE2	0.42	3.07	9	1
1:A:1831:ASP:OD2	1:A:1831:ASP:C	0.41	2.63	18	1
1:A:1869:LEU:CD1	1:A:1877:GLN:OE1	0.41	2.68	20	3
1:A:1883:GLY:O	1:A:1886:VAL:CG2	0.41	2.68	13	2
1:A:1866:GLU:CD	1:A:1866:GLU:C	0.41	2.87	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1866:GLU:O	1:A:1867:PRO:C	0.40	2.63	2	1
1:A:1831:ASP:OD1	1:A:1831:ASP:C	0.40	2.63	10	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	65/141 (46%)	62±1 (95±1%)	3±1 (5±1%)	0±0 (1±1%)	26	74
All	All	1300/2820 (46%)	1234 (95%)	59 (5%)	7 (1%)	26	74

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

Mol	Chain	Res	Type	Models (Total)
1	A	1861	SER	6
1	A	1909	VAL	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	60/126 (48%)	58±0 (96±1%)	2±0 (4±1%)	32	82
All	All	1200/2520 (48%)	1158 (96%)	42 (4%)	32	82

All 5 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	1869	LEU	20

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Mol	Chain	Res	Type	Models (Total)
1	A	1846	THR	19
1	A	1912	VAL	1
1	A	1829	VAL	1
1	A	1861	SER	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 91% 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	1738
Number of shifts mapped to atoms	1737
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1817	ALA	H	8.371	0.007	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	140	-0.25 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	131	0.19 ± 0.04	None needed (< 0.5 ppm)
$^{13}\text{C}'$	132	-0.41 ± 0.06	None needed (< 0.5 ppm)
^{15}N	132	-1.43 ± 0.22	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 93%, i.e. 862 atoms were assigned a chemical shift out of a possible 928. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	316/324 (98%)	129/131 (98%)	126/130 (97%)	61/63 (97%)
Sidechain	468/518 (90%)	317/333 (95%)	146/165 (88%)	5/20 (25%)
Aromatic	78/86 (91%)	39/41 (95%)	39/45 (87%)	0/0 (—%)
Overall	862/928 (93%)	485/505 (96%)	311/340 (91%)	66/83 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1738 atoms were assigned a chemical shift out of a possible 1910. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	687/703 (98%)	283/286 (99%)	272/282 (96%)	132/135 (98%)
Sidechain	965/1112 (87%)	653/712 (92%)	302/348 (87%)	10/52 (19%)
Aromatic	86/95 (91%)	43/45 (96%)	43/50 (86%)	0/0 (—%)
Overall	1738/1910 (91%)	979/1043 (94%)	617/680 (91%)	142/187 (76%)

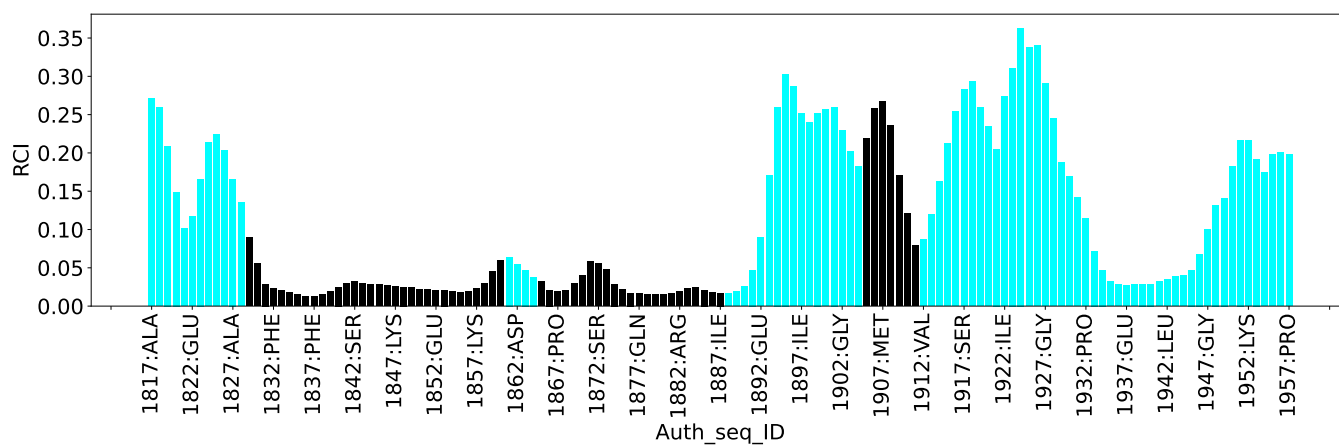
7.1.4 Statistically unusual chemical shifts [i](#)

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	3379
Intra-residue ($ i-j =0$)	1585
Sequential ($ i-j =1$)	717
Medium range ($ i-j >1$ and $ i-j <5$)	623
Long range ($ i-j \geq 5$)	397
Inter-chain	0
Hydrogen bond restraints	57
Disulfide bond restraints	0
Total dihedral-angle restraints	174
Number of unmapped restraints	0
Number of restraints per residue	25.2
Number of long range restraints per residue ¹	2.8

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)	193.2	0.2
0.2-0.5 (Medium)	25.3	0.5
>0.5 (Large)	3.6	5.27

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)	4.0	4.66
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

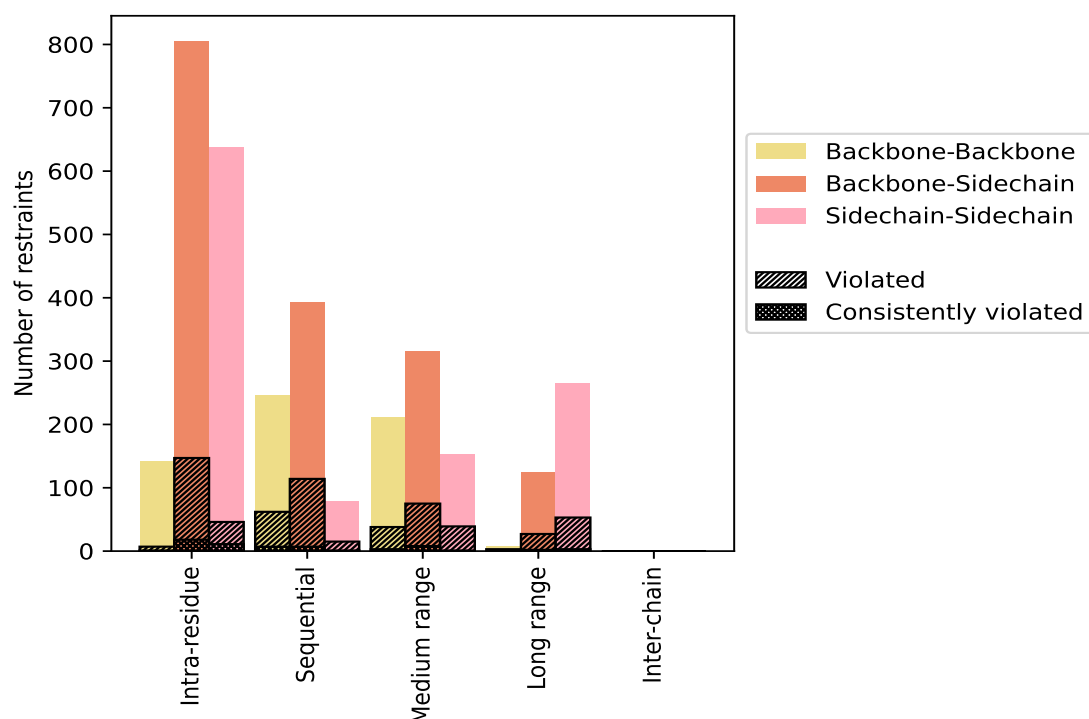
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1585	46.9	200	12.6	5.9	30	1.9	0.9
Backbone-Backbone	142	4.2	7	4.9	0.2	1	0.7	0.0
Backbone-Sidechain	805	23.8	147	18.3	4.4	18	2.2	0.5
Sidechain-Sidechain	638	18.9	46	7.2	1.4	11	1.7	0.3
Sequential ($i-j =1$)	717	21.2	191	26.6	5.7	15	2.1	0.4
Backbone-Backbone	246	7.3	62	25.2	1.8	7	2.8	0.2
Backbone-Sidechain	392	11.6	114	29.1	3.4	7	1.8	0.2
Sidechain-Sidechain	79	2.3	15	19.0	0.4	1	1.3	0.0
Medium range ($i-j >1$ & $i-j <5$)	623	18.4	143	23.0	4.2	6	1.0	0.2
Backbone-Backbone	211	6.2	38	18.0	1.1	3	1.4	0.1
Backbone-Sidechain	260	7.7	66	25.4	2.0	2	0.8	0.1
Sidechain-Sidechain	152	4.5	39	25.7	1.2	1	0.7	0.0
Long range ($i-j \geq 5$)	397	11.7	82	20.7	2.4	4	1.0	0.1
Backbone-Backbone	8	0.2	3	37.5	0.1	0	0.0	0.0
Backbone-Sidechain	124	3.7	26	21.0	0.8	1	0.8	0.0
Sidechain-Sidechain	265	7.8	53	20.0	1.6	3	1.1	0.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	57	1.7	10	17.5	0.3	7	12.3	0.2
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3379	100.0	626	18.5	18.5	62	1.8	1.8
Backbone-Backbone	607	18.0	110	18.1	3.3	11	1.8	0.3
Backbone-Sidechain	1638	48.5	363	22.2	10.7	35	2.1	1.0
Sidechain-Sidechain	1134	33.6	153	13.5	4.5	16	1.4	0.5

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	90	68	60	29	0	247	0.18	5.18	0.33	0.14
2	84	73	60	30	0	247	0.18	5.0	0.32	0.14
3	83	67	58	25	0	233	0.18	5.05	0.33	0.14
4	85	65	60	26	0	236	0.18	5.07	0.33	0.13
5	74	64	61	23	0	222	0.18	5.19	0.35	0.14
6	81	61	55	24	0	221	0.18	5.07	0.34	0.14
7	78	76	62	31	0	247	0.18	4.85	0.31	0.14
8	81	61	61	26	0	229	0.18	4.73	0.31	0.14
9	79	63	69	35	0	246	0.18	5.09	0.33	0.14
10	80	71	59	30	0	240	0.18	5.16	0.34	0.14

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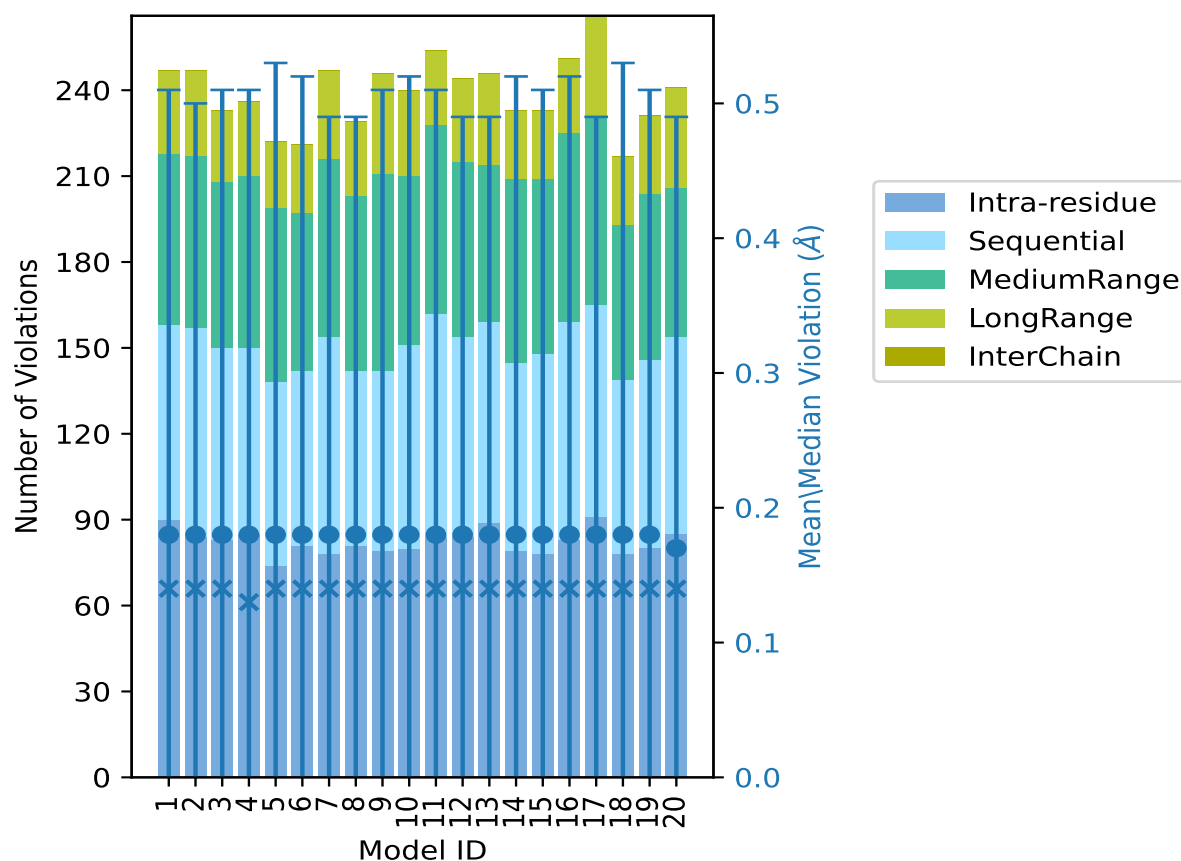
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	84	78	66	26	0	254	0.18	5.11	0.33	0.14
12	84	70	61	29	0	244	0.18	4.88	0.31	0.14
13	89	70	55	32	0	246	0.18	4.86	0.31	0.14
14	79	66	64	24	0	233	0.18	5.11	0.34	0.14
15	78	70	61	24	0	233	0.18	4.9	0.33	0.14
16	83	76	66	26	0	251	0.18	5.27	0.34	0.14
17	91	74	66	35	0	266	0.18	5.02	0.31	0.14
18	78	61	54	24	0	217	0.18	5.09	0.35	0.14
19	80	66	58	27	0	231	0.18	4.92	0.33	0.14
20	85	69	52	35	0	241	0.17	4.98	0.32	0.14

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

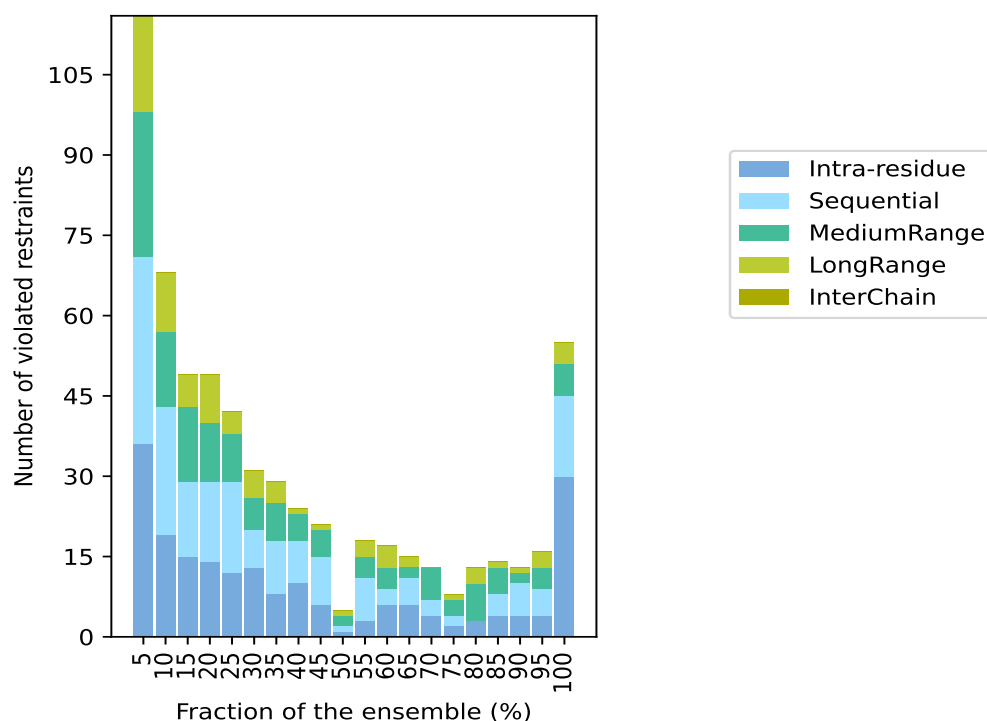
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2706(IR:1385, SQ:526, MR:480, LR:315, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
36	35	27	18	0	116	1	5.0
19	24	14	11	0	68	2	10.0
15	14	14	6	0	49	3	15.0
14	15	11	9	0	49	4	20.0
12	17	9	4	0	42	5	25.0
13	7	6	5	0	31	6	30.0
8	10	7	4	0	29	7	35.0
10	8	5	1	0	24	8	40.0
6	9	5	1	0	21	9	45.0
1	1	2	1	0	5	10	50.0
3	8	4	3	0	18	11	55.0
6	3	4	4	0	17	12	60.0
6	5	2	2	0	15	13	65.0
4	3	6	0	0	13	14	70.0
2	2	3	1	0	8	15	75.0
3	0	7	3	0	13	16	80.0
4	4	5	1	0	14	17	85.0
4	6	2	1	0	13	18	90.0
4	5	4	3	0	16	19	95.0
30	15	6	4	0	55	20	100.0

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

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

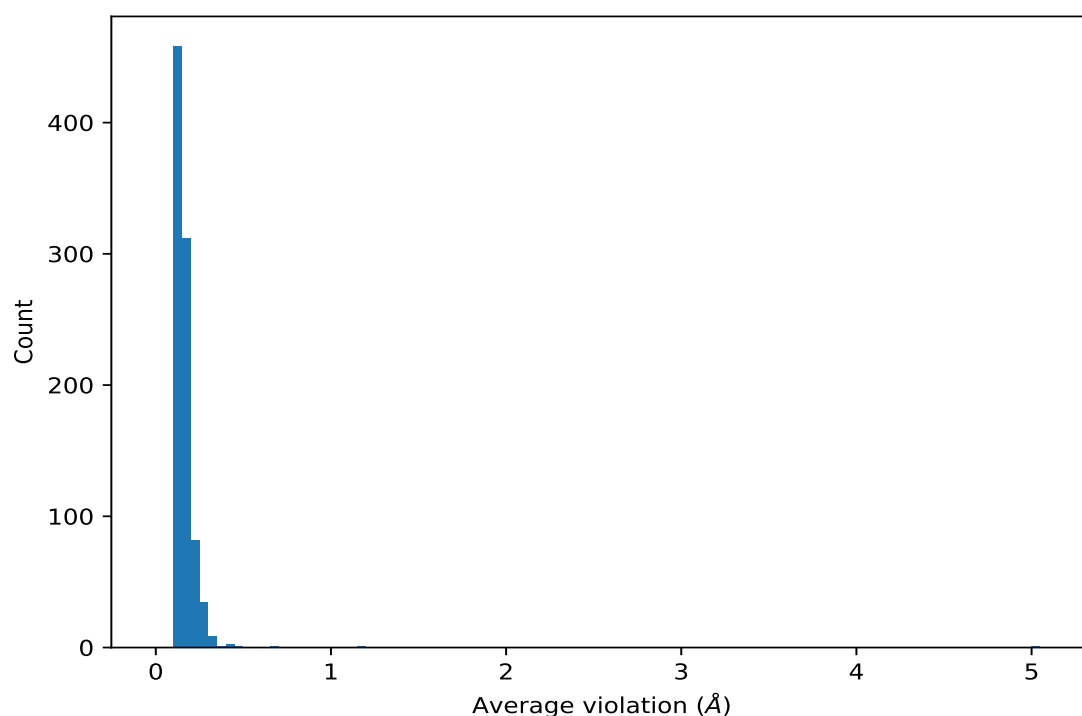
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	20	5.03	0.13	5.06
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	20	1.15	0.12	1.19
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	20	0.69	0.04	0.7
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	20	0.45	0.06	0.44
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	20	0.41	0.04	0.4
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	20	0.32	0.02	0.32
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	20	0.19	0.04	0.19
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	20	0.19	0.01	0.19
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	20	0.18	0.04	0.17
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	20	0.18	0.03	0.19
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	20	0.17	0.0	0.17
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	20	0.17	0.02	0.17
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	20	0.17	0.04	0.16
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	20	0.16	0.02	0.17
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	20	0.16	0.02	0.17
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	20	0.16	0.01	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	20	0.16	0.01	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	20	0.16	0.01	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	20	0.16	0.01	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	20	0.16	0.01	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	20	0.16	0.01	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	20	0.16	0.01	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	20	0.16	0.01	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	20	0.16	0.01	0.16
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	20	0.16	0.01	0.16
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	20	0.16	0.01	0.16
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	20	0.16	0.01	0.16
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	20	0.16	0.01	0.16
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	20	0.16	0.02	0.16
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	20	0.16	0.02	0.16
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	20	0.16	0.02	0.16
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	20	0.16	0.01	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	20	0.16	0.01	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	20	0.16	0.01	0.16
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	20	0.16	0.03	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	20	0.15	0.01	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	20	0.15	0.01	0.15
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	20	0.15	0.02	0.15
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	20	0.15	0.01	0.16
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	20	0.15	0.03	0.15
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	20	0.15	0.03	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	20	0.15	0.0	0.15
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	20	0.15	0.02	0.15
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	20	0.15	0.02	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	20	0.15	0.02	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	20	0.15	0.02	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	20	0.15	0.02	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	20	0.15	0.02	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	20	0.15	0.02	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	20	0.15	0.02	0.15
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	20	0.15	0.01	0.14
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	20	0.15	0.0	0.15
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	20	0.15	0.01	0.15
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	20	0.14	0.0	0.15
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	20	0.14	0.01	0.15
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	20	0.14	0.02	0.15
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	20	0.14	0.0	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	20	0.14	0.0	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	20	0.14	0.0	0.14
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	20	0.14	0.01	0.14
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	20	0.13	0.01	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	20	0.13	0.01	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	20	0.13	0.01	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	20	0.13	0.01	0.13
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	20	0.13	0.01	0.13
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	20	0.13	0.02	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	20	0.13	0.0	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	20	0.13	0.0	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	20	0.13	0.0	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	20	0.13	0.0	0.13
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	20	0.13	0.01	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	20	0.13	0.01	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	20	0.13	0.01	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	20	0.13	0.01	0.13
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	20	0.13	0.01	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	20	0.12	0.01	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	20	0.12	0.01	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	20	0.12	0.01	0.12
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	20	0.12	0.01	0.12
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	20	0.12	0.01	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	20	0.12	0.0	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	20	0.12	0.0	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	20	0.12	0.0	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	20	0.12	0.0	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	20	0.12	0.0	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	20	0.12	0.0	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	20	0.12	0.0	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	20	0.12	0.0	0.12
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	20	0.12	0.01	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	20	0.12	0.01	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	20	0.12	0.01	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	20	0.12	0.0	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	20	0.12	0.0	0.12
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	20	0.12	0.01	0.12
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	20	0.12	0.01	0.12
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	20	0.11	0.01	0.11
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	19	0.18	0.03	0.18
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	19	0.17	0.04	0.16
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	19	0.17	0.04	0.16
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	19	0.17	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	19	0.17	0.03	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	19	0.17	0.03	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	19	0.17	0.03	0.17
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	19	0.16	0.01	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	19	0.16	0.01	0.16
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	19	0.16	0.04	0.16
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	19	0.16	0.04	0.16
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	19	0.15	0.03	0.15
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	19	0.15	0.02	0.15
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	19	0.15	0.01	0.15
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	19	0.15	0.04	0.13
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	19	0.15	0.04	0.13
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	19	0.14	0.01	0.14
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	19	0.14	0.02	0.14
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	19	0.13	0.02	0.12
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	19	0.13	0.02	0.12
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	19	0.13	0.01	0.13
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	19	0.13	0.02	0.13
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	19	0.12	0.01	0.13
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	19	0.12	0.01	0.13
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	19	0.12	0.01	0.12
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	18	0.18	0.01	0.18
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	18	0.16	0.03	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	18	0.16	0.03	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	18	0.16	0.03	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	18	0.16	0.03	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	18	0.16	0.03	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	18	0.16	0.03	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	18	0.16	0.03	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	18	0.16	0.03	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	18	0.16	0.03	0.15
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	18	0.15	0.01	0.15
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	18	0.15	0.01	0.15
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	18	0.15	0.02	0.15
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	18	0.15	0.02	0.15
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	18	0.15	0.02	0.15
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	18	0.14	0.03	0.14
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	18	0.14	0.04	0.13
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	18	0.13	0.01	0.13
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	18	0.13	0.02	0.13
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	18	0.13	0.02	0.12
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	18	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	18	0.12	0.01	0.12
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	18	0.12	0.01	0.12
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	18	0.11	0.01	0.11
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	18	0.11	0.01	0.11
(1,361)	1:1817:A:ALA:HB1	1:1818:A:SER:HA	17	0.26	0.1	0.18
(1,361)	1:1817:A:ALA:HA	1:1818:A:SER:HA	17	0.26	0.1	0.18
(1,361)	1:1817:A:ALA:HB3	1:1818:A:SER:HA	17	0.26	0.1	0.18
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	17	0.19	0.05	0.2
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	17	0.19	0.05	0.2
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	17	0.19	0.05	0.2
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	17	0.17	0.03	0.18
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	17	0.16	0.03	0.15
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	17	0.15	0.03	0.16
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	17	0.15	0.03	0.16
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	17	0.15	0.03	0.16
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	17	0.15	0.03	0.16
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	17	0.15	0.03	0.16
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	17	0.15	0.03	0.16
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	17	0.15	0.03	0.16
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	17	0.15	0.03	0.16
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	17	0.15	0.03	0.16
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	17	0.15	0.01	0.15
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	17	0.15	0.03	0.15
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	17	0.15	0.03	0.15
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	17	0.14	0.02	0.14
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	17	0.13	0.02	0.13
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	17	0.13	0.02	0.13
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	17	0.13	0.02	0.12
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	17	0.13	0.02	0.12
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	17	0.13	0.02	0.12
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	17	0.12	0.03	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	17	0.12	0.03	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	17	0.12	0.03	0.11
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	17	0.12	0.01	0.11
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	17	0.12	0.01	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	17	0.12	0.01	0.12
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	17	0.11	0.01	0.11
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	16	0.35	0.13	0.32
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	16	0.19	0.07	0.19
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	16	0.18	0.04	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	16	0.18	0.02	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	16	0.18	0.02	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	16	0.18	0.02	0.18
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	16	0.17	0.04	0.17
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	16	0.17	0.04	0.17
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	16	0.17	0.04	0.17
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	16	0.17	0.05	0.15
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	16	0.14	0.03	0.13
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	16	0.14	0.01	0.14
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	16	0.14	0.01	0.14
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	16	0.14	0.01	0.14
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	16	0.13	0.01	0.14
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	16	0.13	0.02	0.12
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	16	0.13	0.02	0.12
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	16	0.13	0.02	0.12
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	16	0.12	0.01	0.12
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	16	0.12	0.02	0.12
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	16	0.12	0.01	0.12
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	16	0.12	0.01	0.12
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	16	0.12	0.01	0.12
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE2	15	0.16	0.03	0.16
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE3	15	0.16	0.03	0.16
(1,3258)	1:1862:A:ASP:HA	1:1865:A:ILE:HB	15	0.15	0.02	0.16
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD21	15	0.14	0.02	0.14
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD22	15	0.14	0.02	0.14
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD23	15	0.14	0.02	0.14
(1,330)	1:1827:A:ALA:H	1:1826:A:LYS:HB3	15	0.14	0.04	0.13
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB2	15	0.14	0.04	0.12
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB3	15	0.14	0.04	0.12
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE1	15	0.12	0.01	0.12
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE2	15	0.12	0.01	0.12
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE1	15	0.12	0.01	0.12
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE2	15	0.12	0.01	0.12
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE1	15	0.12	0.01	0.12
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE2	15	0.12	0.01	0.12
(1,2426)	1:1907:A:MET:HA	1:1908:A:GLU:H	15	0.12	0.01	0.12
(1,986)	1:1837:A:PHE:H	1:1840:A:ILE:H	15	0.11	0.01	0.11
(1,573)	1:1817:A:ALA:HB1	1:1819:A:ARG:H	14	0.2	0.05	0.18
(1,573)	1:1817:A:ALA:HB2	1:1819:A:ARG:H	14	0.2	0.05	0.18
(1,573)	1:1817:A:ALA:HB3	1:1819:A:ARG:H	14	0.2	0.05	0.18
(1,3190)	1:1923:A:GLY:H	1:1922:A:ILE:H	14	0.18	0.04	0.2
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG21	14	0.18	0.05	0.19
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG22	14	0.18	0.05	0.19
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG23	14	0.18	0.05	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG21	14	0.18	0.05	0.19
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG22	14	0.18	0.05	0.19
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG23	14	0.18	0.05	0.19
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG21	14	0.18	0.05	0.19
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG22	14	0.18	0.05	0.19
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG23	14	0.18	0.05	0.19
(1,474)	1:1877:A:GLN:HG2	1:1874:A:GLN:HA	14	0.17	0.04	0.17
(1,897)	1:1946:A:CYS:H	1:1945:A:ARG:HB2	14	0.16	0.03	0.16
(1,994)	1:1889:A:MET:HE1	1:1885:A:ARG:HG2	14	0.16	0.03	0.16
(1,994)	1:1889:A:MET:HE2	1:1885:A:ARG:HG2	14	0.16	0.03	0.16
(1,994)	1:1889:A:MET:HE3	1:1885:A:ARG:HG2	14	0.16	0.03	0.16
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE2	14	0.14	0.0	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE3	14	0.14	0.0	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE2	14	0.14	0.0	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE3	14	0.14	0.0	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD11	14	0.14	0.01	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD12	14	0.14	0.01	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD13	14	0.14	0.01	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD11	14	0.14	0.01	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD12	14	0.14	0.01	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD13	14	0.14	0.01	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD11	14	0.14	0.01	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD12	14	0.14	0.01	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD13	14	0.14	0.01	0.14
(1,526)	1:1885:A:ARG:HA	1:1888:A:GLU:HG2	14	0.14	0.03	0.13
(1,1858)	1:1934:A:VAL:HA	1:1937:A:GLU:H	14	0.14	0.02	0.14
(1,1342)	1:1859:A:LYS:H	1:1858:A:LYS:HG3	14	0.12	0.01	0.11
(1,2298)	1:1891:A:ARG:H	1:1891:A:ARG:HB2	14	0.11	0.01	0.12
(1,1029)	1:1836:A:ILE:HA	1:1836:A:ILE:HG13	14	0.1	0.0	0.1
(1,2089)	1:1916:A:THR:H	1:1915:A:PRO:HB2	13	0.2	0.04	0.2
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE2	13	0.18	0.03	0.17
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE3	13	0.18	0.03	0.17
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	13	0.18	0.03	0.17
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	13	0.18	0.03	0.17
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE1	13	0.15	0.04	0.14
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE2	13	0.15	0.04	0.14
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE1	13	0.15	0.04	0.14
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE2	13	0.15	0.04	0.14
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE1	13	0.15	0.04	0.14
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE2	13	0.15	0.04	0.14
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG2	13	0.14	0.05	0.12
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG3	13	0.14	0.05	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1312)	1:1859:A:LYS:HE2	1:1859:A:LYS:HD2	13	0.14	0.0	0.14
(1,1312)	1:1859:A:LYS:HE3	1:1859:A:LYS:HD2	13	0.14	0.0	0.14
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE1	13	0.14	0.03	0.13
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE2	13	0.14	0.03	0.13
(1,1567)	1:1894:A:LYS:H	1:1894:A:LYS:HD2	13	0.14	0.03	0.14
(1,258)	1:1941:A:ILE:HA	1:1941:A:ILE:HG13	13	0.13	0.01	0.13
(1,3159)	1:1822:A:GLU:H	1:1822:A:GLU:HG2	13	0.13	0.04	0.12
(1,828)	1:1851:A:ALA:HB1	1:1852:A:GLU:HG2	13	0.13	0.01	0.13
(1,828)	1:1851:A:ALA:HB2	1:1852:A:GLU:HG2	13	0.13	0.01	0.13
(1,828)	1:1851:A:ALA:HB3	1:1852:A:GLU:HG2	13	0.13	0.01	0.13
(1,2807)	1:1889:A:MET:H	1:1888:A:GLU:HB2	13	0.13	0.02	0.12
(1,509)	1:1865:A:ILE:HG21	1:1866:A:GLU:H	13	0.13	0.02	0.12
(1,509)	1:1865:A:ILE:HG22	1:1866:A:GLU:H	13	0.13	0.02	0.12
(1,509)	1:1865:A:ILE:HG23	1:1866:A:GLU:H	13	0.13	0.02	0.12
(1,2648)	1:1853:A:LEU:HA	1:1856:A:TYR:HB3	13	0.12	0.01	0.11
(1,3032)	1:1835:A:GLU:H	1:1833:A:LEU:HB2	13	0.11	0.01	0.11
(1,2451)	1:1861:A:SER:H	1:1860:A:TYR:HB3	13	0.11	0.01	0.11
(1,807)	1:1907:A:MET:H	1:1906:A:GLN:HG2	12	0.22	0.05	0.22
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG21	12	0.18	0.06	0.18
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG22	12	0.18	0.06	0.18
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG23	12	0.18	0.06	0.18
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG21	12	0.18	0.06	0.18
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG22	12	0.18	0.06	0.18
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG23	12	0.18	0.06	0.18
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG21	12	0.18	0.06	0.18
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG22	12	0.18	0.06	0.18
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG23	12	0.18	0.06	0.18
(1,102)	1:1940:A:LYS:HA	1:1940:A:LYS:HD3	12	0.18	0.03	0.18
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG21	12	0.17	0.04	0.17
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG22	12	0.17	0.04	0.17
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG23	12	0.17	0.04	0.17
(1,125)	1:1822:A:GLU:HG2	1:1823:A:LYS:H	12	0.16	0.05	0.16
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD11	12	0.15	0.03	0.15
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD12	12	0.15	0.03	0.15
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD13	12	0.15	0.03	0.15
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG21	12	0.15	0.02	0.15
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG22	12	0.15	0.02	0.15
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG23	12	0.15	0.02	0.15
(1,2489)	1:1893:A:GLY:H	1:1891:A:ARG:HB2	12	0.15	0.03	0.15
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	12	0.15	0.01	0.14
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	12	0.15	0.01	0.14
(1,3168)	1:1874:A:GLN:HB2	1:1874:A:GLN:HG2	12	0.14	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2606)	1:1840:A:ILE:HD11	1:1850:A:LEU:HA	12	0.14	0.02	0.14
(1,2606)	1:1840:A:ILE:HD12	1:1850:A:LEU:HA	12	0.14	0.02	0.14
(1,2606)	1:1840:A:ILE:HD13	1:1850:A:LEU:HA	12	0.14	0.02	0.14
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD11	12	0.13	0.02	0.14
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD12	12	0.13	0.02	0.14
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD13	12	0.13	0.02	0.14
(1,1806)	1:1840:A:ILE:HB	1:1876:A:PHE:HZ	12	0.13	0.02	0.12
(1,461)	1:1845:A:ASN:HD21	1:1839:A:LYS:HG3	12	0.13	0.01	0.12
(1,2685)	1:1859:A:LYS:HA	1:1859:A:LYS:HG3	12	0.12	0.01	0.12
(1,2502)	1:1892:A:GLU:HG3	1:1892:A:GLU:HB3	12	0.11	0.01	0.1
(1,3134)	1:1852:A:GLU:HG2	1:1852:A:GLU:HB3	12	0.11	0.01	0.1
(3,56)	1:1945:A:ARG:N	1:1941:A:ILE:O	11	0.27	0.16	0.2
(1,697)	1:1956:A:ARG:H	1:1956:A:ARG:HB3	11	0.21	0.05	0.22
(1,2328)	1:1950:A:ASN:H	1:1951:A:THR:H	11	0.21	0.07	0.21
(1,3246)	1:1904:A:SER:H	1:1905:A:PRO:HD2	11	0.18	0.06	0.16
(1,2854)	1:1924:A:ASN:H	1:1924:A:ASN:HA	11	0.18	0.03	0.18
(1,2490)	1:1820:A:ILE:HD11	1:1821:A:ASP:H	11	0.17	0.04	0.18
(1,2490)	1:1820:A:ILE:HD12	1:1821:A:ASP:H	11	0.17	0.04	0.18
(1,2490)	1:1820:A:ILE:HD13	1:1821:A:ASP:H	11	0.17	0.04	0.18
(1,1718)	1:1902:A:GLY:H	1:1901:A:THR:HA	11	0.16	0.03	0.17
(1,3075)	1:1942:A:LEU:HB3	1:1838:A:LYS:HG3	11	0.16	0.05	0.16
(1,239)	1:1896:A:ARG:H	1:1897:A:ILE:HB	11	0.16	0.04	0.14
(1,889)	1:1889:A:MET:H	1:1892:A:GLU:HG3	11	0.14	0.04	0.13
(1,2731)	1:1916:A:THR:HG21	1:1914:A:THR:HB	11	0.14	0.02	0.14
(1,2731)	1:1916:A:THR:HG22	1:1914:A:THR:HB	11	0.14	0.02	0.14
(1,2731)	1:1916:A:THR:HG23	1:1914:A:THR:HB	11	0.14	0.02	0.14
(1,1556)	1:1853:A:LEU:HD11	1:1857:A:LYS:HD2	11	0.14	0.02	0.14
(1,1556)	1:1853:A:LEU:HD12	1:1857:A:LYS:HD2	11	0.14	0.02	0.14
(1,1556)	1:1853:A:LEU:HD13	1:1857:A:LYS:HD2	11	0.14	0.02	0.14
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD11	11	0.14	0.03	0.13
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD12	11	0.14	0.03	0.13
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD13	11	0.14	0.03	0.13
(1,2893)	1:1887:A:ILE:HA	1:1890:A:GLU:HB2	11	0.14	0.02	0.14
(1,2287)	1:1863:A:ALA:H	1:1862:A:ASP:HA	11	0.12	0.02	0.12
(1,2929)	1:1922:A:ILE:HA	1:1922:A:ILE:HB	11	0.12	0.0	0.12
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD11	11	0.11	0.01	0.11
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD12	11	0.11	0.01	0.11
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD13	11	0.11	0.01	0.11
(1,2818)	1:1886:A:VAL:H	1:1885:A:ARG:HG3	11	0.11	0.01	0.11
(1,615)	1:1880:A:VAL:H	1:1881:A:GLU:HB2	11	0.11	0.0	0.11
(1,1952)	1:1840:A:ILE:HG21	1:1846:A:THR:HB	10	0.19	0.06	0.18
(1,1952)	1:1840:A:ILE:HG22	1:1846:A:THR:HB	10	0.19	0.06	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1952)	1:1840:A:ILE:HG23	1:1846:A:THR:HB	10	0.19	0.06	0.18
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG21	10	0.18	0.05	0.16
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG22	10	0.18	0.05	0.16
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG23	10	0.18	0.05	0.16
(1,736)	1:1898:A:SER:H	1:1897:A:ILE:H	10	0.16	0.06	0.15
(1,2179)	1:1940:A:LYS:HA	1:1943:A:ARG:HB2	10	0.14	0.02	0.14
(1,1200)	1:1922:A:ILE:HB	1:1922:A:ILE:H	10	0.12	0.01	0.12
(3,45)	1:1934:A:VAL:N	1:1930:A:VAL:O	9	0.4	0.26	0.31
(1,2265)	1:1824:A:SER:H	1:1823:A:LYS:HB2	9	0.25	0.1	0.26
(1,981)	1:1818:A:SER:HB2	1:1820:A:ILE:H	9	0.22	0.05	0.2
(1,981)	1:1818:A:SER:HB3	1:1820:A:ILE:H	9	0.22	0.05	0.2
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD11	9	0.2	0.06	0.2
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD12	9	0.2	0.06	0.2
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD13	9	0.2	0.06	0.2
(1,558)	1:1929:A:GLU:H	1:1928:A:GLU:HA	9	0.19	0.06	0.2
(1,2515)	1:1898:A:SER:H	1:1897:A:ILE:HB	9	0.19	0.09	0.13
(1,3172)	1:1902:A:GLY:H	1:1901:A:THR:HB	9	0.18	0.07	0.17
(1,1439)	1:1928:A:GLU:HA	1:1928:A:GLU:HB3	9	0.17	0.03	0.16
(1,3020)	1:1948:A:LEU:HA	1:1949:A:ASP:H	9	0.17	0.03	0.17
(1,1272)	1:1895:A:GLY:H	1:1893:A:GLY:H	9	0.16	0.03	0.14
(1,888)	1:1887:A:ILE:HA	1:1890:A:GLU:HG2	9	0.14	0.04	0.13
(1,1121)	1:1820:A:ILE:H	1:1820:A:ILE:HG12	9	0.14	0.02	0.14
(1,3142)	1:1900:A:SER:H	1:1900:A:SER:HA	9	0.14	0.02	0.14
(1,2886)	1:1905:A:PRO:HD2	1:1905:A:PRO:HB2	9	0.14	0.03	0.13
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG21	9	0.13	0.02	0.12
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG22	9	0.13	0.02	0.12
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG23	9	0.13	0.02	0.12
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG21	9	0.13	0.02	0.12
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG22	9	0.13	0.02	0.12
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG23	9	0.13	0.02	0.12
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG21	9	0.13	0.02	0.12
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG22	9	0.13	0.02	0.12
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG23	9	0.13	0.02	0.12
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD11	9	0.13	0.02	0.12
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD12	9	0.13	0.02	0.12
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD13	9	0.13	0.02	0.12
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD11	9	0.13	0.02	0.12
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD12	9	0.13	0.02	0.12
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD13	9	0.13	0.02	0.12
(1,2564)	1:1909:A:VAL:H	1:1910:A:THR:H	9	0.13	0.03	0.11
(1,1000)	1:1917:A:SER:HA	1:1918:A:THR:H	9	0.13	0.02	0.12
(1,952)	1:1949:A:ASP:HA	1:1949:A:ASP:HB3	9	0.12	0.03	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,844)	1:1890:A:GLU:HA	1:1890:A:GLU:HG2	9	0.11	0.01	0.11
(1,325)	1:1936:A:LEU:HB2	1:1933:A:SER:HA	9	0.11	0.01	0.11
(1,3238)	1:1920:A:SER:H	1:1919:A:VAL:H	9	0.11	0.0	0.11
(1,972)	1:1952:A:LYS:H	1:1951:A:THR:HB	8	0.22	0.06	0.2
(1,116)	1:1948:A:LEU:H	1:1949:A:ASP:H	8	0.21	0.05	0.2
(1,1790)	1:1927:A:GLY:H	1:1925:A:THR:HB	8	0.21	0.08	0.2
(1,525)	1:1924:A:ASN:H	1:1923:A:GLY:H	8	0.2	0.06	0.19
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE2	8	0.18	0.0	0.18
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE3	8	0.18	0.0	0.18
(1,3303)	1:1898:A:SER:H	1:1897:A:ILE:HG13	8	0.18	0.03	0.18
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG11	8	0.17	0.05	0.18
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG12	8	0.17	0.05	0.18
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG13	8	0.17	0.05	0.18
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE2	8	0.16	0.02	0.16
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE3	8	0.16	0.02	0.16
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE2	8	0.16	0.02	0.16
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE3	8	0.16	0.02	0.16
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE2	8	0.16	0.02	0.16
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE3	8	0.16	0.02	0.16
(1,2037)	1:1843:A:LYS:HE3	1:1844:A:GLU:HG3	8	0.15	0.03	0.16
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG11	8	0.15	0.03	0.14
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG12	8	0.15	0.03	0.14
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG13	8	0.15	0.03	0.14
(1,3245)	1:1891:A:ARG:HG3	1:1891:A:ARG:HE	8	0.14	0.01	0.14
(1,2504)	1:1867:A:PRO:HA	1:1871:A:ASN:HD21	8	0.14	0.02	0.14
(1,466)	1:1917:A:SER:H	1:1917:A:SER:HB2	8	0.14	0.04	0.12
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD2	8	0.14	0.02	0.13
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD3	8	0.14	0.02	0.13
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD2	8	0.14	0.02	0.13
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD3	8	0.14	0.02	0.13
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD2	8	0.14	0.02	0.13
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD3	8	0.14	0.02	0.13
(1,2261)	1:1906:A:GLN:H	1:1906:A:GLN:HB2	8	0.13	0.02	0.14
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD1	8	0.13	0.01	0.13
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD2	8	0.13	0.01	0.13
(1,2424)	1:1950:A:ASN:HB2	1:1950:A:ASN:HA	8	0.13	0.02	0.12
(1,2907)	1:1894:A:LYS:H	1:1894:A:LYS:HE3	8	0.12	0.01	0.12
(1,1479)	1:1867:A:PRO:HD2	1:1868:A:PHE:H	8	0.12	0.02	0.12
(1,2483)	1:1908:A:GLU:H	1:1908:A:GLU:HG2	8	0.11	0.01	0.12
(1,1395)	1:1893:A:GLY:H	1:1892:A:GLU:HG3	8	0.11	0.01	0.11
(1,1504)	1:1855:A:GLU:HA	1:1858:A:LYS:HE2	8	0.11	0.01	0.11
(1,1187)	1:1838:A:LYS:H	1:1838:A:LYS:HG3	8	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1833)	1:1941:A:ILE:H	1:1941:A:ILE:HA	8	0.11	0.01	0.11
(1,2580)	1:1929:A:GLU:H	1:1928:A:GLU:HG2	7	0.3	0.16	0.27
(1,97)	1:1927:A:GLY:H	1:1929:A:GLU:H	7	0.27	0.13	0.28
(1,2234)	1:1924:A:ASN:H	1:1922:A:ILE:HA	7	0.25	0.1	0.21
(1,2974)	1:1930:A:VAL:H	1:1929:A:GLU:HB3	7	0.23	0.05	0.24
(1,3086)	1:1903:A:ILE:H	1:1900:A:SER:HB3	7	0.21	0.08	0.19
(1,2099)	1:1927:A:GLY:H	1:1928:A:GLU:H	7	0.2	0.04	0.19
(1,1675)	1:1924:A:ASN:H	1:1924:A:ASN:HB2	7	0.19	0.05	0.21
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG21	7	0.17	0.04	0.16
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG22	7	0.17	0.04	0.16
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG23	7	0.17	0.04	0.16
(1,1963)	1:1942:A:LEU:H	1:1941:A:ILE:HG12	7	0.17	0.02	0.18
(1,377)	1:1820:A:ILE:HB	1:1823:A:LYS:HG2	7	0.17	0.06	0.15
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG21	7	0.17	0.03	0.15
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG22	7	0.17	0.03	0.15
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG23	7	0.17	0.03	0.15
(1,2682)	1:1826:A:LYS:HB2	1:1871:A:ASN:HD22	7	0.15	0.04	0.15
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG21	7	0.15	0.05	0.14
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG22	7	0.15	0.05	0.14
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG23	7	0.15	0.05	0.14
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG21	7	0.15	0.05	0.14
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG22	7	0.15	0.05	0.14
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG23	7	0.15	0.05	0.14
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG21	7	0.15	0.05	0.14
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG22	7	0.15	0.05	0.14
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG23	7	0.15	0.05	0.14
(1,1458)	1:1955:A:ASP:H	1:1954:A:ASP:HA	7	0.14	0.02	0.14
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD11	7	0.14	0.03	0.14
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD12	7	0.14	0.03	0.14
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD13	7	0.14	0.03	0.14
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD11	7	0.14	0.03	0.14
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD12	7	0.14	0.03	0.14
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD13	7	0.14	0.03	0.14
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD11	7	0.14	0.03	0.14
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD12	7	0.14	0.03	0.14
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD13	7	0.14	0.03	0.14
(1,2518)	1:1848:A:GLU:HB2	1:1839:A:LYS:HD2	7	0.14	0.02	0.13
(1,1619)	1:1887:A:ILE:HG21	1:1890:A:GLU:HB2	7	0.13	0.02	0.13
(1,1619)	1:1887:A:ILE:HG22	1:1890:A:GLU:HB2	7	0.13	0.02	0.13
(1,1619)	1:1887:A:ILE:HG23	1:1890:A:GLU:HB2	7	0.13	0.02	0.13
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG21	7	0.13	0.03	0.12
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG22	7	0.13	0.03	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG23	7	0.13	0.03	0.12
(1,2737)	1:1823:A:LYS:HA	1:1824:A:SER:H	7	0.13	0.01	0.13
(1,595)	1:1823:A:LYS:HA	1:1823:A:LYS:HB2	7	0.13	0.01	0.12
(1,1978)	1:1941:A:ILE:H	1:1940:A:LYS:H	7	0.12	0.01	0.12
(1,2801)	1:1874:A:GLN:HA	1:1874:A:GLN:HG2	7	0.12	0.01	0.12
(1,2975)	1:1892:A:GLU:H	1:1891:A:ARG:HG3	7	0.12	0.01	0.11
(1,937)	1:1894:A:LYS:H	1:1894:A:LYS:HG3	7	0.11	0.01	0.11
(1,1080)	1:1847:A:LYS:HA	1:1850:A:LEU:HB2	7	0.11	0.01	0.11
(1,2415)	1:1857:A:LYS:HA	1:1857:A:LYS:HG2	7	0.11	0.01	0.11
(1,669)	1:1890:A:GLU:H	1:1890:A:GLU:HG3	7	0.11	0.01	0.11
(1,2055)	1:1922:A:ILE:HA	1:1922:A:ILE:HG12	7	0.11	0.01	0.11
(1,516)	1:1886:A:VAL:HG21	1:1882:A:ARG:HG3	7	0.11	0.01	0.1
(1,516)	1:1886:A:VAL:HG22	1:1882:A:ARG:HG3	7	0.11	0.01	0.1
(1,516)	1:1886:A:VAL:HG23	1:1882:A:ARG:HG3	7	0.11	0.01	0.1
(1,3018)	1:1863:A:ALA:HB1	1:1862:A:ASP:H	6	0.29	0.01	0.3
(1,3018)	1:1863:A:ALA:HB2	1:1862:A:ASP:H	6	0.29	0.01	0.3
(1,3018)	1:1863:A:ALA:HB3	1:1862:A:ASP:H	6	0.29	0.01	0.3
(1,583)	1:1867:A:PRO:HA	1:1870:A:LYS:HB2	6	0.27	0.03	0.29
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG21	6	0.26	0.08	0.3
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG22	6	0.26	0.08	0.3
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG23	6	0.26	0.08	0.3
(1,1598)	1:1955:A:ASP:H	1:1953:A:GLN:HG2	6	0.24	0.13	0.21
(1,2522)	1:1903:A:ILE:H	1:1903:A:ILE:HG13	6	0.24	0.04	0.24
(1,579)	1:1897:A:ILE:H	1:1897:A:ILE:HG12	6	0.22	0.06	0.22
(1,442)	1:1948:A:LEU:HB2	1:1949:A:ASP:H	6	0.2	0.04	0.22
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG21	6	0.2	0.0	0.2
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG22	6	0.2	0.0	0.2
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG23	6	0.2	0.0	0.2
(1,1755)	1:1907:A:MET:H	1:1906:A:GLN:HB2	6	0.19	0.05	0.18
(1,758)	1:1823:A:LYS:H	1:1823:A:LYS:HG3	6	0.19	0.02	0.18
(1,3321)	1:1954:A:ASP:HA	1:1954:A:ASP:HB3	6	0.19	0.04	0.18
(1,90)	1:1945:A:ARG:HA	1:1945:A:ARG:HB2	6	0.18	0.0	0.18
(1,2048)	1:1838:A:LYS:HD2	1:1838:A:LYS:HE3	6	0.18	0.07	0.14
(1,2048)	1:1838:A:LYS:HD3	1:1838:A:LYS:HE3	6	0.18	0.07	0.14
(1,61)	1:1948:A:LEU:HD11	1:1949:A:ASP:H	6	0.17	0.03	0.16
(1,61)	1:1948:A:LEU:HD12	1:1949:A:ASP:H	6	0.17	0.03	0.16
(1,61)	1:1948:A:LEU:HD13	1:1949:A:ASP:H	6	0.17	0.03	0.16
(1,601)	1:1923:A:GLY:H	1:1922:A:ILE:HG13	6	0.16	0.04	0.15
(1,2973)	1:1870:A:LYS:HA	1:1874:A:GLN:HE21	6	0.16	0.05	0.15
(1,2672)	1:1906:A:GLN:HA	1:1906:A:GLN:HG2	6	0.15	0.01	0.15
(1,2672)	1:1906:A:GLN:HA	1:1906:A:GLN:HG3	6	0.15	0.01	0.15
(1,3312)	1:1906:A:GLN:H	1:1906:A:GLN:HB3	6	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,375)	1:1896:A:ARG:HG2	1:1896:A:ARG:HD2	6	0.14	0.06	0.11
(1,375)	1:1896:A:ARG:HG2	1:1896:A:ARG:HD3	6	0.14	0.06	0.11
(1,2165)	1:1841:A:GLY:H	1:1876:A:PHE:HE1	6	0.14	0.03	0.13
(1,2165)	1:1841:A:GLY:H	1:1876:A:PHE:HE2	6	0.14	0.03	0.13
(1,1098)	1:1905:A:PRO:HD2	1:1904:A:SER:HB2	6	0.13	0.02	0.13
(1,1098)	1:1905:A:PRO:HD2	1:1904:A:SER:HB3	6	0.13	0.02	0.13
(1,96)	1:1828:A:LYS:HA	1:1831:A:ASP:HB3	6	0.13	0.02	0.12
(1,2330)	1:1922:A:ILE:HG21	1:1922:A:ILE:H	6	0.13	0.01	0.13
(1,2330)	1:1922:A:ILE:HG22	1:1922:A:ILE:H	6	0.13	0.01	0.13
(1,2330)	1:1922:A:ILE:HG23	1:1922:A:ILE:H	6	0.13	0.01	0.13
(1,135)	1:1939:A:LEU:HD11	1:1839:A:LYS:HD2	6	0.12	0.02	0.13
(1,135)	1:1939:A:LEU:HD12	1:1839:A:LYS:HD2	6	0.12	0.02	0.13
(1,135)	1:1939:A:LEU:HD13	1:1839:A:LYS:HD2	6	0.12	0.02	0.13
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD21	6	0.12	0.02	0.12
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD22	6	0.12	0.02	0.12
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD23	6	0.12	0.02	0.12
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD21	6	0.12	0.02	0.12
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD22	6	0.12	0.02	0.12
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD23	6	0.12	0.02	0.12
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD21	6	0.12	0.02	0.12
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD22	6	0.12	0.02	0.12
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD23	6	0.12	0.02	0.12
(1,1747)	1:1853:A:LEU:HD11	1:1856:A:TYR:HB2	6	0.12	0.01	0.12
(1,1747)	1:1853:A:LEU:HD12	1:1856:A:TYR:HB2	6	0.12	0.01	0.12
(1,1747)	1:1853:A:LEU:HD13	1:1856:A:TYR:HB2	6	0.12	0.01	0.12
(1,2842)	1:1950:A:ASN:HB2	1:1951:A:THR:H	6	0.12	0.01	0.12
(1,472)	1:1894:A:LYS:H	1:1894:A:LYS:HB3	6	0.12	0.0	0.12
(1,1678)	1:1832:A:PHE:HD1	1:1856:A:TYR:HE1	6	0.11	0.01	0.11
(1,1678)	1:1832:A:PHE:HD1	1:1856:A:TYR:HE2	6	0.11	0.01	0.11
(1,1678)	1:1832:A:PHE:HD2	1:1856:A:TYR:HE1	6	0.11	0.01	0.11
(1,1678)	1:1832:A:PHE:HD2	1:1856:A:TYR:HE2	6	0.11	0.01	0.11
(1,2051)	1:1840:A:ILE:HA	1:1846:A:THR:HA	6	0.11	0.01	0.11
(1,2760)	1:1903:A:ILE:HA	1:1903:A:ILE:HG12	6	0.11	0.01	0.11
(1,1703)	1:1821:A:ASP:HB3	1:1823:A:LYS:H	5	0.28	0.05	0.25
(1,1752)	1:1899:A:THR:HG21	1:1899:A:THR:H	5	0.23	0.09	0.2
(1,1752)	1:1899:A:THR:HG22	1:1899:A:THR:H	5	0.23	0.09	0.2
(1,1752)	1:1899:A:THR:HG23	1:1899:A:THR:H	5	0.23	0.09	0.2
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG21	5	0.23	0.1	0.22
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG22	5	0.23	0.1	0.22
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG23	5	0.23	0.1	0.22
(1,2017)	1:1838:A:LYS:HG3	1:1838:A:LYS:HE3	5	0.23	0.06	0.26
(1,3138)	1:1926:A:ASN:H	1:1926:A:ASN:HD22	5	0.22	0.08	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,74)	1:1954:A:ASP:H	1:1953:A:GLN:HG2	5	0.21	0.02	0.22
(1,2924)	1:1900:A:SER:HB2	1:1903:A:ILE:HB	5	0.2	0.03	0.21
(1,679)	1:1954:A:ASP:H	1:1953:A:GLN:HB2	5	0.2	0.08	0.18
(1,1957)	1:1927:A:GLY:H	1:1926:A:ASN:HB2	5	0.2	0.05	0.2
(1,2347)	1:1820:A:ILE:HB	1:1821:A:ASP:H	5	0.2	0.02	0.2
(1,2847)	1:1921:A:SER:HA	1:1922:A:ILE:H	5	0.19	0.02	0.19
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD11	5	0.18	0.02	0.17
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD12	5	0.18	0.02	0.17
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD13	5	0.18	0.02	0.17
(1,1470)	1:1824:A:SER:H	1:1827:A:ALA:H	5	0.18	0.06	0.16
(1,3186)	1:1903:A:ILE:H	1:1902:A:GLY:H	5	0.17	0.08	0.14
(1,612)	1:1900:A:SER:HB3	1:1901:A:THR:H	5	0.17	0.03	0.17
(1,1244)	1:1926:A:ASN:H	1:1926:A:ASN:HB2	5	0.16	0.01	0.16
(1,1255)	1:1865:A:ILE:HD11	1:1857:A:LYS:HE2	5	0.16	0.03	0.17
(1,1255)	1:1865:A:ILE:HD12	1:1857:A:LYS:HE2	5	0.16	0.03	0.17
(1,1255)	1:1865:A:ILE:HD13	1:1857:A:LYS:HE2	5	0.16	0.03	0.17
(1,1664)	1:1847:A:LYS:HD2	1:1847:A:LYS:HE2	5	0.16	0.0	0.16
(1,1664)	1:1847:A:LYS:HD2	1:1847:A:LYS:HE3	5	0.16	0.0	0.16
(1,1664)	1:1847:A:LYS:HD3	1:1847:A:LYS:HE2	5	0.16	0.0	0.16
(1,1664)	1:1847:A:LYS:HD3	1:1847:A:LYS:HE3	5	0.16	0.0	0.16
(1,1770)	1:1914:A:THR:HB	1:1915:A:PRO:HD2	5	0.16	0.02	0.16
(1,3255)	1:1926:A:ASN:H	1:1925:A:THR:HA	5	0.16	0.02	0.17
(1,2028)	1:1824:A:SER:H	1:1823:A:LYS:HG3	5	0.16	0.04	0.17
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG21	5	0.15	0.02	0.14
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG22	5	0.15	0.02	0.14
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG23	5	0.15	0.02	0.14
(1,3111)	1:1931:A:GLY:H	1:1930:A:VAL:HB	5	0.14	0.02	0.13
(1,1307)	1:1821:A:ASP:HA	1:1823:A:LYS:H	5	0.14	0.04	0.13
(1,1689)	1:1928:A:GLU:H	1:1927:A:GLY:HA2	5	0.14	0.01	0.13
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD21	5	0.14	0.01	0.15
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD22	5	0.14	0.01	0.15
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD23	5	0.14	0.01	0.15
(1,450)	1:1896:A:ARG:HB2	1:1890:A:GLU:HG2	5	0.13	0.02	0.13
(1,3015)	1:1938:A:ARG:HB2	1:1845:A:ASN:HD21	5	0.13	0.02	0.14
(1,2245)	1:1954:A:ASP:HA	1:1954:A:ASP:HB2	5	0.12	0.01	0.12
(1,585)	1:1923:A:GLY:H	1:1922:A:ILE:HB	5	0.12	0.01	0.11
(1,2559)	1:1892:A:GLU:H	1:1890:A:GLU:HA	5	0.12	0.01	0.11
(1,2710)	1:1899:A:THR:H	1:1898:A:SER:HA	5	0.12	0.01	0.12
(1,1683)	1:1933:A:SER:H	1:1932:A:PRO:HB2	5	0.12	0.02	0.11
(1,2070)	1:1820:A:ILE:HG12	1:1821:A:ASP:H	5	0.12	0.01	0.11
(1,739)	1:1822:A:GLU:H	1:1822:A:GLU:HG3	5	0.12	0.0	0.12
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD21	5	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD22	5	0.12	0.01	0.12
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD23	5	0.12	0.01	0.12
(1,215)	1:1828:A:LYS:HA	1:1831:A:ASP:HB2	5	0.11	0.01	0.12
(1,878)	1:1820:A:ILE:H	1:1820:A:ILE:HB	5	0.11	0.0	0.11
(1,1090)	1:1852:A:GLU:H	1:1850:A:LEU:H	5	0.11	0.01	0.11
(1,1956)	1:1953:A:GLN:HA	1:1953:A:GLN:HB3	5	0.1	0.01	0.1
(1,1960)	1:1828:A:LYS:HE2	1:1828:A:LYS:HD2	5	0.1	0.0	0.1
(1,1960)	1:1828:A:LYS:HE2	1:1828:A:LYS:HD3	5	0.1	0.0	0.1
(1,1960)	1:1828:A:LYS:HE3	1:1828:A:LYS:HD2	5	0.1	0.0	0.1
(1,1960)	1:1828:A:LYS:HE3	1:1828:A:LYS:HD3	5	0.1	0.0	0.1
(1,2951)	1:1940:A:LYS:HD3	1:1940:A:LYS:HE2	5	0.1	0.0	0.1
(1,2951)	1:1940:A:LYS:HD3	1:1940:A:LYS:HE3	5	0.1	0.0	0.1
(1,1180)	1:1929:A:GLU:HG3	1:1930:A:VAL:HG21	4	0.34	0.05	0.34
(1,1180)	1:1929:A:GLU:HG3	1:1930:A:VAL:HG22	4	0.34	0.05	0.34
(1,1180)	1:1929:A:GLU:HG3	1:1930:A:VAL:HG23	4	0.34	0.05	0.34
(1,89)	1:1924:A:ASN:H	1:1922:A:ILE:HG21	4	0.3	0.09	0.32
(1,89)	1:1924:A:ASN:H	1:1922:A:ILE:HG22	4	0.3	0.09	0.32
(1,89)	1:1924:A:ASN:H	1:1922:A:ILE:HG23	4	0.3	0.09	0.32
(1,1091)	1:1939:A:LEU:HD11	1:1943:A:ARG:HD2	4	0.28	0.03	0.28
(1,1091)	1:1939:A:LEU:HD11	1:1943:A:ARG:HD3	4	0.28	0.03	0.28
(1,1091)	1:1939:A:LEU:HD12	1:1943:A:ARG:HD2	4	0.28	0.03	0.28
(1,1091)	1:1939:A:LEU:HD12	1:1943:A:ARG:HD3	4	0.28	0.03	0.28
(1,1091)	1:1939:A:LEU:HD13	1:1943:A:ARG:HD2	4	0.28	0.03	0.28
(1,1091)	1:1939:A:LEU:HD13	1:1943:A:ARG:HD3	4	0.28	0.03	0.28
(1,3203)	1:1903:A:ILE:H	1:1900:A:SER:HB2	4	0.24	0.09	0.24
(1,2662)	1:1955:A:ASP:H	1:1956:A:ARG:H	4	0.23	0.07	0.26
(1,316)	1:1919:A:VAL:HG21	1:1918:A:THR:HG21	4	0.23	0.13	0.2
(1,316)	1:1919:A:VAL:HG21	1:1918:A:THR:HG22	4	0.23	0.13	0.2
(1,316)	1:1919:A:VAL:HG21	1:1918:A:THR:HG23	4	0.23	0.13	0.2
(1,316)	1:1919:A:VAL:HG22	1:1918:A:THR:HG21	4	0.23	0.13	0.2
(1,316)	1:1919:A:VAL:HG22	1:1918:A:THR:HG22	4	0.23	0.13	0.2
(1,316)	1:1919:A:VAL:HG22	1:1918:A:THR:HG23	4	0.23	0.13	0.2
(1,316)	1:1919:A:VAL:HG23	1:1918:A:THR:HG21	4	0.23	0.13	0.2
(1,316)	1:1919:A:VAL:HG23	1:1918:A:THR:HG22	4	0.23	0.13	0.2
(1,316)	1:1919:A:VAL:HG23	1:1918:A:THR:HG23	4	0.23	0.13	0.2
(1,3271)	1:1870:A:LYS:HD2	1:1870:A:LYS:HG3	4	0.22	0.0	0.22
(1,3271)	1:1870:A:LYS:HD3	1:1870:A:LYS:HG3	4	0.22	0.0	0.22
(1,2745)	1:1929:A:GLU:HG2	1:1930:A:VAL:H	4	0.21	0.07	0.22
(1,3212)	1:1902:A:GLY:H	1:1900:A:SER:HB2	4	0.21	0.07	0.22
(1,2012)	1:1823:A:LYS:H	1:1822:A:GLU:HB3	4	0.2	0.02	0.2
(1,1898)	1:1928:A:GLU:H	1:1928:A:GLU:HB2	4	0.2	0.05	0.18
(1,1604)	1:1930:A:VAL:H	1:1931:A:GLY:H	4	0.19	0.05	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2705)	1:1889:A:MET:HA	1:1894:A:LYS:HB3	4	0.18	0.07	0.18
(1,1261)	1:1927:A:GLY:H	1:1925:A:THR:HG21	4	0.18	0.03	0.18
(1,1261)	1:1927:A:GLY:H	1:1925:A:THR:HG22	4	0.18	0.03	0.18
(1,1261)	1:1927:A:GLY:H	1:1925:A:THR:HG23	4	0.18	0.03	0.18
(1,2268)	1:1824:A:SER:HB3	1:1825:A:SER:H	4	0.18	0.08	0.16
(1,2581)	1:1920:A:SER:H	1:1919:A:VAL:HB	4	0.18	0.02	0.18
(1,2410)	1:1898:A:SER:H	1:1898:A:SER:HB2	4	0.17	0.04	0.16
(1,1131)	1:1824:A:SER:H	1:1827:A:ALA:HB1	4	0.17	0.04	0.16
(1,1131)	1:1824:A:SER:H	1:1827:A:ALA:HB2	4	0.17	0.04	0.16
(1,1131)	1:1824:A:SER:H	1:1827:A:ALA:HB3	4	0.17	0.04	0.16
(1,416)	1:1955:A:ASP:H	1:1954:A:ASP:H	4	0.17	0.04	0.15
(1,2378)	1:1923:A:GLY:H	1:1922:A:ILE:HG12	4	0.17	0.0	0.17
(1,311)	1:1930:A:VAL:H	1:1930:A:VAL:HG21	4	0.17	0.03	0.17
(1,311)	1:1930:A:VAL:H	1:1930:A:VAL:HG22	4	0.17	0.03	0.17
(1,311)	1:1930:A:VAL:H	1:1930:A:VAL:HG23	4	0.17	0.03	0.17
(1,104)	1:1951:A:THR:H	1:1951:A:THR:HB	4	0.16	0.06	0.14
(1,2709)	1:1824:A:SER:HA	1:1825:A:SER:H	4	0.16	0.03	0.15
(1,265)	1:1904:A:SER:HB2	1:1913:A:PRO:HG3	4	0.16	0.04	0.14
(1,229)	1:1823:A:LYS:HA	1:1826:A:LYS:HE2	4	0.15	0.02	0.15
(1,229)	1:1823:A:LYS:HA	1:1826:A:LYS:HE3	4	0.15	0.02	0.15
(1,3098)	1:1920:A:SER:H	1:1920:A:SER:HB3	4	0.15	0.03	0.15
(1,385)	1:1952:A:LYS:H	1:1951:A:THR:HA	4	0.14	0.04	0.14
(1,31)	1:1827:A:ALA:H	1:1826:A:LYS:HB2	4	0.14	0.02	0.15
(1,1081)	1:1826:A:LYS:HB2	1:1826:A:LYS:HD2	4	0.14	0.01	0.14
(1,1081)	1:1826:A:LYS:HB2	1:1826:A:LYS:HD3	4	0.14	0.01	0.14
(1,186)	1:1884:A:LEU:HD11	1:1857:A:LYS:HD3	4	0.14	0.02	0.14
(1,186)	1:1884:A:LEU:HD12	1:1857:A:LYS:HD3	4	0.14	0.02	0.14
(1,186)	1:1884:A:LEU:HD13	1:1857:A:LYS:HD3	4	0.14	0.02	0.14
(1,1379)	1:1939:A:LEU:HD11	1:1839:A:LYS:HB2	4	0.13	0.01	0.14
(1,1379)	1:1939:A:LEU:HD12	1:1839:A:LYS:HB2	4	0.13	0.01	0.14
(1,1379)	1:1939:A:LEU:HD13	1:1839:A:LYS:HB2	4	0.13	0.01	0.14
(1,3062)	1:1872:A:SER:H	1:1870:A:LYS:HB2	4	0.13	0.01	0.13
(1,1239)	1:1890:A:GLU:HA	1:1896:A:ARG:HG3	4	0.12	0.03	0.12
(1,781)	1:1819:A:ARG:HB2	1:1819:A:ARG:HA	4	0.12	0.0	0.12
(1,1305)	1:1837:A:PHE:HE1	1:1876:A:PHE:HE1	4	0.12	0.0	0.12
(1,1305)	1:1837:A:PHE:HE1	1:1876:A:PHE:HE2	4	0.12	0.0	0.12
(1,1305)	1:1837:A:PHE:HE2	1:1876:A:PHE:HE1	4	0.12	0.0	0.12
(1,1305)	1:1837:A:PHE:HE2	1:1876:A:PHE:HE2	4	0.12	0.0	0.12
(1,1666)	1:1907:A:MET:HG2	1:1908:A:GLU:H	4	0.12	0.01	0.12
(1,2162)	1:1858:A:LYS:HE3	1:1854:A:TYR:HE1	4	0.12	0.02	0.12
(1,2162)	1:1858:A:LYS:HE3	1:1854:A:TYR:HE2	4	0.12	0.02	0.12
(1,12)	1:1928:A:GLU:H	1:1928:A:GLU:HG2	4	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,12)	1:1928:A:GLU:H	1:1928:A:GLU:HG3	4	0.12	0.0	0.12
(1,974)	1:1856:A:TYR:HD1	1:1833:A:LEU:HD11	4	0.12	0.01	0.12
(1,974)	1:1856:A:TYR:HD1	1:1833:A:LEU:HD12	4	0.12	0.01	0.12
(1,974)	1:1856:A:TYR:HD1	1:1833:A:LEU:HD13	4	0.12	0.01	0.12
(1,974)	1:1856:A:TYR:HD2	1:1833:A:LEU:HD11	4	0.12	0.01	0.12
(1,974)	1:1856:A:TYR:HD2	1:1833:A:LEU:HD12	4	0.12	0.01	0.12
(1,974)	1:1856:A:TYR:HD2	1:1833:A:LEU:HD13	4	0.12	0.01	0.12
(1,2339)	1:1840:A:ILE:H	1:1849:A:GLY:H	4	0.12	0.01	0.12
(1,1895)	1:1855:A:GLU:H	1:1852:A:GLU:HG2	4	0.12	0.0	0.12
(1,247)	1:1905:A:PRO:HD3	1:1905:A:PRO:HB3	4	0.11	0.0	0.11
(1,55)	1:1874:A:GLN:HB2	1:1874:A:GLN:HE21	4	0.11	0.0	0.11
(1,959)	1:1898:A:SER:H	1:1897:A:ILE:HG12	4	0.11	0.01	0.11
(1,1335)	1:1953:A:GLN:HA	1:1953:A:GLN:HG2	4	0.11	0.01	0.11
(1,2180)	1:1884:A:LEU:H	1:1850:A:LEU:HD11	4	0.11	0.01	0.11
(1,2180)	1:1884:A:LEU:H	1:1850:A:LEU:HD12	4	0.11	0.01	0.11
(1,2180)	1:1884:A:LEU:H	1:1850:A:LEU:HD13	4	0.11	0.01	0.11
(1,2134)	1:1853:A:LEU:H	1:1853:A:LEU:HB3	4	0.11	0.0	0.11
(1,1415)	1:1897:A:ILE:H	1:1897:A:ILE:HG21	4	0.1	0.0	0.1
(1,1415)	1:1897:A:ILE:H	1:1897:A:ILE:HG22	4	0.1	0.0	0.1
(1,1415)	1:1897:A:ILE:H	1:1897:A:ILE:HG23	4	0.1	0.0	0.1
(1,1588)	1:1882:A:ARG:H	1:1880:A:VAL:H	4	0.1	0.0	0.1
(1,129)	1:1820:A:ILE:HB	1:1823:A:LYS:H	3	0.42	0.06	0.45
(1,2100)	1:1822:A:GLU:H	1:1824:A:SER:H	3	0.3	0.11	0.34
(1,308)	1:1897:A:ILE:H	1:1896:A:ARG:HG2	3	0.29	0.08	0.26
(1,925)	1:1955:A:ASP:H	1:1953:A:GLN:HA	3	0.28	0.05	0.29
(1,3021)	1:1919:A:VAL:H	1:1918:A:THR:HG21	3	0.26	0.05	0.23
(1,3021)	1:1919:A:VAL:H	1:1918:A:THR:HG22	3	0.26	0.05	0.23
(1,3021)	1:1919:A:VAL:H	1:1918:A:THR:HG23	3	0.26	0.05	0.23
(1,676)	1:1899:A:THR:H	1:1897:A:ILE:HG21	3	0.26	0.06	0.29
(1,676)	1:1899:A:THR:H	1:1897:A:ILE:HG22	3	0.26	0.06	0.29
(1,676)	1:1899:A:THR:H	1:1897:A:ILE:HG23	3	0.26	0.06	0.29
(1,3320)	1:1900:A:SER:H	1:1899:A:THR:HA	3	0.23	0.02	0.23
(1,2825)	1:1818:A:SER:HB3	1:1821:A:ASP:H	3	0.23	0.04	0.22
(1,1634)	1:1953:A:GLN:HA	1:1953:A:GLN:HG3	3	0.22	0.01	0.23
(1,3144)	1:1845:A:ASN:HA	1:1845:A:ASN:HD21	3	0.21	0.15	0.11
(1,2908)	1:1947:A:GLY:HA2	1:1949:A:ASP:H	3	0.21	0.1	0.18
(1,2908)	1:1947:A:GLY:HA3	1:1949:A:ASP:H	3	0.21	0.1	0.18
(1,1982)	1:1930:A:VAL:HB	1:1930:A:VAL:HA	3	0.2	0.04	0.18
(1,2971)	1:1933:A:SER:HB2	1:1934:A:VAL:H	3	0.2	0.02	0.19
(1,690)	1:1899:A:THR:H	1:1898:A:SER:HB2	3	0.2	0.02	0.19
(1,1361)	1:1862:A:ASP:H	1:1861:A:SER:HB3	3	0.19	0.03	0.21
(1,2688)	1:1938:A:ARG:HD2	1:1934:A:VAL:HG21	3	0.18	0.05	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2688)	1:1938:A:ARG:HD2	1:1934:A:VAL:HG22	3	0.18	0.05	0.15
(1,2688)	1:1938:A:ARG:HD2	1:1934:A:VAL:HG23	3	0.18	0.05	0.15
(1,2688)	1:1938:A:ARG:HD3	1:1934:A:VAL:HG21	3	0.18	0.05	0.15
(1,2688)	1:1938:A:ARG:HD3	1:1934:A:VAL:HG22	3	0.18	0.05	0.15
(1,2688)	1:1938:A:ARG:HD3	1:1934:A:VAL:HG23	3	0.18	0.05	0.15
(1,2503)	1:1873:A:SER:HB2	1:1873:A:SER:H	3	0.18	0.01	0.18
(1,3051)	1:1918:A:THR:H	1:1917:A:SER:HB2	3	0.18	0.02	0.16
(1,2859)	1:1943:A:ARG:HA	1:1838:A:LYS:HE2	3	0.17	0.05	0.16
(1,982)	1:1858:A:LYS:H	1:1858:A:LYS:HG3	3	0.16	0.01	0.16
(1,195)	1:1844:A:GLU:HA	1:1846:A:THR:HG21	3	0.16	0.06	0.13
(1,195)	1:1844:A:GLU:HA	1:1846:A:THR:HG22	3	0.16	0.06	0.13
(1,195)	1:1844:A:GLU:HA	1:1846:A:THR:HG23	3	0.16	0.06	0.13
(1,1410)	1:1951:A:THR:HG21	1:1951:A:THR:H	3	0.16	0.03	0.17
(1,1410)	1:1951:A:THR:HG22	1:1951:A:THR:H	3	0.16	0.03	0.17
(1,1410)	1:1951:A:THR:HG23	1:1951:A:THR:H	3	0.16	0.03	0.17
(1,2960)	1:1858:A:LYS:HB2	1:1855:A:GLU:H	3	0.16	0.01	0.16
(1,2321)	1:1903:A:ILE:H	1:1902:A:GLY:HA2	3	0.16	0.02	0.16
(1,2321)	1:1903:A:ILE:H	1:1902:A:GLY:HA3	3	0.16	0.02	0.16
(1,1514)	1:1896:A:ARG:HB2	1:1889:A:MET:HE1	3	0.16	0.04	0.13
(1,1514)	1:1896:A:ARG:HB2	1:1889:A:MET:HE2	3	0.16	0.04	0.13
(1,1514)	1:1896:A:ARG:HB2	1:1889:A:MET:HE3	3	0.16	0.04	0.13
(1,1462)	1:1924:A:ASN:HB3	1:1924:A:ASN:HA	3	0.15	0.02	0.14
(1,593)	1:1920:A:SER:HA	1:1915:A:PRO:HB3	3	0.14	0.03	0.14
(1,630)	1:1926:A:ASN:HA	1:1926:A:ASN:HB2	3	0.13	0.03	0.12
(1,929)	1:1922:A:ILE:HG13	1:1922:A:ILE:H	3	0.13	0.02	0.14
(1,1532)	1:1822:A:GLU:HG3	1:1823:A:LYS:H	3	0.13	0.01	0.13
(1,1194)	1:1918:A:THR:HA	1:1918:A:THR:HB	3	0.13	0.01	0.12
(1,2668)	1:1925:A:THR:H	1:1924:A:ASN:HB2	3	0.13	0.02	0.13
(1,632)	1:1949:A:ASP:H	1:1949:A:ASP:HB3	3	0.13	0.01	0.13
(1,1056)	1:1927:A:GLY:H	1:1926:A:ASN:HA	3	0.13	0.01	0.13
(1,1120)	1:1941:A:ILE:HD11	1:1944:A:GLN:HE22	3	0.13	0.02	0.11
(1,1120)	1:1941:A:ILE:HD12	1:1944:A:GLN:HE22	3	0.13	0.02	0.11
(1,1120)	1:1941:A:ILE:HD13	1:1944:A:GLN:HE22	3	0.13	0.02	0.11
(1,2765)	1:1878:A:SER:HA	1:1881:A:GLU:HG3	3	0.13	0.01	0.12
(1,1028)	1:1886:A:VAL:HA	1:1888:A:GLU:H	3	0.12	0.0	0.12
(1,1979)	1:1941:A:ILE:HG21	1:1942:A:LEU:HG	3	0.12	0.01	0.12
(1,1979)	1:1941:A:ILE:HG22	1:1942:A:LEU:HG	3	0.12	0.01	0.12
(1,1979)	1:1941:A:ILE:HG23	1:1942:A:LEU:HG	3	0.12	0.01	0.12
(1,2624)	1:1882:A:ARG:HG3	1:1882:A:ARG:HD2	3	0.12	0.0	0.12
(1,2624)	1:1882:A:ARG:HG3	1:1882:A:ARG:HD3	3	0.12	0.0	0.12
(1,2733)	1:1885:A:ARG:HA	1:1889:A:MET:H	3	0.12	0.02	0.11
(1,1907)	1:1858:A:LYS:HA	1:1861:A:SER:HA	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)
(1,444)	1:1872:A:SER:H	1:1877:A:GLN:HG3	3	0.11	0.0	0.11
(1,1381)	1:1922:A:ILE:H	1:1921:A:SER:HB2	3	0.11	0.0	0.11
(1,1750)	1:1924:A:ASN:HB2	1:1924:A:ASN:HA	3	0.11	0.0	0.11
(1,2454)	1:1818:A:SER:HB2	1:1818:A:SER:HA	3	0.11	0.0	0.11
(1,2454)	1:1818:A:SER:HB3	1:1818:A:SER:HA	3	0.11	0.0	0.11
(1,666)	1:1942:A:LEU:HD21	1:1839:A:LYS:HG2	3	0.11	0.0	0.11
(1,666)	1:1942:A:LEU:HD22	1:1839:A:LYS:HG2	3	0.11	0.0	0.11
(1,666)	1:1942:A:LEU:HD23	1:1839:A:LYS:HG2	3	0.11	0.0	0.11
(1,1724)	1:1853:A:LEU:HD21	1:1869:A:LEU:HD11	3	0.11	0.0	0.11
(1,1724)	1:1853:A:LEU:HD21	1:1869:A:LEU:HD12	3	0.11	0.0	0.11
(1,1724)	1:1853:A:LEU:HD21	1:1869:A:LEU:HD13	3	0.11	0.0	0.11
(1,1724)	1:1853:A:LEU:HD22	1:1869:A:LEU:HD11	3	0.11	0.0	0.11
(1,1724)	1:1853:A:LEU:HD22	1:1869:A:LEU:HD12	3	0.11	0.0	0.11
(1,1724)	1:1853:A:LEU:HD22	1:1869:A:LEU:HD13	3	0.11	0.0	0.11
(1,1724)	1:1853:A:LEU:HD23	1:1869:A:LEU:HD11	3	0.11	0.0	0.11
(1,1724)	1:1853:A:LEU:HD23	1:1869:A:LEU:HD12	3	0.11	0.0	0.11
(1,1724)	1:1853:A:LEU:HD23	1:1869:A:LEU:HD13	3	0.11	0.0	0.11
(1,975)	1:1876:A:PHE:H	1:1876:A:PHE:HB3	3	0.1	0.0	0.1
(1,719)	1:1877:A:GLN:H	1:1878:A:SER:HB2	3	0.1	0.0	0.1
(1,1627)	1:1863:A:ALA:H	1:1861:A:SER:HB2	2	0.29	0.08	0.29
(1,2035)	1:1926:A:ASN:HB3	1:1928:A:GLU:H	2	0.28	0.01	0.28
(1,2889)	1:1906:A:GLN:H	1:1907:A:MET:HA	2	0.27	0.0	0.27
(1,413)	1:1923:A:GLY:H	1:1922:A:ILE:HG21	2	0.26	0.01	0.26
(1,413)	1:1923:A:GLY:H	1:1922:A:ILE:HG22	2	0.26	0.01	0.26
(1,413)	1:1923:A:GLY:H	1:1922:A:ILE:HG23	2	0.26	0.01	0.26
(1,1679)	1:1929:A:GLU:H	1:1929:A:GLU:HB2	2	0.24	0.08	0.24
(1,2622)	1:1830:A:ASN:H	1:1829:A:VAL:HB	2	0.24	0.03	0.24
(1,555)	1:1927:A:GLY:H	1:1926:A:ASN:HB3	2	0.24	0.04	0.24
(1,3265)	1:1847:A:LYS:H	1:1846:A:THR:HB	2	0.23	0.12	0.23
(1,293)	1:1897:A:ILE:HD11	1:1890:A:GLU:HG3	2	0.23	0.06	0.23
(1,293)	1:1897:A:ILE:HD12	1:1890:A:GLU:HG3	2	0.23	0.06	0.23
(1,293)	1:1897:A:ILE:HD13	1:1890:A:GLU:HG3	2	0.23	0.06	0.23
(1,995)	1:1953:A:GLN:H	1:1953:A:GLN:HB3	2	0.22	0.06	0.22
(1,798)	1:1822:A:GLU:HB2	1:1823:A:LYS:H	2	0.22	0.02	0.22
(1,2548)	1:1925:A:THR:H	1:1924:A:ASN:HB3	2	0.21	0.03	0.21
(1,1089)	1:1948:A:LEU:H	1:1948:A:LEU:HD11	2	0.2	0.04	0.2
(1,1089)	1:1948:A:LEU:H	1:1948:A:LEU:HD12	2	0.2	0.04	0.2
(1,1089)	1:1948:A:LEU:H	1:1948:A:LEU:HD13	2	0.2	0.04	0.2
(1,3028)	1:1954:A:ASP:H	1:1954:A:ASP:HB2	2	0.2	0.0	0.2
(1,76)	1:1897:A:ILE:H	1:1896:A:ARG:HB2	2	0.2	0.01	0.2
(1,169)	1:1821:A:ASP:HB2	1:1822:A:GLU:H	2	0.2	0.03	0.2
(1,1270)	1:1893:A:GLY:H	1:1894:A:LYS:HD2	2	0.2	0.05	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1105)	1:1838:A:LYS:HD2	1:1943:A:ARG:HA	2	0.19	0.03	0.19
(1,1105)	1:1838:A:LYS:HD3	1:1943:A:ARG:HA	2	0.19	0.03	0.19
(1,1700)	1:1922:A:ILE:HG12	1:1922:A:ILE:H	2	0.18	0.05	0.18
(1,2631)	1:1929:A:GLU:HB2	1:1930:A:VAL:H	2	0.18	0.06	0.18
(1,109)	1:1929:A:GLU:H	1:1927:A:GLY:HA2	2	0.17	0.02	0.17
(1,954)	1:1863:A:ALA:H	1:1863:A:ALA:HA	2	0.17	0.01	0.17
(1,1018)	1:1861:A:SER:HA	1:1862:A:ASP:H	2	0.16	0.01	0.16
(1,1876)	1:1863:A:ALA:HB1	1:1860:A:TYR:HB2	2	0.16	0.02	0.16
(1,1876)	1:1863:A:ALA:HB2	1:1860:A:TYR:HB2	2	0.16	0.02	0.16
(1,1876)	1:1863:A:ALA:HB3	1:1860:A:TYR:HB2	2	0.16	0.02	0.16
(1,2747)	1:1900:A:SER:H	1:1899:A:THR:H	2	0.16	0.0	0.16
(1,111)	1:1894:A:LYS:H	1:1892:A:GLU:HB3	2	0.16	0.04	0.16
(1,957)	1:1936:A:LEU:H	1:1935:A:TYR:HB2	2	0.16	0.01	0.16
(1,957)	1:1936:A:LEU:H	1:1935:A:TYR:HB3	2	0.16	0.01	0.16
(1,1345)	1:1821:A:ASP:H	1:1821:A:ASP:HB3	2	0.16	0.01	0.16
(1,851)	1:1906:A:GLN:HB2	1:1908:A:GLU:H	2	0.15	0.05	0.15
(1,1032)	1:1829:A:VAL:H	1:1829:A:VAL:HG21	2	0.15	0.01	0.15
(1,1032)	1:1829:A:VAL:H	1:1829:A:VAL:HG22	2	0.15	0.01	0.15
(1,1032)	1:1829:A:VAL:H	1:1829:A:VAL:HG23	2	0.15	0.01	0.15
(1,489)	1:1854:A:TYR:H	1:1884:A:LEU:HB3	2	0.15	0.0	0.15
(1,2011)	1:1930:A:VAL:H	1:1929:A:GLU:HG3	2	0.15	0.04	0.15
(1,1565)	1:1838:A:LYS:HA	1:1842:A:SER:H	2	0.14	0.03	0.14
(1,1195)	1:1829:A:VAL:HG21	1:1833:A:LEU:HD11	2	0.14	0.03	0.14
(1,1195)	1:1829:A:VAL:HG21	1:1833:A:LEU:HD12	2	0.14	0.03	0.14
(1,1195)	1:1829:A:VAL:HG21	1:1833:A:LEU:HD13	2	0.14	0.03	0.14
(1,1195)	1:1829:A:VAL:HG22	1:1833:A:LEU:HD11	2	0.14	0.03	0.14
(1,1195)	1:1829:A:VAL:HG22	1:1833:A:LEU:HD12	2	0.14	0.03	0.14
(1,1195)	1:1829:A:VAL:HG22	1:1833:A:LEU:HD13	2	0.14	0.03	0.14
(1,1195)	1:1829:A:VAL:HG23	1:1833:A:LEU:HD11	2	0.14	0.03	0.14
(1,1195)	1:1829:A:VAL:HG23	1:1833:A:LEU:HD12	2	0.14	0.03	0.14
(1,1195)	1:1829:A:VAL:HG23	1:1833:A:LEU:HD13	2	0.14	0.03	0.14
(1,2243)	1:1862:A:ASP:HB2	1:1862:A:ASP:H	2	0.14	0.01	0.14
(1,2616)	1:1919:A:VAL:H	1:1918:A:THR:HB	2	0.14	0.01	0.14
(1,2701)	1:1924:A:ASN:H	1:1923:A:GLY:HA2	2	0.13	0.02	0.13
(1,2701)	1:1924:A:ASN:H	1:1923:A:GLY:HA3	2	0.13	0.02	0.13
(1,3126)	1:1818:A:SER:H	1:1818:A:SER:HB2	2	0.13	0.0	0.13
(1,3126)	1:1818:A:SER:H	1:1818:A:SER:HB3	2	0.13	0.0	0.13
(1,985)	1:1877:A:GLN:HE21	1:1869:A:LEU:HD21	2	0.12	0.02	0.12
(1,985)	1:1877:A:GLN:HE21	1:1869:A:LEU:HD22	2	0.12	0.02	0.12
(1,985)	1:1877:A:GLN:HE21	1:1869:A:LEU:HD23	2	0.12	0.02	0.12
(1,1212)	1:1950:A:ASN:HB3	1:1950:A:ASN:HA	2	0.12	0.02	0.12
(1,1582)	1:1884:A:LEU:HD11	1:1853:A:LEU:HA	2	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1582)	1:1884:A:LEU:HD12	1:1853:A:LEU:HA	2	0.12	0.01	0.12
(1,1582)	1:1884:A:LEU:HD13	1:1853:A:LEU:HA	2	0.12	0.01	0.12
(1,1853)	1:1827:A:ALA:H	1:1826:A:LYS:HG2	2	0.12	0.02	0.12
(1,2955)	1:1905:A:PRO:HD2	1:1904:A:SER:HA	2	0.12	0.02	0.12
(1,874)	1:1823:A:LYS:H	1:1820:A:ILE:HG21	2	0.12	0.01	0.12
(1,874)	1:1823:A:LYS:H	1:1820:A:ILE:HG22	2	0.12	0.01	0.12
(1,874)	1:1823:A:LYS:H	1:1820:A:ILE:HG23	2	0.12	0.01	0.12
(1,1401)	1:1829:A:VAL:HG21	1:1864:A:ASP:HB3	2	0.12	0.0	0.12
(1,1401)	1:1829:A:VAL:HG22	1:1864:A:ASP:HB3	2	0.12	0.0	0.12
(1,1401)	1:1829:A:VAL:HG23	1:1864:A:ASP:HB3	2	0.12	0.0	0.12
(1,2193)	1:1889:A:MET:HB2	1:1894:A:LYS:HE2	2	0.12	0.01	0.12
(1,2724)	1:1864:A:ASP:H	1:1864:A:ASP:HB2	2	0.12	0.01	0.12
(1,324)	1:1889:A:MET:HE1	1:1896:A:ARG:HD2	2	0.12	0.02	0.12
(1,324)	1:1889:A:MET:HE2	1:1896:A:ARG:HD2	2	0.12	0.02	0.12
(1,324)	1:1889:A:MET:HE3	1:1896:A:ARG:HD2	2	0.12	0.02	0.12
(1,815)	1:1911:A:CYS:HA	1:1912:A:VAL:HG11	2	0.12	0.02	0.12
(1,815)	1:1911:A:CYS:HA	1:1912:A:VAL:HG12	2	0.12	0.02	0.12
(1,815)	1:1911:A:CYS:HA	1:1912:A:VAL:HG13	2	0.12	0.02	0.12
(1,1624)	1:1941:A:ILE:HA	1:1944:A:GLN:HB2	2	0.12	0.02	0.12
(1,1624)	1:1941:A:ILE:HA	1:1944:A:GLN:HB3	2	0.12	0.02	0.12
(1,2345)	1:1930:A:VAL:H	1:1930:A:VAL:HG11	2	0.12	0.02	0.12
(1,2345)	1:1930:A:VAL:H	1:1930:A:VAL:HG12	2	0.12	0.02	0.12
(1,2345)	1:1930:A:VAL:H	1:1930:A:VAL:HG13	2	0.12	0.02	0.12
(1,93)	1:1857:A:LYS:HA	1:1865:A:ILE:HD11	2	0.12	0.0	0.12
(1,93)	1:1857:A:LYS:HA	1:1865:A:ILE:HD12	2	0.12	0.0	0.12
(1,93)	1:1857:A:LYS:HA	1:1865:A:ILE:HD13	2	0.12	0.0	0.12
(1,246)	1:1874:A:GLN:H	1:1874:A:GLN:HG2	2	0.12	0.0	0.12
(1,1330)	1:1893:A:GLY:H	1:1892:A:GLU:HB2	2	0.12	0.0	0.12
(1,69)	1:1883:A:GLY:HA2	1:1887:A:ILE:H	2	0.11	0.0	0.11
(1,383)	1:1830:A:ASN:HA	1:1833:A:LEU:HB3	2	0.11	0.0	0.11
(1,675)	1:1890:A:GLU:HB3	1:1890:A:GLU:HG2	2	0.11	0.01	0.11
(1,1189)	1:1956:A:ARG:HB2	1:1956:A:ARG:HD2	2	0.11	0.01	0.11
(1,1189)	1:1956:A:ARG:HB2	1:1956:A:ARG:HD3	2	0.11	0.01	0.11
(1,2418)	1:1891:A:ARG:HA	1:1891:A:ARG:HG2	2	0.11	0.0	0.11
(1,2423)	1:1931:A:GLY:H	1:1930:A:VAL:HA	2	0.11	0.01	0.11
(1,2613)	1:1839:A:LYS:H	1:1838:A:LYS:HG3	2	0.11	0.0	0.11
(1,2651)	1:1823:A:LYS:H	1:1823:A:LYS:HB2	2	0.11	0.0	0.11
(1,362)	1:1854:A:TYR:HA	1:1857:A:LYS:HB2	2	0.11	0.0	0.11
(1,1334)	1:1884:A:LEU:H	1:1882:A:ARG:HB3	2	0.11	0.0	0.11
(1,1638)	1:1869:A:LEU:HD11	1:1876:A:PHE:HE1	2	0.11	0.0	0.11
(1,1638)	1:1869:A:LEU:HD11	1:1876:A:PHE:HE2	2	0.11	0.0	0.11
(1,1638)	1:1869:A:LEU:HD12	1:1876:A:PHE:HE1	2	0.11	0.0	0.11

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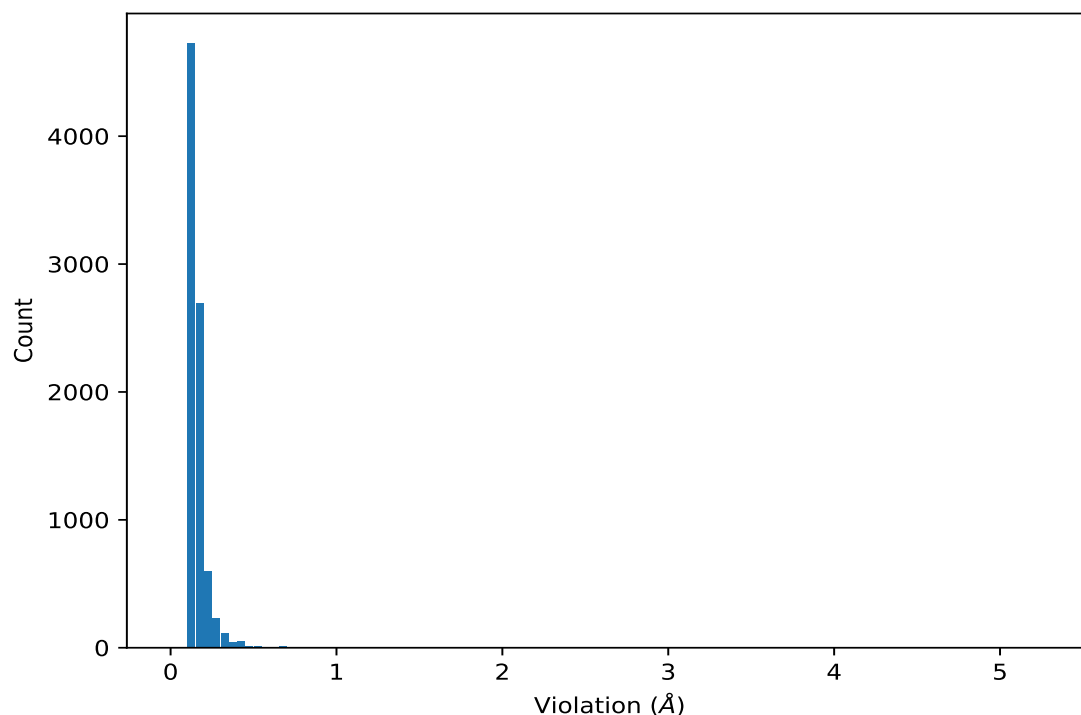
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1638)	1:1869:A:LEU:HD12	1:1876:A:PHE:HE2	2	0.11	0.0	0.11
(1,1638)	1:1869:A:LEU:HD13	1:1876:A:PHE:HE1	2	0.11	0.0	0.11
(1,1638)	1:1869:A:LEU:HD13	1:1876:A:PHE:HE2	2	0.11	0.0	0.11
(1,1870)	1:1956:A:ARG:H	1:1956:A:ARG:HG3	2	0.11	0.0	0.11
(1,2776)	1:1916:A:THR:HB	1:1917:A:SER:H	2	0.11	0.0	0.11
(1,749)	1:1872:A:SER:HB3	1:1877:A:GLN:HE22	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)
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	16	5.27
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	5	5.19
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	1	5.18
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	10	5.16
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	11	5.11
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	14	5.11
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	9	5.09
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	18	5.09
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	4	5.07
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	6	5.07
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	3	5.05
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	17	5.02
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	2	5.0
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	20	4.98
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	19	4.92
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	15	4.9
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	12	4.88
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	13	4.86
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	7	4.85
(3,27)	1:1870:A:LYS:N	1:1864:A:ASP:O	8	4.73
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	1	1.32
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	16	1.31
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	5	1.28
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	10	1.28
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	11	1.24
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	14	1.23
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	18	1.23
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	6	1.21
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	3	1.2
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	4	1.2
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	9	1.18
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	17	1.14
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	2	1.1
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	19	1.1
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	20	1.09
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	15	1.05
(3,45)	1:1934:A:VAL:N	1:1930:A:VAL:O	15	1.03
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	12	1.02
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	13	0.98
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	7	0.95
(3,25)	1:1868:A:PHE:N	1:1864:A:ASP:O	8	0.86
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	2	0.76
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	10	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	16	0.75
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	1	0.73
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	13	0.71
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	17	0.71
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	19	0.71
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	3	0.7
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	15	0.7
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	18	0.7
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	5	0.69
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	12	0.68
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	8	0.67
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	4	0.66
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	6	0.66
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	7	0.66
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	9	0.66
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	20	0.66
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	11	0.64
(3,31)	1:1879:A:TYR:N	1:1875:A:PHE:O	14	0.64
(1,2580)	1:1929:A:GLU:H	1:1928:A:GLU:HG2	18	0.63
(3,56)	1:1945:A:ARG:N	1:1941:A:ILE:O	16	0.62
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	16	0.61
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	5	0.6
(1,2068)	1:1820:A:ILE:H	1:1820:A:ILE:HD11	11	0.58
(1,2068)	1:1820:A:ILE:H	1:1820:A:ILE:HD12	11	0.58
(1,2068)	1:1820:A:ILE:H	1:1820:A:ILE:HD13	11	0.58
(3,45)	1:1934:A:VAL:N	1:1930:A:VAL:O	3	0.54
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	13	0.53
(3,45)	1:1934:A:VAL:N	1:1930:A:VAL:O	12	0.51
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	6	0.51
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	7	0.51
(1,1598)	1:1955:A:ASP:H	1:1953:A:GLN:HG2	9	0.51
(1,97)	1:1927:A:GLY:H	1:1929:A:GLU:H	11	0.51
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	2	0.5
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	2	0.5
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	4	0.5
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	10	0.5
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	3	0.49
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	13	0.49
(3,45)	1:1934:A:VAL:N	1:1930:A:VAL:O	1	0.48
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	5	0.48
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	12	0.47
(1,129)	1:1820:A:ILE:HB	1:1823:A:LYS:H	11	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,56)	1:1945:A:ARG:N	1:1941:A:ILE:O	7	0.46
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	16	0.46
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	1	0.46
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	7	0.46
(1,129)	1:1820:A:ILE:HB	1:1823:A:LYS:H	13	0.45
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	15	0.44
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	17	0.44
(1,361)	1:1817:A:ALA:HB3	1:1818:A:SER:HA	4	0.44
(1,361)	1:1817:A:ALA:HA	1:1818:A:SER:HA	13	0.44
(3,56)	1:1945:A:ARG:N	1:1941:A:ILE:O	17	0.43
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	8	0.43
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	11	0.43
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	15	0.43
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	6	0.43
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	18	0.43
(1,3144)	1:1845:A:ASN:HA	1:1845:A:ASN:HD21	10	0.43
(1,2580)	1:1929:A:GLU:H	1:1928:A:GLU:HG2	19	0.43
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	12	0.42
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	20	0.42
(1,316)	1:1919:A:VAL:HG21	1:1918:A:THR:HG21	3	0.42
(1,316)	1:1919:A:VAL:HG21	1:1918:A:THR:HG22	3	0.42
(1,316)	1:1919:A:VAL:HG21	1:1918:A:THR:HG23	3	0.42
(1,316)	1:1919:A:VAL:HG22	1:1918:A:THR:HG21	3	0.42
(1,316)	1:1919:A:VAL:HG22	1:1918:A:THR:HG22	3	0.42
(1,316)	1:1919:A:VAL:HG22	1:1918:A:THR:HG23	3	0.42
(1,316)	1:1919:A:VAL:HG23	1:1918:A:THR:HG21	3	0.42
(1,316)	1:1919:A:VAL:HG23	1:1918:A:THR:HG22	3	0.42
(1,316)	1:1919:A:VAL:HG23	1:1918:A:THR:HG23	3	0.42
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	2	0.41
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	9	0.41
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	9	0.41
(1,2210)	1:1840:A:ILE:HG21	1:1846:A:THR:HG21	12	0.41
(1,2210)	1:1840:A:ILE:HG21	1:1846:A:THR:HG22	12	0.41
(1,2210)	1:1840:A:ILE:HG21	1:1846:A:THR:HG23	12	0.41
(1,2210)	1:1840:A:ILE:HG22	1:1846:A:THR:HG21	12	0.41
(1,2210)	1:1840:A:ILE:HG22	1:1846:A:THR:HG22	12	0.41
(1,2210)	1:1840:A:ILE:HG22	1:1846:A:THR:HG23	12	0.41
(1,2210)	1:1840:A:ILE:HG23	1:1846:A:THR:HG21	12	0.41
(1,2210)	1:1840:A:ILE:HG23	1:1846:A:THR:HG22	12	0.41
(1,2210)	1:1840:A:ILE:HG23	1:1846:A:THR:HG23	12	0.41
(1,1180)	1:1929:A:GLU:HG3	1:1930:A:VAL:HG21	10	0.41
(1,1180)	1:1929:A:GLU:HG3	1:1930:A:VAL:HG22	10	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1180)	1:1929:A:GLU:HG3	1:1930:A:VAL:HG23	10	0.41
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	3	0.4
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	8	0.4
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	13	0.4
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	14	0.4
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	12	0.4
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	19	0.4
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	20	0.4
(1,2100)	1:1822:A:GLU:H	1:1824:A:SER:H	16	0.4
(1,361)	1:1817:A:ALA:HA	1:1818:A:SER:HA	8	0.4
(1,308)	1:1897:A:ILE:H	1:1896:A:ARG:HG2	11	0.4
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	16	0.39
(1,2265)	1:1824:A:SER:H	1:1823:A:LYS:HB2	13	0.39
(1,1752)	1:1899:A:THR:HG21	1:1899:A:THR:H	18	0.39
(1,1752)	1:1899:A:THR:HG22	1:1899:A:THR:H	18	0.39
(1,1752)	1:1899:A:THR:HG23	1:1899:A:THR:H	18	0.39
(1,361)	1:1817:A:ALA:HA	1:1818:A:SER:HA	14	0.39
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	10	0.38
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	18	0.38
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	19	0.38
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	11	0.38
(1,2515)	1:1898:A:SER:H	1:1897:A:ILE:HB	15	0.38
(1,2265)	1:1824:A:SER:H	1:1823:A:LYS:HB2	15	0.38
(1,2234)	1:1924:A:ASN:H	1:1922:A:ILE:HA	8	0.38
(1,89)	1:1924:A:ASN:H	1:1922:A:ILE:HG21	14	0.38
(1,89)	1:1924:A:ASN:H	1:1922:A:ILE:HG22	14	0.38
(1,89)	1:1924:A:ASN:H	1:1922:A:ILE:HG23	14	0.38
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	3	0.37
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	1	0.37
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	17	0.37
(1,2265)	1:1824:A:SER:H	1:1823:A:LYS:HB2	8	0.37
(1,2234)	1:1924:A:ASN:H	1:1922:A:ILE:HA	7	0.37
(1,1703)	1:1821:A:ASP:HB3	1:1823:A:LYS:H	15	0.37
(1,1627)	1:1863:A:ALA:H	1:1861:A:SER:HB2	17	0.37
(1,97)	1:1927:A:GLY:H	1:1929:A:GLU:H	9	0.37
(1,89)	1:1924:A:ASN:H	1:1922:A:ILE:HG21	17	0.37
(1,89)	1:1924:A:ASN:H	1:1922:A:ILE:HG22	17	0.37
(1,89)	1:1924:A:ASN:H	1:1922:A:ILE:HG23	17	0.37
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	5	0.36
(1,1180)	1:1929:A:GLU:HG3	1:1930:A:VAL:HG21	17	0.36
(1,1180)	1:1929:A:GLU:HG3	1:1930:A:VAL:HG22	17	0.36
(1,1180)	1:1929:A:GLU:HG3	1:1930:A:VAL:HG23	17	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,37)	1:1885:A:ARG:N	1:1881:A:GLU:O	4	0.35
(1,3265)	1:1847:A:LYS:H	1:1846:A:THR:HB	12	0.35
(1,3203)	1:1903:A:ILE:H	1:1900:A:SER:HB2	16	0.35
(1,2908)	1:1947:A:GLY:HA2	1:1949:A:ASP:H	9	0.35
(1,2908)	1:1947:A:GLY:HA3	1:1949:A:ASP:H	9	0.35
(1,2328)	1:1950:A:ASN:H	1:1951:A:THR:H	2	0.35
(1,972)	1:1952:A:LYS:H	1:1951:A:THR:HB	13	0.35
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG21	11	0.35
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG22	11	0.35
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG23	11	0.35
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	18	0.34
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	1	0.34
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	6	0.34
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	11	0.34
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	19	0.34
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	8	0.34
(3,30)	1:1878:A:SER:N	1:1874:A:GLN:O	14	0.34
(1,3172)	1:1902:A:GLY:H	1:1901:A:THR:HB	4	0.34
(1,2234)	1:1924:A:ASN:H	1:1922:A:ILE:HA	10	0.34
(1,2100)	1:1822:A:GLU:H	1:1824:A:SER:H	4	0.34
(1,1952)	1:1840:A:ILE:HG21	1:1846:A:THR:HB	12	0.34
(1,1952)	1:1840:A:ILE:HG22	1:1846:A:THR:HB	12	0.34
(1,1952)	1:1840:A:ILE:HG23	1:1846:A:THR:HB	12	0.34
(1,1790)	1:1927:A:GLY:H	1:1925:A:THR:HB	18	0.34
(1,679)	1:1954:A:ASP:H	1:1953:A:GLN:HB2	16	0.34
(1,665)	1:1929:A:GLU:H	1:1930:A:VAL:H	10	0.34
(1,129)	1:1820:A:ILE:HB	1:1823:A:LYS:H	14	0.34
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	3	0.33
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	15	0.33
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	16	0.33
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	18	0.33
(1,3138)	1:1926:A:ASN:H	1:1926:A:ASN:HD22	5	0.33
(1,3086)	1:1903:A:ILE:H	1:1900:A:SER:HB3	15	0.33
(1,3021)	1:1919:A:VAL:H	1:1918:A:THR:HG21	3	0.33
(1,3021)	1:1919:A:VAL:H	1:1918:A:THR:HG22	3	0.33
(1,3021)	1:1919:A:VAL:H	1:1918:A:THR:HG23	3	0.33
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG21	6	0.33
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG22	6	0.33
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG23	6	0.33
(1,1091)	1:1939:A:LEU:HD11	1:1943:A:ARG:HD2	11	0.33
(1,1091)	1:1939:A:LEU:HD11	1:1943:A:ARG:HD3	11	0.33
(1,1091)	1:1939:A:LEU:HD12	1:1943:A:ARG:HD2	11	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1091)	1:1939:A:LEU:HD12	1:1943:A:ARG:HD3	11	0.33
(1,1091)	1:1939:A:LEU:HD13	1:1943:A:ARG:HD2	11	0.33
(1,1091)	1:1939:A:LEU:HD13	1:1943:A:ARG:HD3	11	0.33
(1,925)	1:1955:A:ASP:H	1:1953:A:GLN:HA	5	0.33
(1,525)	1:1924:A:ASN:H	1:1923:A:GLY:H	8	0.33
(1,361)	1:1817:A:ALA:HA	1:1818:A:SER:HA	2	0.33
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG21	16	0.33
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG22	16	0.33
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG23	16	0.33
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	2	0.32
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	7	0.32
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	9	0.32
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	10	0.32
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	12	0.32
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	13	0.32
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	20	0.32
(1,3186)	1:1903:A:ILE:H	1:1902:A:GLY:H	19	0.32
(1,2580)	1:1929:A:GLU:H	1:1928:A:GLU:HG2	6	0.32
(1,1679)	1:1929:A:GLU:H	1:1929:A:GLU:HB2	13	0.32
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG21	9	0.32
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG22	9	0.32
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG23	9	0.32
(1,97)	1:1927:A:GLY:H	1:1929:A:GLU:H	2	0.32
(3,45)	1:1934:A:VAL:N	1:1930:A:VAL:O	14	0.31
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	14	0.31
(1,3212)	1:1902:A:GLY:H	1:1900:A:SER:HB2	12	0.31
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	5	0.31
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	8	0.31
(1,3086)	1:1903:A:ILE:H	1:1900:A:SER:HB3	10	0.31
(1,3018)	1:1863:A:ALA:HB1	1:1862:A:ASP:H	8	0.31
(1,3018)	1:1863:A:ALA:HB2	1:1862:A:ASP:H	8	0.31
(1,3018)	1:1863:A:ALA:HB3	1:1862:A:ASP:H	8	0.31
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	19	0.31
(1,2328)	1:1950:A:ASN:H	1:1951:A:THR:H	8	0.31
(1,2048)	1:1838:A:LYS:HD2	1:1838:A:LYS:HE3	17	0.31
(1,2048)	1:1838:A:LYS:HD3	1:1838:A:LYS:HE3	17	0.31
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	9	0.31
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	9	0.31
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG21	2	0.31
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG22	2	0.31
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG23	2	0.31
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD11	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD12	9	0.31
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD13	9	0.31
(1,1180)	1:1929:A:GLU:HG3	1:1930:A:VAL:HG21	4	0.31
(1,1180)	1:1929:A:GLU:HG3	1:1930:A:VAL:HG22	4	0.31
(1,1180)	1:1929:A:GLU:HG3	1:1930:A:VAL:HG23	4	0.31
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG21	19	0.31
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG22	19	0.31
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG23	19	0.31
(1,676)	1:1899:A:THR:H	1:1897:A:ILE:HG21	11	0.31
(1,676)	1:1899:A:THR:H	1:1897:A:ILE:HG22	11	0.31
(1,676)	1:1899:A:THR:H	1:1897:A:ILE:HG23	11	0.31
(1,361)	1:1817:A:ALA:HA	1:1818:A:SER:HA	12	0.31
(1,361)	1:1817:A:ALA:HA	1:1818:A:SER:HA	20	0.31
(1,116)	1:1948:A:LEU:H	1:1949:A:ASP:H	2	0.31
(3,56)	1:1945:A:ARG:N	1:1941:A:ILE:O	19	0.3
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	1	0.3
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	5	0.3
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	17	0.3
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	1	0.3
(1,3018)	1:1863:A:ALA:HB1	1:1862:A:ASP:H	16	0.3
(1,3018)	1:1863:A:ALA:HB2	1:1862:A:ASP:H	16	0.3
(1,3018)	1:1863:A:ALA:HB3	1:1862:A:ASP:H	16	0.3
(1,3018)	1:1863:A:ALA:HB1	1:1862:A:ASP:H	20	0.3
(1,3018)	1:1863:A:ALA:HB2	1:1862:A:ASP:H	20	0.3
(1,3018)	1:1863:A:ALA:HB3	1:1862:A:ASP:H	20	0.3
(1,2745)	1:1929:A:GLU:HG2	1:1930:A:VAL:H	2	0.3
(1,2522)	1:1903:A:ILE:H	1:1903:A:ILE:HG13	18	0.3
(1,2268)	1:1824:A:SER:HB3	1:1825:A:SER:H	14	0.3
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG21	7	0.3
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG22	7	0.3
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG23	7	0.3
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG21	7	0.3
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG22	7	0.3
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG23	7	0.3
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG21	7	0.3
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG22	7	0.3
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG23	7	0.3
(1,736)	1:1898:A:SER:H	1:1897:A:ILE:H	7	0.3
(1,697)	1:1956:A:ARG:H	1:1956:A:ARG:HB3	19	0.3
(1,583)	1:1867:A:PRO:HA	1:1870:A:LYS:HB2	4	0.3
(1,583)	1:1867:A:PRO:HA	1:1870:A:LYS:HB2	7	0.3
(1,579)	1:1897:A:ILE:H	1:1897:A:ILE:HG12	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:1817:A:ALA:HA	1:1818:A:SER:HA	6	0.3
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	8	0.29
(1,3246)	1:1904:A:SER:H	1:1905:A:PRO:HD2	12	0.29
(1,3018)	1:1863:A:ALA:HB1	1:1862:A:ASP:H	11	0.29
(1,3018)	1:1863:A:ALA:HB2	1:1862:A:ASP:H	11	0.29
(1,3018)	1:1863:A:ALA:HB3	1:1862:A:ASP:H	11	0.29
(1,2662)	1:1955:A:ASP:H	1:1956:A:ARG:H	11	0.29
(1,2035)	1:1926:A:ASN:HB3	1:1928:A:GLU:H	9	0.29
(1,1703)	1:1821:A:ASP:HB3	1:1823:A:LYS:H	2	0.29
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG21	1	0.29
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG22	1	0.29
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG23	1	0.29
(1,1091)	1:1939:A:LEU:HD11	1:1943:A:ARG:HD2	9	0.29
(1,1091)	1:1939:A:LEU:HD11	1:1943:A:ARG:HD3	9	0.29
(1,1091)	1:1939:A:LEU:HD12	1:1943:A:ARG:HD2	9	0.29
(1,1091)	1:1939:A:LEU:HD12	1:1943:A:ARG:HD3	9	0.29
(1,1091)	1:1939:A:LEU:HD13	1:1943:A:ARG:HD2	9	0.29
(1,1091)	1:1939:A:LEU:HD13	1:1943:A:ARG:HD3	9	0.29
(1,995)	1:1953:A:GLN:H	1:1953:A:GLN:HB3	4	0.29
(1,981)	1:1818:A:SER:HB2	1:1820:A:ILE:H	1	0.29
(1,981)	1:1818:A:SER:HB3	1:1820:A:ILE:H	1	0.29
(1,981)	1:1818:A:SER:HB2	1:1820:A:ILE:H	11	0.29
(1,981)	1:1818:A:SER:HB3	1:1820:A:ILE:H	11	0.29
(1,925)	1:1955:A:ASP:H	1:1953:A:GLN:HA	4	0.29
(1,807)	1:1907:A:MET:H	1:1906:A:GLN:HG2	7	0.29
(1,676)	1:1899:A:THR:H	1:1897:A:ILE:HG21	10	0.29
(1,676)	1:1899:A:THR:H	1:1897:A:ILE:HG22	10	0.29
(1,676)	1:1899:A:THR:H	1:1897:A:ILE:HG23	10	0.29
(1,583)	1:1867:A:PRO:HA	1:1870:A:LYS:HB2	14	0.29
(1,573)	1:1817:A:ALA:HB1	1:1819:A:ARG:H	16	0.29
(1,573)	1:1817:A:ALA:HB2	1:1819:A:ARG:H	16	0.29
(1,573)	1:1817:A:ALA:HB3	1:1819:A:ARG:H	16	0.29
(1,437)	1:1940:A:LYS:HD3	1:1943:A:ARG:HD2	7	0.29
(1,437)	1:1940:A:LYS:HD3	1:1943:A:ARG:HD3	7	0.29
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	10	0.29
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	10	0.29
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	10	0.29
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	15	0.28
(3,38)	1:1886:A:VAL:N	1:1882:A:ARG:O	4	0.28
(1,3203)	1:1903:A:ILE:H	1:1900:A:SER:HB2	7	0.28
(1,3018)	1:1863:A:ALA:HB1	1:1862:A:ASP:H	2	0.28
(1,3018)	1:1863:A:ALA:HB2	1:1862:A:ASP:H	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3018)	1:1863:A:ALA:HB3	1:1862:A:ASP:H	2	0.28
(1,3018)	1:1863:A:ALA:HB1	1:1862:A:ASP:H	17	0.28
(1,3018)	1:1863:A:ALA:HB2	1:1862:A:ASP:H	17	0.28
(1,3018)	1:1863:A:ALA:HB3	1:1862:A:ASP:H	17	0.28
(1,2825)	1:1818:A:SER:HB3	1:1821:A:ASP:H	13	0.28
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	7	0.28
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	7	0.28
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	7	0.28
(1,2705)	1:1889:A:MET:HA	1:1894:A:LYS:HB3	18	0.28
(1,2515)	1:1898:A:SER:H	1:1897:A:ILE:HB	11	0.28
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	8	0.28
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	8	0.28
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	8	0.28
(1,2143)	1:1863:A:ALA:HB1	1:1864:A:ASP:H	17	0.28
(1,2143)	1:1863:A:ALA:HB2	1:1864:A:ASP:H	17	0.28
(1,2143)	1:1863:A:ALA:HB3	1:1864:A:ASP:H	17	0.28
(1,2099)	1:1927:A:GLY:H	1:1928:A:GLU:H	11	0.28
(1,1898)	1:1928:A:GLU:H	1:1928:A:GLU:HB2	18	0.28
(1,1470)	1:1824:A:SER:H	1:1827:A:ALA:H	9	0.28
(1,1180)	1:1929:A:GLU:HG3	1:1930:A:VAL:HG21	7	0.28
(1,1180)	1:1929:A:GLU:HG3	1:1930:A:VAL:HG22	7	0.28
(1,1180)	1:1929:A:GLU:HG3	1:1930:A:VAL:HG23	7	0.28
(1,807)	1:1907:A:MET:H	1:1906:A:GLN:HG2	4	0.28
(1,583)	1:1867:A:PRO:HA	1:1870:A:LYS:HB2	8	0.28
(1,573)	1:1817:A:ALA:HB1	1:1819:A:ARG:H	9	0.28
(1,573)	1:1817:A:ALA:HB2	1:1819:A:ARG:H	9	0.28
(1,573)	1:1817:A:ALA:HB3	1:1819:A:ARG:H	9	0.28
(1,558)	1:1929:A:GLU:H	1:1928:A:GLU:HA	11	0.28
(1,555)	1:1927:A:GLY:H	1:1926:A:ASN:HB3	7	0.28
(1,375)	1:1896:A:ARG:HG2	1:1896:A:ARG:HD2	11	0.28
(1,375)	1:1896:A:ARG:HG2	1:1896:A:ARG:HD3	11	0.28
(1,293)	1:1897:A:ILE:HD11	1:1890:A:GLU:HG3	13	0.28
(1,293)	1:1897:A:ILE:HD12	1:1890:A:GLU:HG3	13	0.28
(1,293)	1:1897:A:ILE:HD13	1:1890:A:GLU:HG3	13	0.28
(1,116)	1:1948:A:LEU:H	1:1949:A:ASP:H	13	0.28
(1,102)	1:1940:A:LYS:HA	1:1940:A:LYS:HD3	7	0.28
(1,97)	1:1927:A:GLY:H	1:1929:A:GLU:H	10	0.28
(1,89)	1:1924:A:ASN:H	1:1922:A:ILE:HG21	13	0.28
(1,89)	1:1924:A:ASN:H	1:1922:A:ILE:HG22	13	0.28
(1,89)	1:1924:A:ASN:H	1:1922:A:ILE:HG23	13	0.28
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	10	0.27
(1,3246)	1:1904:A:SER:H	1:1905:A:PRO:HD2	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3138)	1:1926:A:ASN:H	1:1926:A:ASN:HD22	17	0.27
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	15	0.27
(1,3075)	1:1942:A:LEU:HB3	1:1838:A:LYS:HG3	9	0.27
(1,2974)	1:1930:A:VAL:H	1:1929:A:GLU:HB3	6	0.27
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	16	0.27
(1,2889)	1:1906:A:GLN:H	1:1907:A:MET:HA	16	0.27
(1,2889)	1:1906:A:GLN:H	1:1907:A:MET:HA	19	0.27
(1,2662)	1:1955:A:ASP:H	1:1956:A:ARG:H	9	0.27
(1,2622)	1:1830:A:ASN:H	1:1829:A:VAL:HB	9	0.27
(1,2580)	1:1929:A:GLU:H	1:1928:A:GLU:HG2	4	0.27
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG21	6	0.27
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG22	6	0.27
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG23	6	0.27
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG21	6	0.27
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG22	6	0.27
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG23	6	0.27
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG21	6	0.27
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG22	6	0.27
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG23	6	0.27
(1,2089)	1:1916:A:THR:H	1:1915:A:PRO:HB2	7	0.27
(1,2017)	1:1838:A:LYS:HG3	1:1838:A:LYS:HE3	15	0.27
(1,1790)	1:1927:A:GLY:H	1:1925:A:THR:HB	16	0.27
(1,1755)	1:1907:A:MET:H	1:1906:A:GLN:HB2	19	0.27
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE2	13	0.27
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE3	13	0.27
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	13	0.27
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	13	0.27
(1,972)	1:1952:A:LYS:H	1:1951:A:THR:HB	15	0.27
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB2	7	0.27
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB3	7	0.27
(1,573)	1:1817:A:ALA:HB1	1:1819:A:ARG:H	15	0.27
(1,573)	1:1817:A:ALA:HB2	1:1819:A:ARG:H	15	0.27
(1,573)	1:1817:A:ALA:HB3	1:1819:A:ARG:H	15	0.27
(1,413)	1:1923:A:GLY:H	1:1922:A:ILE:HG21	16	0.27
(1,413)	1:1923:A:GLY:H	1:1922:A:ILE:HG22	16	0.27
(1,413)	1:1923:A:GLY:H	1:1922:A:ILE:HG23	16	0.27
(1,316)	1:1919:A:VAL:HG21	1:1918:A:THR:HG21	1	0.27
(1,316)	1:1919:A:VAL:HG21	1:1918:A:THR:HG22	1	0.27
(1,316)	1:1919:A:VAL:HG21	1:1918:A:THR:HG23	1	0.27
(1,316)	1:1919:A:VAL:HG22	1:1918:A:THR:HG21	1	0.27
(1,316)	1:1919:A:VAL:HG22	1:1918:A:THR:HG22	1	0.27
(1,316)	1:1919:A:VAL:HG22	1:1918:A:THR:HG23	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,316)	1:1919:A:VAL:HG23	1:1918:A:THR:HG21	1	0.27
(1,316)	1:1919:A:VAL:HG23	1:1918:A:THR:HG22	1	0.27
(1,316)	1:1919:A:VAL:HG23	1:1918:A:THR:HG23	1	0.27
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	11	0.26
(1,3320)	1:1900:A:SER:H	1:1899:A:THR:HA	5	0.26
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG2	4	0.26
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG3	4	0.26
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG2	8	0.26
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG3	8	0.26
(1,3159)	1:1822:A:GLU:H	1:1822:A:GLU:HG2	13	0.26
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	14	0.26
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	13	0.26
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	14	0.26
(1,2974)	1:1930:A:VAL:H	1:1929:A:GLU:HB3	14	0.26
(1,2974)	1:1930:A:VAL:H	1:1929:A:GLU:HB3	15	0.26
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	10	0.26
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	10	0.26
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	10	0.26
(1,2662)	1:1955:A:ASP:H	1:1956:A:ARG:H	15	0.26
(1,2522)	1:1903:A:ILE:H	1:1903:A:ILE:HG13	17	0.26
(1,2328)	1:1950:A:ASN:H	1:1951:A:THR:H	13	0.26
(1,2265)	1:1824:A:SER:H	1:1823:A:LYS:HB2	9	0.26
(1,2265)	1:1824:A:SER:H	1:1823:A:LYS:HB2	20	0.26
(1,2089)	1:1916:A:THR:H	1:1915:A:PRO:HB2	8	0.26
(1,2035)	1:1926:A:ASN:HB3	1:1928:A:GLU:H	7	0.26
(1,2017)	1:1838:A:LYS:HG3	1:1838:A:LYS:HE3	1	0.26
(1,2017)	1:1838:A:LYS:HG3	1:1838:A:LYS:HE3	18	0.26
(1,1982)	1:1930:A:VAL:HB	1:1930:A:VAL:HA	9	0.26
(1,1790)	1:1927:A:GLY:H	1:1925:A:THR:HB	19	0.26
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD11	4	0.26
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD12	4	0.26
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD13	4	0.26
(1,1091)	1:1939:A:LEU:HD11	1:1943:A:ARG:HD2	20	0.26
(1,1091)	1:1939:A:LEU:HD11	1:1943:A:ARG:HD3	20	0.26
(1,1091)	1:1939:A:LEU:HD12	1:1943:A:ARG:HD2	20	0.26
(1,1091)	1:1939:A:LEU:HD12	1:1943:A:ARG:HD3	20	0.26
(1,1091)	1:1939:A:LEU:HD13	1:1943:A:ARG:HD2	20	0.26
(1,1091)	1:1939:A:LEU:HD13	1:1943:A:ARG:HD3	20	0.26
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	5	0.26
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	20	0.26
(1,579)	1:1897:A:ILE:H	1:1897:A:ILE:HG12	16	0.26
(1,558)	1:1929:A:GLU:H	1:1928:A:GLU:HA	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:1923:A:GLY:H	1:1922:A:ILE:HG21	3	0.26
(1,413)	1:1923:A:GLY:H	1:1922:A:ILE:HG22	3	0.26
(1,413)	1:1923:A:GLY:H	1:1922:A:ILE:HG23	3	0.26
(1,308)	1:1897:A:ILE:H	1:1896:A:ARG:HG2	6	0.26
(1,104)	1:1951:A:THR:H	1:1951:A:THR:HB	3	0.26
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	6	0.25
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	17	0.25
(1,3172)	1:1902:A:GLY:H	1:1901:A:THR:HB	14	0.25
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG21	19	0.25
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG22	19	0.25
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG23	19	0.25
(1,3086)	1:1903:A:ILE:H	1:1900:A:SER:HB3	7	0.25
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	7	0.25
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	7	0.25
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	2	0.25
(1,2924)	1:1900:A:SER:HB2	1:1903:A:ILE:HB	12	0.25
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	16	0.25
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	16	0.25
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	16	0.25
(1,2688)	1:1938:A:ARG:HD2	1:1934:A:VAL:HG21	6	0.25
(1,2688)	1:1938:A:ARG:HD2	1:1934:A:VAL:HG22	6	0.25
(1,2688)	1:1938:A:ARG:HD2	1:1934:A:VAL:HG23	6	0.25
(1,2688)	1:1938:A:ARG:HD3	1:1934:A:VAL:HG21	6	0.25
(1,2688)	1:1938:A:ARG:HD3	1:1934:A:VAL:HG22	6	0.25
(1,2688)	1:1938:A:ARG:HD3	1:1934:A:VAL:HG23	6	0.25
(1,2631)	1:1929:A:GLU:HB2	1:1930:A:VAL:H	20	0.25
(1,2522)	1:1903:A:ILE:H	1:1903:A:ILE:HG13	1	0.25
(1,2328)	1:1950:A:ASN:H	1:1951:A:THR:H	7	0.25
(1,2328)	1:1950:A:ASN:H	1:1951:A:THR:H	15	0.25
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	9	0.25
(1,1957)	1:1927:A:GLY:H	1:1926:A:ASN:HB2	3	0.25
(1,1957)	1:1927:A:GLY:H	1:1926:A:ASN:HB2	14	0.25
(1,1703)	1:1821:A:ASP:HB3	1:1823:A:LYS:H	11	0.25
(1,1598)	1:1955:A:ASP:H	1:1953:A:GLN:HG2	14	0.25
(1,1270)	1:1893:A:GLY:H	1:1894:A:LYS:HD2	19	0.25
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG11	12	0.25
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG12	12	0.25
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG13	12	0.25
(1,1091)	1:1939:A:LEU:HD11	1:1943:A:ARG:HD2	4	0.25
(1,1091)	1:1939:A:LEU:HD11	1:1943:A:ARG:HD3	4	0.25
(1,1091)	1:1939:A:LEU:HD12	1:1943:A:ARG:HD2	4	0.25
(1,1091)	1:1939:A:LEU:HD12	1:1943:A:ARG:HD3	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1091)	1:1939:A:LEU:HD13	1:1943:A:ARG:HD2	4	0.25
(1,1091)	1:1939:A:LEU:HD13	1:1943:A:ARG:HD3	4	0.25
(1,1089)	1:1948:A:LEU:H	1:1948:A:LEU:HD11	6	0.25
(1,1089)	1:1948:A:LEU:H	1:1948:A:LEU:HD12	6	0.25
(1,1089)	1:1948:A:LEU:H	1:1948:A:LEU:HD13	6	0.25
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	9	0.25
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	9	0.25
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	9	0.25
(1,994)	1:1889:A:MET:HE1	1:1885:A:ARG:HG2	19	0.25
(1,994)	1:1889:A:MET:HE2	1:1885:A:ARG:HG2	19	0.25
(1,994)	1:1889:A:MET:HE3	1:1885:A:ARG:HG2	19	0.25
(1,981)	1:1818:A:SER:HB2	1:1820:A:ILE:H	6	0.25
(1,981)	1:1818:A:SER:HB3	1:1820:A:ILE:H	6	0.25
(1,807)	1:1907:A:MET:H	1:1906:A:GLN:HG2	3	0.25
(1,807)	1:1907:A:MET:H	1:1906:A:GLN:HG2	6	0.25
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	7	0.25
(1,442)	1:1948:A:LEU:HB2	1:1949:A:ASP:H	10	0.25
(1,377)	1:1820:A:ILE:HB	1:1823:A:LYS:HG2	17	0.25
(1,330)	1:1827:A:ALA:H	1:1826:A:LYS:HB3	13	0.25
(1,173)	1:1845:A:ASN:HA	1:1845:A:ASN:HD22	10	0.25
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	9	0.24
(1,3321)	1:1954:A:ASP:HA	1:1954:A:ASP:HB3	15	0.24
(1,3303)	1:1898:A:SER:H	1:1897:A:ILE:HG13	11	0.24
(1,3212)	1:1902:A:GLY:H	1:1900:A:SER:HB2	10	0.24
(1,3138)	1:1926:A:ASN:H	1:1926:A:ASN:HD22	10	0.24
(1,2983)	1:1838:A:LYS:HD2	1:1838:A:LYS:HG3	12	0.24
(1,2983)	1:1838:A:LYS:HD3	1:1838:A:LYS:HG3	12	0.24
(1,2974)	1:1930:A:VAL:H	1:1929:A:GLU:HB3	4	0.24
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	1	0.24
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	1	0.24
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	1	0.24
(1,2745)	1:1929:A:GLU:HG2	1:1930:A:VAL:H	8	0.24
(1,2548)	1:1925:A:THR:H	1:1924:A:ASN:HB3	15	0.24
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	18	0.24
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	10	0.24
(1,1790)	1:1927:A:GLY:H	1:1925:A:THR:HB	9	0.24
(1,1752)	1:1899:A:THR:HG21	1:1899:A:THR:H	3	0.24
(1,1752)	1:1899:A:THR:HG22	1:1899:A:THR:H	3	0.24
(1,1752)	1:1899:A:THR:HG23	1:1899:A:THR:H	3	0.24
(1,1703)	1:1821:A:ASP:HB3	1:1823:A:LYS:H	19	0.24
(1,1700)	1:1922:A:ILE:HG12	1:1922:A:ILE:H	1	0.24
(1,1675)	1:1924:A:ASN:H	1:1924:A:ASN:HB2	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1604)	1:1930:A:VAL:H	1:1931:A:GLY:H	14	0.24
(1,1604)	1:1930:A:VAL:H	1:1931:A:GLY:H	17	0.24
(1,1131)	1:1824:A:SER:H	1:1827:A:ALA:HB1	14	0.24
(1,1131)	1:1824:A:SER:H	1:1827:A:ALA:HB2	14	0.24
(1,1131)	1:1824:A:SER:H	1:1827:A:ALA:HB3	14	0.24
(1,807)	1:1907:A:MET:H	1:1906:A:GLN:HG2	2	0.24
(1,798)	1:1822:A:GLU:HB2	1:1823:A:LYS:H	10	0.24
(1,697)	1:1956:A:ARG:H	1:1956:A:ARG:HB3	9	0.24
(1,697)	1:1956:A:ARG:H	1:1956:A:ARG:HB3	13	0.24
(1,601)	1:1923:A:GLY:H	1:1922:A:ILE:HG13	3	0.24
(1,583)	1:1867:A:PRO:HA	1:1870:A:LYS:HB2	17	0.24
(1,525)	1:1924:A:ASN:H	1:1923:A:GLY:H	2	0.24
(1,525)	1:1924:A:ASN:H	1:1923:A:GLY:H	16	0.24
(1,474)	1:1877:A:GLN:HG2	1:1874:A:GLN:HA	5	0.24
(1,416)	1:1955:A:ASP:H	1:1954:A:ASP:H	2	0.24
(1,377)	1:1820:A:ILE:HB	1:1823:A:LYS:HG2	3	0.24
(1,195)	1:1844:A:GLU:HA	1:1846:A:THR:HG21	12	0.24
(1,195)	1:1844:A:GLU:HA	1:1846:A:THR:HG22	12	0.24
(1,195)	1:1844:A:GLU:HA	1:1846:A:THR:HG23	12	0.24
(1,74)	1:1954:A:ASP:H	1:1953:A:GLN:HG2	12	0.24
(3,56)	1:1945:A:ARG:N	1:1941:A:ILE:O	18	0.23
(1,3321)	1:1954:A:ASP:HA	1:1954:A:ASP:HB3	12	0.23
(1,3320)	1:1900:A:SER:H	1:1899:A:THR:HA	8	0.23
(1,3246)	1:1904:A:SER:H	1:1905:A:PRO:HD2	18	0.23
(1,3190)	1:1923:A:GLY:H	1:1922:A:ILE:H	17	0.23
(1,3190)	1:1923:A:GLY:H	1:1922:A:ILE:H	19	0.23
(1,3190)	1:1923:A:GLY:H	1:1922:A:ILE:H	20	0.23
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	11	0.23
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	11	0.23
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	11	0.23
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	3	0.23
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	17	0.23
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	17	0.23
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	7	0.23
(1,3021)	1:1919:A:VAL:H	1:1918:A:THR:HG21	17	0.23
(1,3021)	1:1919:A:VAL:H	1:1918:A:THR:HG22	17	0.23
(1,3021)	1:1919:A:VAL:H	1:1918:A:THR:HG23	17	0.23
(1,3021)	1:1919:A:VAL:H	1:1918:A:THR:HG21	19	0.23
(1,3021)	1:1919:A:VAL:H	1:1918:A:THR:HG22	19	0.23
(1,3021)	1:1919:A:VAL:H	1:1918:A:THR:HG23	19	0.23
(1,2974)	1:1930:A:VAL:H	1:1929:A:GLU:HB3	1	0.23
(1,2971)	1:1933:A:SER:HB2	1:1934:A:VAL:H	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2859)	1:1943:A:ARG:HA	1:1838:A:LYS:HE2	17	0.23
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	6	0.23
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	6	0.23
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	6	0.23
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	18	0.23
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	18	0.23
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	18	0.23
(1,2665)	1:1900:A:SER:H	1:1899:A:THR:HG21	15	0.23
(1,2665)	1:1900:A:SER:H	1:1899:A:THR:HG22	15	0.23
(1,2665)	1:1900:A:SER:H	1:1899:A:THR:HG23	15	0.23
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE1	17	0.23
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE2	17	0.23
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE1	17	0.23
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE2	17	0.23
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE1	17	0.23
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE2	17	0.23
(1,2522)	1:1903:A:ILE:H	1:1903:A:ILE:HG13	3	0.23
(1,2515)	1:1898:A:SER:H	1:1897:A:ILE:HB	6	0.23
(1,2410)	1:1898:A:SER:H	1:1898:A:SER:HB2	3	0.23
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	5	0.23
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	5	0.23
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	5	0.23
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	5	0.23
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	5	0.23
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	5	0.23
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	5	0.23
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	5	0.23
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	5	0.23
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	5	0.23
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG21	12	0.23
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG22	12	0.23
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG23	12	0.23
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG21	12	0.23
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG22	12	0.23
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG23	12	0.23
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG21	12	0.23
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG22	12	0.23
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG23	12	0.23
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG21	12	0.23
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG22	12	0.23
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG23	12	0.23
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG21	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG22	12	0.23
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG23	12	0.23
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG21	12	0.23
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG22	12	0.23
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG23	12	0.23
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	19	0.23
(1,2089)	1:1916:A:THR:H	1:1915:A:PRO:HB2	13	0.23
(1,2089)	1:1916:A:THR:H	1:1915:A:PRO:HB2	14	0.23
(1,2045)	1:1924:A:ASN:H	1:1924:A:ASN:HB3	18	0.23
(1,2017)	1:1838:A:LYS:HG3	1:1838:A:LYS:HE3	7	0.23
(1,1755)	1:1907:A:MET:H	1:1906:A:GLN:HB2	16	0.23
(1,1703)	1:1821:A:ASP:HB3	1:1823:A:LYS:H	1	0.23
(1,1675)	1:1924:A:ASN:H	1:1924:A:ASN:HB2	4	0.23
(1,1675)	1:1924:A:ASN:H	1:1924:A:ASN:HB2	14	0.23
(1,1634)	1:1953:A:GLN:HA	1:1953:A:GLN:HG3	10	0.23
(1,1634)	1:1953:A:GLN:HA	1:1953:A:GLN:HG3	13	0.23
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE2	9	0.23
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE3	9	0.23
(1,1272)	1:1895:A:GLY:H	1:1893:A:GLY:H	11	0.23
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD11	1	0.23
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD12	1	0.23
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD13	1	0.23
(1,888)	1:1887:A:ILE:HA	1:1890:A:GLU:HG2	1	0.23
(1,807)	1:1907:A:MET:H	1:1906:A:GLN:HG2	10	0.23
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG21	6	0.23
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG22	6	0.23
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG23	6	0.23
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG21	6	0.23
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG22	6	0.23
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG23	6	0.23
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG21	6	0.23
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG22	6	0.23
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG23	6	0.23
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG21	8	0.23
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG22	8	0.23
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG23	8	0.23
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG21	8	0.23
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG22	8	0.23
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG23	8	0.23
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG21	8	0.23
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG22	8	0.23
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG23	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG21	12	0.23
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG22	12	0.23
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG23	12	0.23
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG21	12	0.23
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG22	12	0.23
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG23	12	0.23
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG21	12	0.23
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG22	12	0.23
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG23	12	0.23
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG21	2	0.23
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG22	2	0.23
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG23	2	0.23
(1,697)	1:1956:A:ARG:H	1:1956:A:ARG:HB3	2	0.23
(1,697)	1:1956:A:ARG:H	1:1956:A:ARG:HB3	6	0.23
(1,679)	1:1954:A:ASP:H	1:1953:A:GLN:HB2	6	0.23
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	1	0.23
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	16	0.23
(1,558)	1:1929:A:GLU:H	1:1928:A:GLU:HA	3	0.23
(1,558)	1:1929:A:GLU:H	1:1928:A:GLU:HA	17	0.23
(1,442)	1:1948:A:LEU:HB2	1:1949:A:ASP:H	11	0.23
(1,367)	1:1940:A:LYS:HA	1:1943:A:ARG:HD2	7	0.23
(1,367)	1:1940:A:LYS:HA	1:1943:A:ARG:HD3	7	0.23
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	16	0.23
(1,265)	1:1904:A:SER:HB2	1:1913:A:PRO:HG3	19	0.23
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	9	0.23
(1,169)	1:1821:A:ASP:HB2	1:1822:A:GLU:H	7	0.23
(1,125)	1:1822:A:GLU:HG2	1:1823:A:LYS:H	20	0.23
(1,74)	1:1954:A:ASP:H	1:1953:A:GLN:HG2	11	0.23
(1,61)	1:1948:A:LEU:HD11	1:1949:A:ASP:H	7	0.23
(1,61)	1:1948:A:LEU:HD12	1:1949:A:ASP:H	7	0.23
(1,61)	1:1948:A:LEU:HD13	1:1949:A:ASP:H	7	0.23
(3,45)	1:1934:A:VAL:N	1:1930:A:VAL:O	20	0.22
(1,3271)	1:1870:A:LYS:HD2	1:1870:A:LYS:HG3	13	0.22
(1,3271)	1:1870:A:LYS:HD3	1:1870:A:LYS:HG3	13	0.22
(1,3271)	1:1870:A:LYS:HD2	1:1870:A:LYS:HG3	17	0.22
(1,3271)	1:1870:A:LYS:HD3	1:1870:A:LYS:HG3	17	0.22
(1,3271)	1:1870:A:LYS:HD2	1:1870:A:LYS:HG3	18	0.22
(1,3271)	1:1870:A:LYS:HD3	1:1870:A:LYS:HG3	18	0.22
(1,3271)	1:1870:A:LYS:HD2	1:1870:A:LYS:HG3	20	0.22
(1,3271)	1:1870:A:LYS:HD3	1:1870:A:LYS:HG3	20	0.22
(1,3246)	1:1904:A:SER:H	1:1905:A:PRO:HD2	20	0.22
(1,3190)	1:1923:A:GLY:H	1:1922:A:ILE:H	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3190)	1:1923:A:GLY:H	1:1922:A:ILE:H	15	0.22
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	10	0.22
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG21	14	0.22
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG22	14	0.22
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG23	14	0.22
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	8	0.22
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	8	0.22
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	8	0.22
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	6	0.22
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	16	0.22
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	17	0.22
(1,3075)	1:1942:A:LEU:HB3	1:1838:A:LYS:HG3	20	0.22
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	2	0.22
(1,2973)	1:1870:A:LYS:HA	1:1874:A:GLN:HE21	16	0.22
(1,2924)	1:1900:A:SER:HB2	1:1903:A:ILE:HB	14	0.22
(1,2825)	1:1818:A:SER:HB3	1:1821:A:ASP:H	19	0.22
(1,2709)	1:1824:A:SER:HA	1:1825:A:SER:H	4	0.22
(1,2705)	1:1889:A:MET:HA	1:1894:A:LYS:HB3	19	0.22
(1,2622)	1:1830:A:ASN:H	1:1829:A:VAL:HB	5	0.22
(1,2564)	1:1909:A:VAL:H	1:1910:A:THR:H	12	0.22
(1,2490)	1:1820:A:ILE:HD11	1:1821:A:ASP:H	9	0.22
(1,2490)	1:1820:A:ILE:HD12	1:1821:A:ASP:H	9	0.22
(1,2490)	1:1820:A:ILE:HD13	1:1821:A:ASP:H	9	0.22
(1,2490)	1:1820:A:ILE:HD11	1:1821:A:ASP:H	20	0.22
(1,2490)	1:1820:A:ILE:HD12	1:1821:A:ASP:H	20	0.22
(1,2490)	1:1820:A:ILE:HD13	1:1821:A:ASP:H	20	0.22
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	17	0.22
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	17	0.22
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	17	0.22
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD11	13	0.22
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD12	13	0.22
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD13	13	0.22
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG21	2	0.22
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG22	2	0.22
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG23	2	0.22
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG21	2	0.22
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG22	2	0.22
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG23	2	0.22
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG21	2	0.22
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG22	2	0.22
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG23	2	0.22
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	13	0.22
(1,2089)	1:1916:A:THR:H	1:1915:A:PRO:HB2	4	0.22
(1,2012)	1:1823:A:LYS:H	1:1822:A:GLU:HB3	10	0.22
(1,1952)	1:1840:A:ILE:HG21	1:1846:A:THR:HB	6	0.22
(1,1952)	1:1840:A:ILE:HG22	1:1846:A:THR:HB	6	0.22
(1,1952)	1:1840:A:ILE:HG23	1:1846:A:THR:HB	6	0.22
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG21	14	0.22
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG22	14	0.22
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG23	14	0.22
(1,1718)	1:1902:A:GLY:H	1:1901:A:THR:HA	12	0.22
(1,1598)	1:1955:A:ASP:H	1:1953:A:GLN:HG2	5	0.22
(1,1439)	1:1928:A:GLU:HA	1:1928:A:GLU:HB3	7	0.22
(1,1361)	1:1862:A:ASP:H	1:1861:A:SER:HB3	19	0.22
(1,1261)	1:1927:A:GLY:H	1:1925:A:THR:HG21	13	0.22
(1,1261)	1:1927:A:GLY:H	1:1925:A:THR:HG22	13	0.22
(1,1261)	1:1927:A:GLY:H	1:1925:A:THR:HG23	13	0.22
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD11	20	0.22
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD12	20	0.22
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD13	20	0.22
(1,1105)	1:1838:A:LYS:HD2	1:1943:A:ARG:HA	20	0.22
(1,1105)	1:1838:A:LYS:HD3	1:1943:A:ARG:HA	20	0.22
(1,981)	1:1818:A:SER:HB2	1:1820:A:ILE:H	18	0.22
(1,981)	1:1818:A:SER:HB3	1:1820:A:ILE:H	18	0.22
(1,972)	1:1952:A:LYS:H	1:1951:A:THR:HB	14	0.22
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB2	16	0.22
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB3	16	0.22
(1,758)	1:1823:A:LYS:H	1:1823:A:LYS:HG3	15	0.22
(1,736)	1:1898:A:SER:H	1:1897:A:ILE:H	2	0.22
(1,697)	1:1956:A:ARG:H	1:1956:A:ARG:HB3	1	0.22
(1,697)	1:1956:A:ARG:H	1:1956:A:ARG:HB3	8	0.22
(1,690)	1:1899:A:THR:H	1:1898:A:SER:HB2	11	0.22
(1,583)	1:1867:A:PRO:HA	1:1870:A:LYS:HB2	9	0.22
(1,579)	1:1897:A:ILE:H	1:1897:A:ILE:HG12	15	0.22
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	16	0.22
(1,442)	1:1948:A:LEU:HB2	1:1949:A:ASP:H	5	0.22
(1,308)	1:1897:A:ILE:H	1:1896:A:ARG:HG2	2	0.22
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG21	15	0.22
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG22	15	0.22
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG23	15	0.22
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	19	0.22
(1,125)	1:1822:A:GLU:HG2	1:1823:A:LYS:H	9	0.22
(1,125)	1:1822:A:GLU:HG2	1:1823:A:LYS:H	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:1954:A:ASP:H	1:1953:A:GLN:HG2	7	0.22
(1,3320)	1:1900:A:SER:H	1:1899:A:THR:HA	15	0.21
(1,3303)	1:1898:A:SER:H	1:1897:A:ILE:HG13	12	0.21
(1,3190)	1:1923:A:GLY:H	1:1922:A:ILE:H	2	0.21
(1,3190)	1:1923:A:GLY:H	1:1922:A:ILE:H	4	0.21
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	16	0.21
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	16	0.21
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	6	0.21
(1,3051)	1:1918:A:THR:H	1:1917:A:SER:HB2	8	0.21
(1,3028)	1:1954:A:ASP:H	1:1954:A:ASP:HB2	12	0.21
(1,2973)	1:1870:A:LYS:HA	1:1874:A:GLN:HE21	4	0.21
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	19	0.21
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	19	0.21
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	19	0.21
(1,2924)	1:1900:A:SER:HB2	1:1903:A:ILE:HB	16	0.21
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	17	0.21
(1,2854)	1:1924:A:ASN:H	1:1924:A:ASN:HA	1	0.21
(1,2854)	1:1924:A:ASN:H	1:1924:A:ASN:HA	9	0.21
(1,2847)	1:1921:A:SER:HA	1:1922:A:ILE:H	11	0.21
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	13	0.21
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	13	0.21
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	13	0.21
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	17	0.21
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	17	0.21
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	17	0.21
(1,2745)	1:1929:A:GLU:HG2	1:1930:A:VAL:H	13	0.21
(1,2682)	1:1826:A:LYS:HB2	1:1871:A:ASN:HD22	7	0.21
(1,2580)	1:1929:A:GLU:H	1:1928:A:GLU:HG2	7	0.21
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	20	0.21
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	9	0.21
(1,2490)	1:1820:A:ILE:HD11	1:1821:A:ASP:H	10	0.21
(1,2490)	1:1820:A:ILE:HD12	1:1821:A:ASP:H	10	0.21
(1,2490)	1:1820:A:ILE:HD13	1:1821:A:ASP:H	10	0.21
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	14	0.21
(1,2347)	1:1820:A:ILE:HB	1:1821:A:ASP:H	3	0.21
(1,2347)	1:1820:A:ILE:HB	1:1821:A:ASP:H	17	0.21
(1,2328)	1:1950:A:ASN:H	1:1951:A:THR:H	6	0.21
(1,2268)	1:1824:A:SER:HB3	1:1825:A:SER:H	10	0.21
(1,2234)	1:1924:A:ASN:H	1:1922:A:ILE:HA	19	0.21
(1,2099)	1:1927:A:GLY:H	1:1928:A:GLU:H	2	0.21
(1,2048)	1:1838:A:LYS:HD2	1:1838:A:LYS:HE3	5	0.21
(1,2048)	1:1838:A:LYS:HD3	1:1838:A:LYS:HE3	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2028)	1:1824:A:SER:H	1:1823:A:LYS:HG3	7	0.21
(1,2012)	1:1823:A:LYS:H	1:1822:A:GLU:HB3	7	0.21
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD11	4	0.21
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD12	4	0.21
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD13	4	0.21
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD11	19	0.21
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD12	19	0.21
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD13	19	0.21
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG21	13	0.21
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG22	13	0.21
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG23	13	0.21
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG21	16	0.21
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG22	16	0.21
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG23	16	0.21
(1,1675)	1:1924:A:ASN:H	1:1924:A:ASN:HB2	6	0.21
(1,1627)	1:1863:A:ALA:H	1:1861:A:SER:HB2	1	0.21
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG21	10	0.21
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG22	10	0.21
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG23	10	0.21
(1,1514)	1:1896:A:ARG:HB2	1:1889:A:MET:HE1	7	0.21
(1,1514)	1:1896:A:ARG:HB2	1:1889:A:MET:HE2	7	0.21
(1,1514)	1:1896:A:ARG:HB2	1:1889:A:MET:HE3	7	0.21
(1,1470)	1:1824:A:SER:H	1:1827:A:ALA:H	10	0.21
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	4	0.21
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	11	0.21
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	18	0.21
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	13	0.21
(1,1361)	1:1862:A:ASP:H	1:1861:A:SER:HB3	9	0.21
(1,1272)	1:1895:A:GLY:H	1:1893:A:GLY:H	15	0.21
(1,972)	1:1952:A:LYS:H	1:1951:A:THR:HB	2	0.21
(1,925)	1:1955:A:ASP:H	1:1953:A:GLN:HA	13	0.21
(1,897)	1:1946:A:CYS:H	1:1945:A:ARG:HB2	13	0.21
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	2	0.21
(1,807)	1:1907:A:MET:H	1:1906:A:GLN:HG2	1	0.21
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG21	15	0.21
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG22	15	0.21
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG23	15	0.21
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG21	15	0.21
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG22	15	0.21
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG23	15	0.21
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG21	15	0.21
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG22	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG23	15	0.21
(1,697)	1:1956:A:ARG:H	1:1956:A:ARG:HB3	17	0.21
(1,612)	1:1900:A:SER:HB3	1:1901:A:THR:H	18	0.21
(1,579)	1:1897:A:ILE:H	1:1897:A:ILE:HG12	8	0.21
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	17	0.21
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	17	0.21
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	17	0.21
(1,525)	1:1924:A:ASN:H	1:1923:A:GLY:H	5	0.21
(1,474)	1:1877:A:GLN:HG2	1:1874:A:GLN:HA	17	0.21
(1,442)	1:1948:A:LEU:HB2	1:1949:A:ASP:H	18	0.21
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	7	0.21
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	17	0.21
(1,311)	1:1930:A:VAL:H	1:1930:A:VAL:HG21	14	0.21
(1,311)	1:1930:A:VAL:H	1:1930:A:VAL:HG22	14	0.21
(1,311)	1:1930:A:VAL:H	1:1930:A:VAL:HG23	14	0.21
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD11	10	0.21
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD12	10	0.21
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD13	10	0.21
(1,239)	1:1896:A:ARG:H	1:1897:A:ILE:HB	8	0.21
(1,239)	1:1896:A:ARG:H	1:1897:A:ILE:HB	15	0.21
(1,76)	1:1897:A:ILE:H	1:1896:A:ARG:HB2	2	0.21
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	15	0.21
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	15	0.21
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	15	0.21
(3,56)	1:1945:A:ARG:N	1:1941:A:ILE:O	10	0.2
(3,56)	1:1945:A:ARG:N	1:1941:A:ILE:O	15	0.2
(3,45)	1:1934:A:VAL:N	1:1930:A:VAL:O	9	0.2
(3,45)	1:1934:A:VAL:N	1:1930:A:VAL:O	19	0.2
(1,3303)	1:1898:A:SER:H	1:1897:A:ILE:HG13	6	0.2
(1,3203)	1:1903:A:ILE:H	1:1900:A:SER:HB2	6	0.2
(1,3190)	1:1923:A:GLY:H	1:1922:A:ILE:H	5	0.2
(1,3190)	1:1923:A:GLY:H	1:1922:A:ILE:H	12	0.2
(1,3172)	1:1902:A:GLY:H	1:1901:A:THR:HB	10	0.2
(1,3172)	1:1902:A:GLY:H	1:1901:A:THR:HB	16	0.2
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	11	0.2
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	10	0.2
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	10	0.2
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	10	0.2
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	11	0.2
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	18	0.2
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	4	0.2
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	6	0.2
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	6	0.2
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	13	0.2
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	13	0.2
(1,3075)	1:1942:A:LEU:HB3	1:1838:A:LYS:HG3	17	0.2
(1,3028)	1:1954:A:ASP:H	1:1954:A:ASP:HB2	15	0.2
(1,3020)	1:1948:A:LEU:HA	1:1949:A:ASP:H	14	0.2
(1,2974)	1:1930:A:VAL:H	1:1929:A:GLU:HB3	12	0.2
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	5	0.2
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	5	0.2
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	5	0.2
(1,2854)	1:1924:A:ASN:H	1:1924:A:ASN:HA	2	0.2
(1,2847)	1:1921:A:SER:HA	1:1922:A:ILE:H	5	0.2
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	1	0.2
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	19	0.2
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	19	0.2
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	19	0.2
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE1	16	0.2
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE2	16	0.2
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE1	16	0.2
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE2	16	0.2
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE1	16	0.2
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE2	16	0.2
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	7	0.2
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	15	0.2
(1,2522)	1:1903:A:ILE:H	1:1903:A:ILE:HG13	11	0.2
(1,2522)	1:1903:A:ILE:H	1:1903:A:ILE:HG13	20	0.2
(1,2489)	1:1893:A:GLY:H	1:1891:A:ARG:HB2	12	0.2
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	7	0.2
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	17	0.2
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	17	0.2
(1,2347)	1:1820:A:ILE:HB	1:1821:A:ASP:H	4	0.2
(1,2347)	1:1820:A:ILE:HB	1:1821:A:ASP:H	8	0.2
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	18	0.2
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	18	0.2
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	18	0.2
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	18	0.2
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	18	0.2
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	18	0.2
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	18	0.2
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	18	0.2
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	7	0.2
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	7	0.2
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	7	0.2
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	9	0.2
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	9	0.2
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	9	0.2
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	13	0.2
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	13	0.2
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	13	0.2
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	20	0.2
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	20	0.2
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	20	0.2
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG21	3	0.2
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG22	3	0.2
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG23	3	0.2
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG21	3	0.2
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG22	3	0.2
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG23	3	0.2
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG21	3	0.2
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG22	3	0.2
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG23	3	0.2
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG21	13	0.2
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG22	13	0.2
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG23	13	0.2
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG21	13	0.2
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG22	13	0.2
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG23	13	0.2
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG21	13	0.2
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG22	13	0.2
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG23	13	0.2
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG21	14	0.2
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG22	14	0.2
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG23	14	0.2
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG21	14	0.2
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG22	14	0.2
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG23	14	0.2
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG21	14	0.2
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG22	14	0.2
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG23	14	0.2
(1,2165)	1:1841:A:GLY:H	1:1876:A:PHE:HE1	7	0.2
(1,2165)	1:1841:A:GLY:H	1:1876:A:PHE:HE2	7	0.2
(1,2099)	1:1927:A:GLY:H	1:1928:A:GLU:H	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2089)	1:1916:A:THR:H	1:1915:A:PRO:HB2	2	0.2
(1,2089)	1:1916:A:THR:H	1:1915:A:PRO:HB2	6	0.2
(1,2037)	1:1843:A:LYS:HE3	1:1844:A:GLU:HG3	14	0.2
(1,1963)	1:1942:A:LEU:H	1:1941:A:ILE:HG12	12	0.2
(1,1957)	1:1927:A:GLY:H	1:1926:A:ASN:HB2	5	0.2
(1,1952)	1:1840:A:ILE:HG21	1:1846:A:THR:HB	14	0.2
(1,1952)	1:1840:A:ILE:HG22	1:1846:A:THR:HB	14	0.2
(1,1952)	1:1840:A:ILE:HG23	1:1846:A:THR:HB	14	0.2
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG21	2	0.2
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG22	2	0.2
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG23	2	0.2
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG21	11	0.2
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG22	11	0.2
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG23	11	0.2
(1,1898)	1:1928:A:GLU:H	1:1928:A:GLU:HB2	11	0.2
(1,1752)	1:1899:A:THR:HG21	1:1899:A:THR:H	6	0.2
(1,1752)	1:1899:A:THR:HG22	1:1899:A:THR:H	6	0.2
(1,1752)	1:1899:A:THR:HG23	1:1899:A:THR:H	6	0.2
(1,1752)	1:1899:A:THR:HG21	1:1899:A:THR:H	20	0.2
(1,1752)	1:1899:A:THR:HG22	1:1899:A:THR:H	20	0.2
(1,1752)	1:1899:A:THR:HG23	1:1899:A:THR:H	20	0.2
(1,1675)	1:1924:A:ASN:H	1:1924:A:ASN:HB2	2	0.2
(1,1634)	1:1953:A:GLN:HA	1:1953:A:GLN:HG3	5	0.2
(1,1598)	1:1955:A:ASP:H	1:1953:A:GLN:HG2	6	0.2
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	10	0.2
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	5	0.2
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	5	0.2
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	8	0.2
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	18	0.2
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	16	0.2
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	16	0.2
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG21	2	0.2
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG22	2	0.2
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG23	2	0.2
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG21	14	0.2
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG22	14	0.2
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG23	14	0.2
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG21	17	0.2
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG22	17	0.2
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG23	17	0.2
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG21	18	0.2
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG22	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG23	18	0.2
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG21	20	0.2
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG22	20	0.2
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG23	20	0.2
(1,1307)	1:1821:A:ASP:HA	1:1823:A:LYS:H	13	0.2
(1,1255)	1:1865:A:ILE:HD11	1:1857:A:LYS:HE2	4	0.2
(1,1255)	1:1865:A:ILE:HD12	1:1857:A:LYS:HE2	4	0.2
(1,1255)	1:1865:A:ILE:HD13	1:1857:A:LYS:HE2	4	0.2
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	13	0.2
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	13	0.2
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD11	16	0.2
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD12	16	0.2
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD13	16	0.2
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG11	4	0.2
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG12	4	0.2
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG13	4	0.2
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG11	7	0.2
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG12	7	0.2
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG13	7	0.2
(1,981)	1:1818:A:SER:HB2	1:1820:A:ILE:H	17	0.2
(1,981)	1:1818:A:SER:HB3	1:1820:A:ILE:H	17	0.2
(1,972)	1:1952:A:LYS:H	1:1951:A:THR:HB	17	0.2
(1,972)	1:1952:A:LYS:H	1:1951:A:THR:HB	20	0.2
(1,889)	1:1889:A:MET:H	1:1892:A:GLU:HG3	2	0.2
(1,889)	1:1889:A:MET:H	1:1892:A:GLU:HG3	6	0.2
(1,889)	1:1889:A:MET:H	1:1892:A:GLU:HG3	11	0.2
(1,851)	1:1906:A:GLN:HB2	1:1908:A:GLU:H	19	0.2
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	4	0.2
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	15	0.2
(1,807)	1:1907:A:MET:H	1:1906:A:GLN:HG2	12	0.2
(1,807)	1:1907:A:MET:H	1:1906:A:GLN:HG2	13	0.2
(1,807)	1:1907:A:MET:H	1:1906:A:GLN:HG2	15	0.2
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG21	3	0.2
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG22	3	0.2
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG23	3	0.2
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG21	3	0.2
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG22	3	0.2
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG23	3	0.2
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG21	3	0.2
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG22	3	0.2
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG23	3	0.2
(1,758)	1:1823:A:LYS:H	1:1823:A:LYS:HG3	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:1898:A:SER:H	1:1897:A:ILE:H	8	0.2
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG21	14	0.2
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG22	14	0.2
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG23	14	0.2
(1,664)	1:1954:A:ASP:H	1:1953:A:GLN:HA	20	0.2
(1,579)	1:1897:A:ILE:H	1:1897:A:ILE:HG12	11	0.2
(1,573)	1:1817:A:ALA:HB1	1:1819:A:ARG:H	6	0.2
(1,573)	1:1817:A:ALA:HB2	1:1819:A:ARG:H	6	0.2
(1,573)	1:1817:A:ALA:HB3	1:1819:A:ARG:H	6	0.2
(1,558)	1:1929:A:GLU:H	1:1928:A:GLU:HA	9	0.2
(1,555)	1:1927:A:GLY:H	1:1926:A:ASN:HB3	17	0.2
(1,474)	1:1877:A:GLN:HG2	1:1874:A:GLN:HA	19	0.2
(1,466)	1:1917:A:SER:H	1:1917:A:SER:HB2	12	0.2
(1,385)	1:1952:A:LYS:H	1:1951:A:THR:HA	1	0.2
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	1	0.2
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	10	0.2
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	18	0.2
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG11	11	0.2
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG12	11	0.2
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG13	11	0.2
(1,239)	1:1896:A:ARG:H	1:1897:A:ILE:HB	12	0.2
(1,228)	1:1848:A:GLU:H	1:1846:A:THR:HG21	12	0.2
(1,228)	1:1848:A:GLU:H	1:1846:A:THR:HG22	12	0.2
(1,228)	1:1848:A:GLU:H	1:1846:A:THR:HG23	12	0.2
(1,125)	1:1822:A:GLU:HG2	1:1823:A:LYS:H	6	0.2
(1,116)	1:1948:A:LEU:H	1:1949:A:ASP:H	9	0.2
(1,116)	1:1948:A:LEU:H	1:1949:A:ASP:H	17	0.2
(1,74)	1:1954:A:ASP:H	1:1953:A:GLN:HG2	15	0.2
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	12	0.19
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG21	10	0.19
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG22	10	0.19
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG23	10	0.19
(1,3258)	1:1862:A:ASP:HA	1:1865:A:ILE:HB	9	0.19
(1,3258)	1:1862:A:ASP:HA	1:1865:A:ILE:HB	13	0.19
(1,3255)	1:1926:A:ASN:H	1:1925:A:THR:HA	8	0.19
(1,3212)	1:1902:A:GLY:H	1:1900:A:SER:HB2	5	0.19
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	1	0.19
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	18	0.19
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	5	0.19
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	5	0.19
(1,3086)	1:1903:A:ILE:H	1:1900:A:SER:HB3	16	0.19
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	12	0.19
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	20	0.19
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	20	0.19
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	3	0.19
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	5	0.19
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	8	0.19
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	12	0.19
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	20	0.19
(1,3020)	1:1948:A:LEU:HA	1:1949:A:ASP:H	7	0.19
(1,3020)	1:1948:A:LEU:HA	1:1949:A:ASP:H	20	0.19
(1,2971)	1:1933:A:SER:HB2	1:1934:A:VAL:H	13	0.19
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	7	0.19
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	7	0.19
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	7	0.19
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	20	0.19
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	20	0.19
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	20	0.19
(1,2886)	1:1905:A:PRO:HD2	1:1905:A:PRO:HB2	2	0.19
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	8	0.19
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	8	0.19
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	8	0.19
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	8	0.19
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	8	0.19
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	8	0.19
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	8	0.19
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	8	0.19
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	8	0.19
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	12	0.19
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	12	0.19
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	12	0.19
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	12	0.19
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	12	0.19
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	12	0.19
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	12	0.19
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	12	0.19
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	12	0.19
(1,2854)	1:1924:A:ASN:H	1:1924:A:ASN:HA	7	0.19
(1,2847)	1:1921:A:SER:HA	1:1922:A:ILE:H	2	0.19
(1,2847)	1:1921:A:SER:HA	1:1922:A:ILE:H	15	0.19
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	16	0.19
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	19	0.19
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	8	0.19
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	8	0.19
(1,2682)	1:1826:A:LYS:HB2	1:1871:A:ASN:HD22	13	0.19
(1,2581)	1:1920:A:SER:H	1:1919:A:VAL:HB	1	0.19
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	9	0.19
(1,2503)	1:1873:A:SER:HB2	1:1873:A:SER:H	9	0.19
(1,2490)	1:1820:A:ILE:HD11	1:1821:A:ASP:H	2	0.19
(1,2490)	1:1820:A:ILE:HD12	1:1821:A:ASP:H	2	0.19
(1,2490)	1:1820:A:ILE:HD13	1:1821:A:ASP:H	2	0.19
(1,2490)	1:1820:A:ILE:HD11	1:1821:A:ASP:H	12	0.19
(1,2490)	1:1820:A:ILE:HD12	1:1821:A:ASP:H	12	0.19
(1,2490)	1:1820:A:ILE:HD13	1:1821:A:ASP:H	12	0.19
(1,2489)	1:1893:A:GLY:H	1:1891:A:ARG:HB2	16	0.19
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	12	0.19
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	20	0.19
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	1	0.19
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	10	0.19
(1,2328)	1:1950:A:ASN:H	1:1951:A:THR:H	16	0.19
(1,2309)	1:1845:A:ASN:HD22	1:1844:A:GLU:HB3	10	0.19
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	13	0.19
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	13	0.19
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	13	0.19
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	13	0.19
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	13	0.19
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	13	0.19
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	13	0.19
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	13	0.19
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	13	0.19
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	5	0.19
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	5	0.19
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	5	0.19
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE2	14	0.19
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE3	14	0.19
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG21	5	0.19
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG22	5	0.19
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG23	5	0.19
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG21	5	0.19
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG22	5	0.19
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG23	5	0.19
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG21	5	0.19
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG22	5	0.19
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG23	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG21	20	0.19
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG22	20	0.19
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG23	20	0.19
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG21	20	0.19
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG22	20	0.19
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG23	20	0.19
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG21	20	0.19
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG22	20	0.19
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG23	20	0.19
(1,2179)	1:1940:A:LYS:HA	1:1943:A:ARG:HB2	8	0.19
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	16	0.19
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	15	0.19
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	15	0.19
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	15	0.19
(1,2099)	1:1927:A:GLY:H	1:1928:A:GLU:H	5	0.19
(1,2099)	1:1927:A:GLY:H	1:1928:A:GLU:H	6	0.19
(1,2089)	1:1916:A:THR:H	1:1915:A:PRO:HB2	3	0.19
(1,2012)	1:1823:A:LYS:H	1:1822:A:GLU:HB3	20	0.19
(1,2011)	1:1930:A:VAL:H	1:1929:A:GLU:HG3	3	0.19
(1,1952)	1:1840:A:ILE:HG21	1:1846:A:THR:HB	13	0.19
(1,1952)	1:1840:A:ILE:HG22	1:1846:A:THR:HB	13	0.19
(1,1952)	1:1840:A:ILE:HG23	1:1846:A:THR:HB	13	0.19
(1,1806)	1:1840:A:ILE:HB	1:1876:A:PHE:HZ	10	0.19
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD21	5	0.19
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD22	5	0.19
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD23	5	0.19
(1,1770)	1:1914:A:THR:HB	1:1915:A:PRO:HD2	7	0.19
(1,1755)	1:1907:A:MET:H	1:1906:A:GLN:HB2	11	0.19
(1,1718)	1:1902:A:GLY:H	1:1901:A:THR:HA	18	0.19
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG21	3	0.19
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG22	3	0.19
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG23	3	0.19
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	17	0.19
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	19	0.19
(1,1439)	1:1928:A:GLU:HA	1:1928:A:GLU:HB3	13	0.19
(1,1410)	1:1951:A:THR:HG21	1:1951:A:THR:H	12	0.19
(1,1410)	1:1951:A:THR:HG22	1:1951:A:THR:H	12	0.19
(1,1410)	1:1951:A:THR:HG23	1:1951:A:THR:H	12	0.19
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	1	0.19
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	2	0.19
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	3	0.19
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	5	0.19
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	10	0.19
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	11	0.19
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	14	0.19
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	15	0.19
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	16	0.19
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	20	0.19
(1,1341)	1:1857:A:LYS:HA	1:1862:A:ASP:H	16	0.19
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG21	15	0.19
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG22	15	0.19
(1,1339)	1:1951:A:THR:HA	1:1951:A:THR:HG23	15	0.19
(1,1261)	1:1927:A:GLY:H	1:1925:A:THR:HG21	10	0.19
(1,1261)	1:1927:A:GLY:H	1:1925:A:THR:HG22	10	0.19
(1,1261)	1:1927:A:GLY:H	1:1925:A:THR:HG23	10	0.19
(1,1255)	1:1865:A:ILE:HD11	1:1857:A:LYS:HE2	1	0.19
(1,1255)	1:1865:A:ILE:HD12	1:1857:A:LYS:HE2	1	0.19
(1,1255)	1:1865:A:ILE:HD13	1:1857:A:LYS:HE2	1	0.19
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	7	0.19
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	7	0.19
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	12	0.19
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	12	0.19
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE2	14	0.19
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE3	14	0.19
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	14	0.19
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	14	0.19
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD11	8	0.19
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD12	8	0.19
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD13	8	0.19
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG11	10	0.19
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG12	10	0.19
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG13	10	0.19
(1,1123)	1:1955:A:ASP:H	1:1954:A:ASP:HB3	13	0.19
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	5	0.19
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	5	0.19
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	9	0.19
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	12	0.19
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	15	0.19
(1,994)	1:1889:A:MET:HE1	1:1885:A:ARG:HG2	7	0.19
(1,994)	1:1889:A:MET:HE2	1:1885:A:ARG:HG2	7	0.19
(1,994)	1:1889:A:MET:HE3	1:1885:A:ARG:HG2	7	0.19
(1,981)	1:1818:A:SER:HB2	1:1820:A:ILE:H	3	0.19
(1,981)	1:1818:A:SER:HB3	1:1820:A:ILE:H	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,981)	1:1818:A:SER:HB2	1:1820:A:ILE:H	7	0.19
(1,981)	1:1818:A:SER:HB3	1:1820:A:ILE:H	7	0.19
(1,972)	1:1952:A:LYS:H	1:1951:A:THR:HB	18	0.19
(1,897)	1:1946:A:CYS:H	1:1945:A:ARG:HB2	8	0.19
(1,897)	1:1946:A:CYS:H	1:1945:A:ARG:HB2	20	0.19
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	1	0.19
(1,798)	1:1822:A:GLU:HB2	1:1823:A:LYS:H	7	0.19
(1,758)	1:1823:A:LYS:H	1:1823:A:LYS:HG3	8	0.19
(1,697)	1:1956:A:ARG:H	1:1956:A:ARG:HB3	16	0.19
(1,690)	1:1899:A:THR:H	1:1898:A:SER:HB2	20	0.19
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	20	0.19
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	10	0.19
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	14	0.19
(1,612)	1:1900:A:SER:HB3	1:1901:A:THR:H	5	0.19
(1,573)	1:1817:A:ALA:HB1	1:1819:A:ARG:H	3	0.19
(1,573)	1:1817:A:ALA:HB2	1:1819:A:ARG:H	3	0.19
(1,573)	1:1817:A:ALA:HB3	1:1819:A:ARG:H	3	0.19
(1,573)	1:1817:A:ALA:HB1	1:1819:A:ARG:H	11	0.19
(1,573)	1:1817:A:ALA:HB2	1:1819:A:ARG:H	11	0.19
(1,573)	1:1817:A:ALA:HB3	1:1819:A:ARG:H	11	0.19
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	1	0.19
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	1	0.19
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	1	0.19
(1,526)	1:1885:A:ARG:HA	1:1888:A:GLU:HG2	8	0.19
(1,526)	1:1885:A:ARG:HA	1:1888:A:GLU:HG2	17	0.19
(1,474)	1:1877:A:GLN:HG2	1:1874:A:GLN:HA	11	0.19
(1,442)	1:1948:A:LEU:HB2	1:1949:A:ASP:H	20	0.19
(1,377)	1:1820:A:ILE:HB	1:1823:A:LYS:HG2	11	0.19
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	2	0.19
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	5	0.19
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	11	0.19
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	13	0.19
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	19	0.19
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	20	0.19
(1,330)	1:1827:A:ALA:H	1:1826:A:LYS:HB3	12	0.19
(1,311)	1:1930:A:VAL:H	1:1930:A:VAL:HG21	4	0.19
(1,311)	1:1930:A:VAL:H	1:1930:A:VAL:HG22	4	0.19
(1,311)	1:1930:A:VAL:H	1:1930:A:VAL:HG23	4	0.19
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD11	20	0.19
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD12	20	0.19
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD13	20	0.19
(1,239)	1:1896:A:ARG:H	1:1897:A:ILE:HB	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	8	0.19
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	10	0.19
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	14	0.19
(1,125)	1:1822:A:GLU:HG2	1:1823:A:LYS:H	7	0.19
(1,116)	1:1948:A:LEU:H	1:1949:A:ASP:H	14	0.19
(1,116)	1:1948:A:LEU:H	1:1949:A:ASP:H	15	0.19
(1,111)	1:1894:A:LYS:H	1:1892:A:GLU:HB3	19	0.19
(1,109)	1:1929:A:GLU:H	1:1927:A:GLY:HA2	20	0.19
(1,102)	1:1940:A:LYS:HA	1:1940:A:LYS:HD3	9	0.19
(1,90)	1:1945:A:ARG:HA	1:1945:A:ARG:HB2	9	0.19
(1,76)	1:1897:A:ILE:H	1:1896:A:ARG:HB2	6	0.19
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	1	0.19
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	1	0.19
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	1	0.19
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	8	0.19
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	8	0.19
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	8	0.19
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	14	0.19
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	14	0.19
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	14	0.19
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	1	0.18
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	13	0.18
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	17	0.18
(1,3321)	1:1954:A:ASP:HA	1:1954:A:ASP:HB3	7	0.18
(1,3303)	1:1898:A:SER:H	1:1897:A:ILE:HG13	16	0.18
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	3	0.18
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	8	0.18
(1,3159)	1:1822:A:GLU:H	1:1822:A:GLU:HG2	6	0.18
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	3	0.18
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	3	0.18
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	3	0.18
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	16	0.18
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	16	0.18
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	16	0.18
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	9	0.18
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	5	0.18
(1,3098)	1:1920:A:SER:H	1:1920:A:SER:HB3	2	0.18
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	15	0.18
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	15	0.18
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	4	0.18
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	10	0.18
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3020)	1:1948:A:LEU:HA	1:1949:A:ASP:H	4	0.18
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	1	0.18
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	20	0.18
(1,2973)	1:1870:A:LYS:HA	1:1874:A:GLN:HE21	5	0.18
(1,2971)	1:1933:A:SER:HB2	1:1934:A:VAL:H	12	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	3	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	3	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	3	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	4	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	4	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	4	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	11	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	11	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	11	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	12	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	12	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	12	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	13	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	13	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	13	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	16	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	16	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	16	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	17	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	17	0.18
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	17	0.18
(1,2924)	1:1900:A:SER:HB2	1:1903:A:ILE:HB	2	0.18
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	9	0.18
(1,2908)	1:1947:A:GLY:HA2	1:1949:A:ASP:H	1	0.18
(1,2908)	1:1947:A:GLY:HA3	1:1949:A:ASP:H	1	0.18
(1,2893)	1:1887:A:ILE:HA	1:1890:A:GLU:HB2	15	0.18
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	7	0.18
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	7	0.18
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	7	0.18
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	7	0.18
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	7	0.18
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	7	0.18
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	7	0.18
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	7	0.18
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	7	0.18
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	15	0.18
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	15	0.18
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	15	0.18
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	15	0.18
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	15	0.18
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	15	0.18
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	15	0.18
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	15	0.18
(1,2854)	1:1924:A:ASN:H	1:1924:A:ASN:HA	6	0.18
(1,2854)	1:1924:A:ASN:H	1:1924:A:ASN:HA	8	0.18
(1,2854)	1:1924:A:ASN:H	1:1924:A:ASN:HA	11	0.18
(1,2854)	1:1924:A:ASN:H	1:1924:A:ASN:HA	19	0.18
(1,2825)	1:1818:A:SER:HB3	1:1821:A:ASP:H	14	0.18
(1,2807)	1:1889:A:MET:H	1:1888:A:GLU:HB2	3	0.18
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	7	0.18
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	14	0.18
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	15	0.18
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	18	0.18
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	12	0.18
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	12	0.18
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	12	0.18
(1,2731)	1:1916:A:THR:HG21	1:1914:A:THR:HB	7	0.18
(1,2731)	1:1916:A:THR:HG22	1:1914:A:THR:HB	7	0.18
(1,2731)	1:1916:A:THR:HG23	1:1914:A:THR:HB	7	0.18
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE1	1	0.18
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE2	1	0.18
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE1	1	0.18
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE2	1	0.18
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE1	1	0.18
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE2	1	0.18
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE1	4	0.18
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE2	4	0.18
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE1	4	0.18
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE2	4	0.18
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE1	4	0.18
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE2	4	0.18
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE1	6	0.18
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE2	6	0.18
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE1	6	0.18
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE2	6	0.18
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE1	6	0.18
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE2	6	0.18
(1,2606)	1:1840:A:ILE:HD11	1:1850:A:LEU:HA	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:1840:A:ILE:HD12	1:1850:A:LEU:HA	7	0.18
(1,2606)	1:1840:A:ILE:HD13	1:1850:A:LEU:HA	7	0.18
(1,2581)	1:1920:A:SER:H	1:1919:A:VAL:HB	10	0.18
(1,2581)	1:1920:A:SER:H	1:1919:A:VAL:HB	13	0.18
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	16	0.18
(1,2548)	1:1925:A:THR:H	1:1924:A:ASN:HB3	5	0.18
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	2	0.18
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	5	0.18
(1,2504)	1:1867:A:PRO:HA	1:1871:A:ASN:HD21	17	0.18
(1,2503)	1:1873:A:SER:HB2	1:1873:A:SER:H	11	0.18
(1,2490)	1:1820:A:ILE:HD11	1:1821:A:ASP:H	1	0.18
(1,2490)	1:1820:A:ILE:HD12	1:1821:A:ASP:H	1	0.18
(1,2490)	1:1820:A:ILE:HD13	1:1821:A:ASP:H	1	0.18
(1,2490)	1:1820:A:ILE:HD11	1:1821:A:ASP:H	6	0.18
(1,2490)	1:1820:A:ILE:HD12	1:1821:A:ASP:H	6	0.18
(1,2490)	1:1820:A:ILE:HD13	1:1821:A:ASP:H	6	0.18
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE1	6	0.18
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE2	6	0.18
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE1	7	0.18
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE2	7	0.18
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE1	13	0.18
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE2	13	0.18
(1,2410)	1:1898:A:SER:H	1:1898:A:SER:HB2	1	0.18
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	9	0.18
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	11	0.18
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	4	0.18
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	8	0.18
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	9	0.18
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	11	0.18
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	20	0.18
(1,2321)	1:1903:A:ILE:H	1:1902:A:GLY:HA2	19	0.18
(1,2321)	1:1903:A:ILE:H	1:1902:A:GLY:HA3	19	0.18
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	1	0.18
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	1	0.18
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	1	0.18
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	1	0.18
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	1	0.18
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	1	0.18
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	1	0.18
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	1	0.18
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	1	0.18
(1,2287)	1:1863:A:ALA:H	1:1862:A:ASP:HA	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG21	17	0.18
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG22	17	0.18
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG23	17	0.18
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE2	3	0.18
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE3	3	0.18
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE2	5	0.18
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE3	5	0.18
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE2	7	0.18
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE3	7	0.18
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE2	9	0.18
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE3	9	0.18
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE2	10	0.18
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE3	10	0.18
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE2	11	0.18
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE3	11	0.18
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE2	13	0.18
(1,2269)	1:1857:A:LYS:HD2	1:1857:A:LYS:HE3	13	0.18
(1,2234)	1:1924:A:ASN:H	1:1922:A:ILE:HA	18	0.18
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD11	11	0.18
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD12	11	0.18
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD13	11	0.18
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG21	2	0.18
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG22	2	0.18
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG23	2	0.18
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG21	3	0.18
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG22	3	0.18
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG23	3	0.18
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG21	3	0.18
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG22	3	0.18
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG23	3	0.18
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG21	3	0.18
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG22	3	0.18
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG23	3	0.18
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	4	0.18
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	5	0.18
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	10	0.18
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	10	0.18
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	10	0.18
(1,2099)	1:1927:A:GLY:H	1:1928:A:GLU:H	3	0.18
(1,2089)	1:1916:A:THR:H	1:1915:A:PRO:HB2	1	0.18
(1,2089)	1:1916:A:THR:H	1:1915:A:PRO:HB2	15	0.18
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	14	0.18
(1,2012)	1:1823:A:LYS:H	1:1822:A:GLU:HB3	12	0.18
(1,1982)	1:1930:A:VAL:HB	1:1930:A:VAL:HA	20	0.18
(1,1963)	1:1942:A:LEU:H	1:1941:A:ILE:HG12	8	0.18
(1,1963)	1:1942:A:LEU:H	1:1941:A:ILE:HG12	9	0.18
(1,1963)	1:1942:A:LEU:H	1:1941:A:ILE:HG12	10	0.18
(1,1952)	1:1840:A:ILE:HG21	1:1846:A:THR:HB	7	0.18
(1,1952)	1:1840:A:ILE:HG22	1:1846:A:THR:HB	7	0.18
(1,1952)	1:1840:A:ILE:HG23	1:1846:A:THR:HB	7	0.18
(1,1952)	1:1840:A:ILE:HG21	1:1846:A:THR:HB	15	0.18
(1,1952)	1:1840:A:ILE:HG22	1:1846:A:THR:HB	15	0.18
(1,1952)	1:1840:A:ILE:HG23	1:1846:A:THR:HB	15	0.18
(1,1876)	1:1863:A:ALA:HB1	1:1860:A:TYR:HB2	17	0.18
(1,1876)	1:1863:A:ALA:HB2	1:1860:A:TYR:HB2	17	0.18
(1,1876)	1:1863:A:ALA:HB3	1:1860:A:TYR:HB2	17	0.18
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD21	19	0.18
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD22	19	0.18
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD23	19	0.18
(1,1755)	1:1907:A:MET:H	1:1906:A:GLN:HB2	7	0.18
(1,1718)	1:1902:A:GLY:H	1:1901:A:THR:HA	1	0.18
(1,1718)	1:1902:A:GLY:H	1:1901:A:THR:HA	11	0.18
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG21	13	0.18
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG22	13	0.18
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG23	13	0.18
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE2	6	0.18
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE3	6	0.18
(1,1565)	1:1838:A:LYS:HA	1:1842:A:SER:H	12	0.18
(1,1556)	1:1853:A:LEU:HD11	1:1857:A:LYS:HD2	11	0.18
(1,1556)	1:1853:A:LEU:HD12	1:1857:A:LYS:HD2	11	0.18
(1,1556)	1:1853:A:LEU:HD13	1:1857:A:LYS:HD2	11	0.18
(1,1505)	1:1909:A:VAL:HB	1:1910:A:THR:H	12	0.18
(1,1486)	1:1950:A:ASN:HA	1:1951:A:THR:H	14	0.18
(1,1462)	1:1924:A:ASN:HB3	1:1924:A:ASN:HA	15	0.18
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	1	0.18
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	13	0.18
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	20	0.18
(1,1439)	1:1928:A:GLU:HA	1:1928:A:GLU:HB3	9	0.18
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	6	0.18
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	7	0.18
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	9	0.18
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	12	0.18
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1387)	1:1829:A:VAL:H	1:1828:A:LYS:HG2	19	0.18
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	7	0.18
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	7	0.18
(1,1322)	1:1904:A:SER:HB2	1:1903:A:ILE:HG21	14	0.18
(1,1322)	1:1904:A:SER:HB2	1:1903:A:ILE:HG22	14	0.18
(1,1322)	1:1904:A:SER:HB2	1:1903:A:ILE:HG23	14	0.18
(1,1322)	1:1904:A:SER:HB3	1:1903:A:ILE:HG21	14	0.18
(1,1322)	1:1904:A:SER:HB3	1:1903:A:ILE:HG22	14	0.18
(1,1322)	1:1904:A:SER:HB3	1:1903:A:ILE:HG23	14	0.18
(1,1272)	1:1895:A:GLY:H	1:1893:A:GLY:H	4	0.18
(1,1244)	1:1926:A:ASN:H	1:1926:A:ASN:HB2	11	0.18
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	12	0.18
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	17	0.18
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	18	0.18
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	3	0.18
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	3	0.18
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	6	0.18
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	6	0.18
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	11	0.18
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	11	0.18
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	15	0.18
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	15	0.18
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE2	7	0.18
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE3	7	0.18
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	7	0.18
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	7	0.18
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE2	8	0.18
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE3	8	0.18
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	8	0.18
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	8	0.18
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE2	19	0.18
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE3	19	0.18
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	19	0.18
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	19	0.18
(1,1098)	1:1905:A:PRO:HD2	1:1904:A:SER:HB2	7	0.18
(1,1098)	1:1905:A:PRO:HD2	1:1904:A:SER:HB3	7	0.18
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	10	0.18
(1,982)	1:1858:A:LYS:H	1:1858:A:LYS:HG3	8	0.18
(1,954)	1:1863:A:ALA:H	1:1863:A:ALA:HA	1	0.18
(1,897)	1:1946:A:CYS:H	1:1945:A:ARG:HB2	11	0.18
(1,888)	1:1887:A:ILE:HA	1:1890:A:GLU:HG2	10	0.18
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	1	0.18
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	1	0.18
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	1	0.18
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	1	0.18
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	1	0.18
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	1	0.18
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	1	0.18
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	1	0.18
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	16	0.18
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	16	0.18
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	16	0.18
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	16	0.18
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	16	0.18
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	16	0.18
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	16	0.18
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	16	0.18
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	16	0.18
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	17	0.18
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	17	0.18
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	17	0.18
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	17	0.18
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	17	0.18
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	17	0.18
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	17	0.18
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	17	0.18
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	17	0.18
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	19	0.18
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	19	0.18
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	19	0.18
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	19	0.18
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	19	0.18
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	19	0.18
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	19	0.18
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	19	0.18
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	19	0.18
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	9	0.18
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	6	0.18
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	10	0.18
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	12	0.18
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	19	0.18
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	7	0.18
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:1823:A:LYS:H	1:1823:A:LYS:HG3	1	0.18
(1,758)	1:1823:A:LYS:H	1:1823:A:LYS:HG3	19	0.18
(1,736)	1:1898:A:SER:H	1:1897:A:ILE:H	16	0.18
(1,690)	1:1899:A:THR:H	1:1898:A:SER:HB2	17	0.18
(1,679)	1:1954:A:ASP:H	1:1953:A:GLN:HB2	18	0.18
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	7	0.18
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	10	0.18
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	10	0.18
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	10	0.18
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	20	0.18
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	20	0.18
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	20	0.18
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	8	0.18
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	9	0.18
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	18	0.18
(1,573)	1:1817:A:ALA:HB1	1:1819:A:ARG:H	17	0.18
(1,573)	1:1817:A:ALA:HB2	1:1819:A:ARG:H	17	0.18
(1,573)	1:1817:A:ALA:HB3	1:1819:A:ARG:H	17	0.18
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	2	0.18
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	2	0.18
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	2	0.18
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE2	7	0.18
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE3	7	0.18
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE2	7	0.18
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE3	7	0.18
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE2	7	0.18
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE3	7	0.18
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE2	11	0.18
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE3	11	0.18
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE2	11	0.18
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE3	11	0.18
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE2	11	0.18
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE3	11	0.18
(1,526)	1:1885:A:ARG:HA	1:1888:A:GLU:HG2	6	0.18
(1,509)	1:1865:A:ILE:HG21	1:1866:A:GLU:H	2	0.18
(1,509)	1:1865:A:ILE:HG22	1:1866:A:GLU:H	2	0.18
(1,509)	1:1865:A:ILE:HG23	1:1866:A:GLU:H	2	0.18
(1,474)	1:1877:A:GLN:HG2	1:1874:A:GLN:HA	7	0.18
(1,474)	1:1877:A:GLN:HG2	1:1874:A:GLN:HA	9	0.18
(1,466)	1:1917:A:SER:H	1:1917:A:SER:HB2	19	0.18
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	9	0.18
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,406)	1:1956:A:ARG:H	1:1955:A:ASP:HB2	19	0.18
(1,406)	1:1956:A:ARG:H	1:1955:A:ASP:HB3	19	0.18
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	6	0.18
(1,361)	1:1817:A:ALA:HB1	1:1818:A:SER:HA	1	0.18
(1,361)	1:1817:A:ALA:HA	1:1818:A:SER:HA	9	0.18
(1,361)	1:1817:A:ALA:HA	1:1818:A:SER:HA	15	0.18
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG11	4	0.18
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG12	4	0.18
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG13	4	0.18
(1,239)	1:1896:A:ARG:H	1:1897:A:ILE:HB	16	0.18
(1,229)	1:1823:A:LYS:HA	1:1826:A:LYS:HE2	15	0.18
(1,229)	1:1823:A:LYS:HA	1:1826:A:LYS:HE3	15	0.18
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	4	0.18
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	5	0.18
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	7	0.18
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	12	0.18
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	13	0.18
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	16	0.18
(1,125)	1:1822:A:GLU:HG2	1:1823:A:LYS:H	12	0.18
(1,116)	1:1948:A:LEU:H	1:1949:A:ASP:H	3	0.18
(1,102)	1:1940:A:LYS:HA	1:1940:A:LYS:HD3	1	0.18
(1,102)	1:1940:A:LYS:HA	1:1940:A:LYS:HD3	2	0.18
(1,102)	1:1940:A:LYS:HA	1:1940:A:LYS:HD3	3	0.18
(1,102)	1:1940:A:LYS:HA	1:1940:A:LYS:HD3	10	0.18
(1,102)	1:1940:A:LYS:HA	1:1940:A:LYS:HD3	16	0.18
(1,102)	1:1940:A:LYS:HA	1:1940:A:LYS:HD3	19	0.18
(1,90)	1:1945:A:ARG:HA	1:1945:A:ARG:HB2	1	0.18
(1,90)	1:1945:A:ARG:HA	1:1945:A:ARG:HB2	3	0.18
(1,90)	1:1945:A:ARG:HA	1:1945:A:ARG:HB2	4	0.18
(1,90)	1:1945:A:ARG:HA	1:1945:A:ARG:HB2	5	0.18
(1,90)	1:1945:A:ARG:HA	1:1945:A:ARG:HB2	14	0.18
(1,74)	1:1954:A:ASP:H	1:1953:A:GLN:HG2	17	0.18
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	20	0.18
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	20	0.18
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	20	0.18
(3,56)	1:1945:A:ARG:N	1:1941:A:ILE:O	1	0.17
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	2	0.17
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	6	0.17
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	7	0.17
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	10	0.17
(1,3321)	1:1954:A:ASP:HA	1:1954:A:ASP:HB3	2	0.17
(1,3312)	1:1906:A:GLN:H	1:1906:A:GLN:HB3	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3303)	1:1898:A:SER:H	1:1897:A:ILE:HG13	15	0.17
(1,3258)	1:1862:A:ASP:HA	1:1865:A:ILE:HB	10	0.17
(1,3258)	1:1862:A:ASP:HA	1:1865:A:ILE:HB	16	0.17
(1,3258)	1:1862:A:ASP:HA	1:1865:A:ILE:HB	18	0.17
(1,3255)	1:1926:A:ASN:H	1:1925:A:THR:HA	3	0.17
(1,3255)	1:1926:A:ASN:H	1:1925:A:THR:HA	13	0.17
(1,3246)	1:1904:A:SER:H	1:1905:A:PRO:HD2	15	0.17
(1,3186)	1:1903:A:ILE:H	1:1902:A:GLY:H	9	0.17
(1,3172)	1:1902:A:GLY:H	1:1901:A:THR:HB	13	0.17
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	2	0.17
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	9	0.17
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG21	3	0.17
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG22	3	0.17
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG23	3	0.17
(1,3142)	1:1900:A:SER:H	1:1900:A:SER:HA	8	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	4	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	4	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	4	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	5	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	5	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	5	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	14	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	14	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	14	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	15	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	15	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	15	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	19	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	19	0.17
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	19	0.17
(1,3111)	1:1931:A:GLY:H	1:1930:A:VAL:HB	12	0.17
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	4	0.17
(1,3098)	1:1920:A:SER:H	1:1920:A:SER:HB3	13	0.17
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	6	0.17
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	6	0.17
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	5	0.17
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	5	0.17
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	14	0.17
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	14	0.17
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	1	0.17
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	15	0.17
(1,3075)	1:1942:A:LEU:HB3	1:1838:A:LYS:HG3	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3075)	1:1942:A:LEU:HB3	1:1838:A:LYS:HG3	11	0.17
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	4	0.17
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	17	0.17
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	18	0.17
(1,3020)	1:1948:A:LEU:HA	1:1949:A:ASP:H	10	0.17
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG21	16	0.17
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG22	16	0.17
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG23	16	0.17
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG21	16	0.17
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG22	16	0.17
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG23	16	0.17
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG21	16	0.17
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG22	16	0.17
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG23	16	0.17
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG21	18	0.17
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG22	18	0.17
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG23	18	0.17
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG21	18	0.17
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG22	18	0.17
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG23	18	0.17
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG21	18	0.17
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG22	18	0.17
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG23	18	0.17
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	5	0.17
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	9	0.17
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	10	0.17
(1,2960)	1:1858:A:LYS:HB2	1:1855:A:GLU:H	16	0.17
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	2	0.17
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	2	0.17
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	2	0.17
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	8	0.17
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	8	0.17
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	8	0.17
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	14	0.17
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	14	0.17
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	14	0.17
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	7	0.17
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	13	0.17
(1,2886)	1:1905:A:PRO:HD2	1:1905:A:PRO:HB2	14	0.17
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	10	0.17
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	10	0.17
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	10	0.17
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	10	0.17
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	10	0.17
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	10	0.17
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	10	0.17
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	10	0.17
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	20	0.17
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	20	0.17
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	20	0.17
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	20	0.17
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	20	0.17
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	20	0.17
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	20	0.17
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	20	0.17
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	20	0.17
(1,2807)	1:1889:A:MET:H	1:1888:A:GLU:HB2	18	0.17
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	3	0.17
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	5	0.17
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	6	0.17
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	12	0.17
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	13	0.17
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	5	0.17
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	5	0.17
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	5	0.17
(1,2682)	1:1826:A:LYS:HB2	1:1871:A:ASN:HD22	17	0.17
(1,2606)	1:1840:A:ILE:HD11	1:1850:A:LEU:HA	15	0.17
(1,2606)	1:1840:A:ILE:HD12	1:1850:A:LEU:HA	15	0.17
(1,2606)	1:1840:A:ILE:HD13	1:1850:A:LEU:HA	15	0.17
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	10	0.17
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	5	0.17
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	6	0.17
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	7	0.17
(1,2518)	1:1848:A:GLU:HB2	1:1839:A:LYS:HD2	20	0.17
(1,2515)	1:1898:A:SER:H	1:1897:A:ILE:HB	12	0.17
(1,2503)	1:1873:A:SER:HB2	1:1873:A:SER:H	5	0.17
(1,2489)	1:1893:A:GLY:H	1:1891:A:ARG:HB2	3	0.17
(1,2489)	1:1893:A:GLY:H	1:1891:A:ARG:HB2	7	0.17
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE1	20	0.17
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE2	20	0.17
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	10	0.17
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	12	0.17
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	14	0.17
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	15	0.17
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	19	0.17
(1,2378)	1:1923:A:GLY:H	1:1922:A:ILE:HG12	7	0.17
(1,2378)	1:1923:A:GLY:H	1:1922:A:ILE:HG12	9	0.17
(1,2378)	1:1923:A:GLY:H	1:1922:A:ILE:HG12	14	0.17
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	1	0.17
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	3	0.17
(1,2328)	1:1950:A:ASN:H	1:1951:A:THR:H	12	0.17
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	2	0.17
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	3	0.17
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	6	0.17
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	10	0.17
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	12	0.17
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	16	0.17
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	3	0.17
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	3	0.17
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	3	0.17
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	3	0.17
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	3	0.17
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	3	0.17
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	3	0.17
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	3	0.17
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	3	0.17
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	14	0.17
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	14	0.17
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	14	0.17
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	14	0.17
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	14	0.17
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	14	0.17
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	14	0.17
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	14	0.17
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	14	0.17
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	11	0.17
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	11	0.17
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	11	0.17
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	15	0.17
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	15	0.17
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	15	0.17
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG21	6	0.17
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG22	6	0.17
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG23	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG21	13	0.17
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG22	13	0.17
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG23	13	0.17
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG21	14	0.17
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG22	14	0.17
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG23	14	0.17
(1,2265)	1:1824:A:SER:H	1:1823:A:LYS:HB2	10	0.17
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD11	1	0.17
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD12	1	0.17
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD13	1	0.17
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD11	18	0.17
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD12	18	0.17
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD13	18	0.17
(1,2226)	1:1924:A:ASN:H	1:1925:A:THR:HG21	6	0.17
(1,2226)	1:1924:A:ASN:H	1:1925:A:THR:HG22	6	0.17
(1,2226)	1:1924:A:ASN:H	1:1925:A:THR:HG23	6	0.17
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG21	19	0.17
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG22	19	0.17
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG23	19	0.17
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG21	17	0.17
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG22	17	0.17
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG23	17	0.17
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG21	17	0.17
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG22	17	0.17
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG23	17	0.17
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG21	17	0.17
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG22	17	0.17
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG23	17	0.17
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG21	6	0.17
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG22	6	0.17
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG23	6	0.17
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG21	6	0.17
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG22	6	0.17
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG23	6	0.17
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG21	6	0.17
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG22	6	0.17
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG23	6	0.17
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	7	0.17
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	7	0.17
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	7	0.17
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	3	0.17
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	18	0.17
(1,2089)	1:1916:A:THR:H	1:1915:A:PRO:HB2	12	0.17
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	9	0.17
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	16	0.17
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	20	0.17
(1,2037)	1:1843:A:LYS:HE3	1:1844:A:GLU:HG3	9	0.17
(1,2037)	1:1843:A:LYS:HE3	1:1844:A:GLU:HG3	15	0.17
(1,2028)	1:1824:A:SER:H	1:1823:A:LYS:HG3	2	0.17
(1,2028)	1:1824:A:SER:H	1:1823:A:LYS:HG3	20	0.17
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	5	0.17
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	5	0.17
(1,1982)	1:1930:A:VAL:HB	1:1930:A:VAL:HA	1	0.17
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD11	1	0.17
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD12	1	0.17
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD13	1	0.17
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD11	12	0.17
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD12	12	0.17
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD13	12	0.17
(1,1963)	1:1942:A:LEU:H	1:1941:A:ILE:HG12	1	0.17
(1,1957)	1:1927:A:GLY:H	1:1926:A:ASN:HB2	11	0.17
(1,1952)	1:1840:A:ILE:HG21	1:1846:A:THR:HB	17	0.17
(1,1952)	1:1840:A:ILE:HG22	1:1846:A:THR:HB	17	0.17
(1,1952)	1:1840:A:ILE:HG23	1:1846:A:THR:HB	17	0.17
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG21	4	0.17
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG22	4	0.17
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG23	4	0.17
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG21	6	0.17
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG22	6	0.17
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG23	6	0.17
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	10	0.17
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	10	0.17
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	14	0.17
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	14	0.17
(1,1858)	1:1934:A:VAL:HA	1:1937:A:GLU:H	6	0.17
(1,1858)	1:1934:A:VAL:HA	1:1937:A:GLU:H	16	0.17
(1,1790)	1:1927:A:GLY:H	1:1925:A:THR:HB	8	0.17
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD21	18	0.17
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD22	18	0.17
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD23	18	0.17
(1,1770)	1:1914:A:THR:HB	1:1915:A:PRO:HD2	20	0.17
(1,1749)	1:1845:A:ASN:HB3	1:1842:A:SER:HB2	10	0.17
(1,1749)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1718)	1:1902:A:GLY:H	1:1901:A:THR:HA	2	0.17
(1,1718)	1:1902:A:GLY:H	1:1901:A:THR:HA	5	0.17
(1,1708)	1:1820:A:ILE:HG13	1:1821:A:ASP:H	16	0.17
(1,1679)	1:1929:A:GLU:H	1:1929:A:GLU:HB2	1	0.17
(1,1619)	1:1887:A:ILE:HG21	1:1890:A:GLU:HB2	19	0.17
(1,1619)	1:1887:A:ILE:HG22	1:1890:A:GLU:HB2	19	0.17
(1,1619)	1:1887:A:ILE:HG23	1:1890:A:GLU:HB2	19	0.17
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD11	7	0.17
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD12	7	0.17
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD13	7	0.17
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD11	7	0.17
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD12	7	0.17
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD13	7	0.17
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD11	7	0.17
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD12	7	0.17
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD13	7	0.17
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD11	17	0.17
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD12	17	0.17
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD13	17	0.17
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD11	17	0.17
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD12	17	0.17
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD13	17	0.17
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD11	17	0.17
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD12	17	0.17
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD13	17	0.17
(1,1598)	1:1955:A:ASP:H	1:1953:A:GLN:HG2	17	0.17
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE2	11	0.17
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE3	11	0.17
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE2	13	0.17
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE3	13	0.17
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE2	16	0.17
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE3	16	0.17
(1,1567)	1:1894:A:LYS:H	1:1894:A:LYS:HD2	9	0.17
(1,1567)	1:1894:A:LYS:H	1:1894:A:LYS:HD2	10	0.17
(1,1567)	1:1894:A:LYS:H	1:1894:A:LYS:HD2	13	0.17
(1,1567)	1:1894:A:LYS:H	1:1894:A:LYS:HD2	17	0.17
(1,1556)	1:1853:A:LEU:HD11	1:1857:A:LYS:HD2	7	0.17
(1,1556)	1:1853:A:LEU:HD12	1:1857:A:LYS:HD2	7	0.17
(1,1556)	1:1853:A:LEU:HD13	1:1857:A:LYS:HD2	7	0.17
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	3	0.17
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	5	0.17
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1439)	1:1928:A:GLU:HA	1:1928:A:GLU:HB3	18	0.17
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	13	0.17
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	13	0.17
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	20	0.17
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	20	0.17
(1,1410)	1:1951:A:THR:HG21	1:1951:A:THR:H	10	0.17
(1,1410)	1:1951:A:THR:HG22	1:1951:A:THR:H	10	0.17
(1,1410)	1:1951:A:THR:HG23	1:1951:A:THR:H	10	0.17
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	8	0.17
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	8	0.17
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	9	0.17
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	9	0.17
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	10	0.17
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	10	0.17
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	18	0.17
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	18	0.17
(1,1272)	1:1895:A:GLY:H	1:1893:A:GLY:H	8	0.17
(1,1261)	1:1927:A:GLY:H	1:1925:A:THR:HG21	9	0.17
(1,1261)	1:1927:A:GLY:H	1:1925:A:THR:HG22	9	0.17
(1,1261)	1:1927:A:GLY:H	1:1925:A:THR:HG23	9	0.17
(1,1255)	1:1865:A:ILE:HD11	1:1857:A:LYS:HE2	16	0.17
(1,1255)	1:1865:A:ILE:HD12	1:1857:A:LYS:HE2	16	0.17
(1,1255)	1:1865:A:ILE:HD13	1:1857:A:LYS:HE2	16	0.17
(1,1244)	1:1926:A:ASN:H	1:1926:A:ASN:HB2	20	0.17
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	5	0.17
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	8	0.17
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	9	0.17
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	11	0.17
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	19	0.17
(1,1239)	1:1890:A:GLU:HA	1:1896:A:ARG:HG3	1	0.17
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	1	0.17
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	1	0.17
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	16	0.17
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	16	0.17
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	17	0.17
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	17	0.17
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	18	0.17
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	18	0.17
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE2	2	0.17
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE3	2	0.17
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	2	0.17
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE2	3	0.17
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE3	3	0.17
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	3	0.17
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	3	0.17
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE2	5	0.17
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE3	5	0.17
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	5	0.17
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	5	0.17
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE2	12	0.17
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE3	12	0.17
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	12	0.17
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	12	0.17
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE2	15	0.17
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE3	15	0.17
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	15	0.17
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	15	0.17
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE2	16	0.17
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE3	16	0.17
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	16	0.17
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	16	0.17
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE2	20	0.17
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE3	20	0.17
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	20	0.17
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	20	0.17
(1,1195)	1:1829:A:VAL:HG21	1:1833:A:LEU:HD11	5	0.17
(1,1195)	1:1829:A:VAL:HG21	1:1833:A:LEU:HD12	5	0.17
(1,1195)	1:1829:A:VAL:HG21	1:1833:A:LEU:HD13	5	0.17
(1,1195)	1:1829:A:VAL:HG22	1:1833:A:LEU:HD11	5	0.17
(1,1195)	1:1829:A:VAL:HG22	1:1833:A:LEU:HD12	5	0.17
(1,1195)	1:1829:A:VAL:HG22	1:1833:A:LEU:HD13	5	0.17
(1,1195)	1:1829:A:VAL:HG23	1:1833:A:LEU:HD11	5	0.17
(1,1195)	1:1829:A:VAL:HG23	1:1833:A:LEU:HD12	5	0.17
(1,1195)	1:1829:A:VAL:HG23	1:1833:A:LEU:HD13	5	0.17
(1,1131)	1:1824:A:SER:H	1:1827:A:ALA:HB1	9	0.17
(1,1131)	1:1824:A:SER:H	1:1827:A:ALA:HB2	9	0.17
(1,1131)	1:1824:A:SER:H	1:1827:A:ALA:HB3	9	0.17
(1,1018)	1:1861:A:SER:HA	1:1862:A:ASP:H	2	0.17
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	6	0.17
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	14	0.17
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	17	0.17
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	20	0.17
(1,994)	1:1889:A:MET:HE1	1:1885:A:ARG:HG2	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:1889:A:MET:HE2	1:1885:A:ARG:HG2	3	0.17
(1,994)	1:1889:A:MET:HE3	1:1885:A:ARG:HG2	3	0.17
(1,994)	1:1889:A:MET:HE1	1:1885:A:ARG:HG2	4	0.17
(1,994)	1:1889:A:MET:HE2	1:1885:A:ARG:HG2	4	0.17
(1,994)	1:1889:A:MET:HE3	1:1885:A:ARG:HG2	4	0.17
(1,994)	1:1889:A:MET:HE1	1:1885:A:ARG:HG2	13	0.17
(1,994)	1:1889:A:MET:HE2	1:1885:A:ARG:HG2	13	0.17
(1,994)	1:1889:A:MET:HE3	1:1885:A:ARG:HG2	13	0.17
(1,994)	1:1889:A:MET:HE1	1:1885:A:ARG:HG2	18	0.17
(1,994)	1:1889:A:MET:HE2	1:1885:A:ARG:HG2	18	0.17
(1,994)	1:1889:A:MET:HE3	1:1885:A:ARG:HG2	18	0.17
(1,981)	1:1818:A:SER:HB2	1:1820:A:ILE:H	20	0.17
(1,981)	1:1818:A:SER:HB3	1:1820:A:ILE:H	20	0.17
(1,952)	1:1949:A:ASP:HA	1:1949:A:ASP:HB3	6	0.17
(1,952)	1:1949:A:ASP:HA	1:1949:A:ASP:HB3	15	0.17
(1,897)	1:1946:A:CYS:H	1:1945:A:ARG:HB2	10	0.17
(1,897)	1:1946:A:CYS:H	1:1945:A:ARG:HB2	12	0.17
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	3	0.17
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	3	0.17
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	3	0.17
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	3	0.17
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	3	0.17
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	3	0.17
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	3	0.17
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	3	0.17
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	3	0.17
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	5	0.17
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	5	0.17
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	5	0.17
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	5	0.17
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	5	0.17
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	5	0.17
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	5	0.17
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	5	0.17
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	5	0.17
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	12	0.17
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	12	0.17
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	12	0.17
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	12	0.17
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	12	0.17
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	12	0.17
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	12	0.17
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	12	0.17
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	13	0.17
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	13	0.17
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	13	0.17
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	13	0.17
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	13	0.17
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	13	0.17
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	13	0.17
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	13	0.17
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	13	0.17
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	18	0.17
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	18	0.17
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	18	0.17
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	18	0.17
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	18	0.17
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	18	0.17
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	18	0.17
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	18	0.17
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	18	0.17
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	3	0.17
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	3	0.17
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	8	0.17
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	8	0.17
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	15	0.17
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	15	0.17
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	17	0.17
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	17	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	1	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	2	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	3	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	4	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	5	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	6	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	8	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	10	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	11	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	12	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	13	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	14	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	15	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	17	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	18	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	19	0.17
(1,778)	1:1830:A:ASN:HA	1:1831:A:ASP:H	20	0.17
(1,758)	1:1823:A:LYS:H	1:1823:A:LYS:HG3	17	0.17
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	10	0.17
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	10	0.17
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	10	0.17
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	10	0.17
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	10	0.17
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	10	0.17
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	19	0.17
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	19	0.17
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	19	0.17
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	19	0.17
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	19	0.17
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	19	0.17
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG21	12	0.17
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG22	12	0.17
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG23	12	0.17
(1,697)	1:1956:A:ARG:H	1:1956:A:ARG:HB3	11	0.17
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	4	0.17
(1,676)	1:1899:A:THR:H	1:1897:A:ILE:HG21	6	0.17
(1,676)	1:1899:A:THR:H	1:1897:A:ILE:HG22	6	0.17
(1,676)	1:1899:A:THR:H	1:1897:A:ILE:HG23	6	0.17
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	1	0.17
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	1	0.17
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	1	0.17
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	17	0.17
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	17	0.17
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	17	0.17
(1,630)	1:1926:A:ASN:HA	1:1926:A:ASN:HB2	13	0.17
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	5	0.17
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	15	0.17
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	17	0.17
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	19	0.17
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	8	0.17
(1,612)	1:1900:A:SER:HB3	1:1901:A:THR:H	12	0.17
(1,593)	1:1920:A:SER:HA	1:1915:A:PRO:HB3	13	0.17
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	2	0.17
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	19	0.17
(1,573)	1:1817:A:ALA:HB1	1:1819:A:ARG:H	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:1817:A:ALA:HB2	1:1819:A:ARG:H	5	0.17
(1,573)	1:1817:A:ALA:HB3	1:1819:A:ARG:H	5	0.17
(1,573)	1:1817:A:ALA:HB1	1:1819:A:ARG:H	7	0.17
(1,573)	1:1817:A:ALA:HB2	1:1819:A:ARG:H	7	0.17
(1,573)	1:1817:A:ALA:HB3	1:1819:A:ARG:H	7	0.17
(1,573)	1:1817:A:ALA:HB1	1:1819:A:ARG:H	18	0.17
(1,573)	1:1817:A:ALA:HB2	1:1819:A:ARG:H	18	0.17
(1,573)	1:1817:A:ALA:HB3	1:1819:A:ARG:H	18	0.17
(1,573)	1:1817:A:ALA:HB1	1:1819:A:ARG:H	20	0.17
(1,573)	1:1817:A:ALA:HB2	1:1819:A:ARG:H	20	0.17
(1,573)	1:1817:A:ALA:HB3	1:1819:A:ARG:H	20	0.17
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	5	0.17
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	5	0.17
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	5	0.17
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	12	0.17
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	12	0.17
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	12	0.17
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	13	0.17
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	13	0.17
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	13	0.17
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	15	0.17
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	15	0.17
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	15	0.17
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE2	9	0.17
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE3	9	0.17
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE2	9	0.17
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE3	9	0.17
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE2	9	0.17
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE3	9	0.17
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE2	10	0.17
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE3	10	0.17
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE2	10	0.17
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE3	10	0.17
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE2	10	0.17
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE3	10	0.17
(1,525)	1:1924:A:ASN:H	1:1923:A:GLY:H	14	0.17
(1,525)	1:1924:A:ASN:H	1:1923:A:GLY:H	20	0.17
(1,474)	1:1877:A:GLN:HG2	1:1874:A:GLN:HA	12	0.17
(1,474)	1:1877:A:GLN:HG2	1:1874:A:GLN:HA	18	0.17
(1,461)	1:1845:A:ASN:HD21	1:1839:A:LYS:HG3	12	0.17
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	3	0.17
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	13	0.17
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	17	0.17
(1,447)	1:1928:A:GLU:H	1:1927:A:GLY:HA3	7	0.17
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	7	0.17
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	7	0.17
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	13	0.17
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	13	0.17
(1,385)	1:1952:A:LYS:H	1:1951:A:THR:HA	14	0.17
(1,361)	1:1817:A:ALA:HA	1:1818:A:SER:HA	3	0.17
(1,361)	1:1817:A:ALA:HA	1:1818:A:SER:HA	5	0.17
(1,361)	1:1817:A:ALA:HA	1:1818:A:SER:HA	7	0.17
(1,361)	1:1817:A:ALA:HA	1:1818:A:SER:HA	11	0.17
(1,361)	1:1817:A:ALA:HA	1:1818:A:SER:HA	17	0.17
(1,361)	1:1817:A:ALA:HA	1:1818:A:SER:HA	18	0.17
(1,330)	1:1827:A:ALA:H	1:1826:A:LYS:HB3	2	0.17
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG11	16	0.17
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG12	16	0.17
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG13	16	0.17
(1,293)	1:1897:A:ILE:HD11	1:1890:A:GLU:HG3	20	0.17
(1,293)	1:1897:A:ILE:HD12	1:1890:A:GLU:HG3	20	0.17
(1,293)	1:1897:A:ILE:HD13	1:1890:A:GLU:HG3	20	0.17
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	8	0.17
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	8	0.17
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	9	0.17
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	9	0.17
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	1	0.17
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	11	0.17
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	15	0.17
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	17	0.17
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	18	0.17
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	20	0.17
(1,169)	1:1821:A:ASP:HB2	1:1822:A:GLU:H	20	0.17
(1,102)	1:1940:A:LYS:HA	1:1940:A:LYS:HD3	18	0.17
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD2	6	0.17
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD3	6	0.17
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD2	6	0.17
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD3	6	0.17
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD2	6	0.17
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD3	6	0.17
(1,61)	1:1948:A:LEU:HD11	1:1949:A:ASP:H	1	0.17
(1,61)	1:1948:A:LEU:HD12	1:1949:A:ASP:H	1	0.17
(1,61)	1:1948:A:LEU:HD13	1:1949:A:ASP:H	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,61)	1:1948:A:LEU:HD11	1:1949:A:ASP:H	5	0.17
(1,61)	1:1948:A:LEU:HD12	1:1949:A:ASP:H	5	0.17
(1,61)	1:1948:A:LEU:HD13	1:1949:A:ASP:H	5	0.17
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	14	0.17
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	14	0.17
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	2	0.17
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	2	0.17
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	2	0.17
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	13	0.17
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	13	0.17
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	13	0.17
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	17	0.17
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	17	0.17
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	17	0.17
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	3	0.16
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	11	0.16
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	14	0.16
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	15	0.16
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	19	0.16
(1,3321)	1:1954:A:ASP:HA	1:1954:A:ASP:HB3	11	0.16
(1,3312)	1:1906:A:GLN:H	1:1906:A:GLN:HB3	4	0.16
(1,3303)	1:1898:A:SER:H	1:1897:A:ILE:HG13	7	0.16
(1,3258)	1:1862:A:ASP:HA	1:1865:A:ILE:HB	4	0.16
(1,3258)	1:1862:A:ASP:HA	1:1865:A:ILE:HB	6	0.16
(1,3258)	1:1862:A:ASP:HA	1:1865:A:ILE:HB	8	0.16
(1,3246)	1:1904:A:SER:H	1:1905:A:PRO:HD2	16	0.16
(1,3245)	1:1891:A:ARG:HG3	1:1891:A:ARG:HE	18	0.16
(1,3168)	1:1874:A:GLN:HB2	1:1874:A:GLN:HG2	13	0.16
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	6	0.16
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	16	0.16
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG21	15	0.16
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG22	15	0.16
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG23	15	0.16
(1,3142)	1:1900:A:SER:H	1:1900:A:SER:HA	19	0.16
(1,3138)	1:1926:A:ASN:H	1:1926:A:ASN:HD22	7	0.16
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	6	0.16
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	6	0.16
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	6	0.16
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	1	0.16
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	3	0.16
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	4	0.16
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3111)	1:1931:A:GLY:H	1:1930:A:VAL:HB	18	0.16
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	2	0.16
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	19	0.16
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	2	0.16
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	2	0.16
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	8	0.16
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	8	0.16
(1,3086)	1:1903:A:ILE:H	1:1900:A:SER:HB3	17	0.16
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	1	0.16
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	1	0.16
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	2	0.16
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	2	0.16
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	15	0.16
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	15	0.16
(1,3075)	1:1942:A:LEU:HB3	1:1838:A:LYS:HG3	10	0.16
(1,3051)	1:1918:A:THR:H	1:1917:A:SER:HB2	12	0.16
(1,3051)	1:1918:A:THR:H	1:1917:A:SER:HB2	18	0.16
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	2	0.16
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	5	0.16
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	10	0.16
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	15	0.16
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	16	0.16
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	20	0.16
(1,3015)	1:1938:A:ARG:HB2	1:1845:A:ASN:HD21	2	0.16
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	14	0.16
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	17	0.16
(1,2960)	1:1858:A:LYS:HB2	1:1855:A:GLU:H	8	0.16
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	6	0.16
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	6	0.16
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	6	0.16
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	3	0.16
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	5	0.16
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	10	0.16
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	12	0.16
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	3	0.16
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	3	0.16
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	3	0.16
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	3	0.16
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	3	0.16
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	3	0.16
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	3	0.16
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	3	0.16
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	6	0.16
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	6	0.16
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	6	0.16
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	6	0.16
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	6	0.16
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	6	0.16
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	6	0.16
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	6	0.16
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	6	0.16
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	9	0.16
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	9	0.16
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	9	0.16
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	9	0.16
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	9	0.16
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	9	0.16
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	9	0.16
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	9	0.16
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	9	0.16
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	11	0.16
(1,2859)	1:1943:A:ARG:HA	1:1838:A:LYS:HE2	1	0.16
(1,2854)	1:1924:A:ASN:H	1:1924:A:ASN:HA	4	0.16
(1,2854)	1:1924:A:ASN:H	1:1924:A:ASN:HA	13	0.16
(1,2847)	1:1921:A:SER:HA	1:1922:A:ILE:H	13	0.16
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	2	0.16
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	8	0.16
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	17	0.16
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	1	0.16
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	8	0.16
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	12	0.16
(1,2747)	1:1900:A:SER:H	1:1899:A:THR:H	8	0.16
(1,2747)	1:1900:A:SER:H	1:1899:A:THR:H	10	0.16
(1,2737)	1:1823:A:LYS:HA	1:1824:A:SER:H	16	0.16
(1,2731)	1:1916:A:THR:HG21	1:1914:A:THR:HB	1	0.16
(1,2731)	1:1916:A:THR:HG22	1:1914:A:THR:HB	1	0.16
(1,2731)	1:1916:A:THR:HG23	1:1914:A:THR:HB	1	0.16
(1,2668)	1:1925:A:THR:H	1:1924:A:ASN:HB2	3	0.16
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	5	0.16
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	11	0.16
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	17	0.16
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	18	0.16
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	2	0.16
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	11	0.16
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	14	0.16
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	16	0.16
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	18	0.16
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	4	0.16
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	14	0.16
(1,2518)	1:1848:A:GLU:HB2	1:1839:A:LYS:HD2	9	0.16
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	12	0.16
(1,2504)	1:1867:A:PRO:HA	1:1871:A:ASN:HD21	8	0.16
(1,2489)	1:1893:A:GLY:H	1:1891:A:ARG:HB2	14	0.16
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	3	0.16
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	7	0.16
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	11	0.16
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	17	0.16
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	2	0.16
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	3	0.16
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	14	0.16
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	15	0.16
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	5	0.16
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	16	0.16
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	18	0.16
(1,2378)	1:1923:A:GLY:H	1:1922:A:ILE:HG12	8	0.16
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	4	0.16
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	15	0.16
(1,2347)	1:1820:A:ILE:HB	1:1821:A:ASP:H	16	0.16
(1,2321)	1:1903:A:ILE:H	1:1902:A:GLY:HA2	6	0.16
(1,2321)	1:1903:A:ILE:H	1:1902:A:GLY:HA3	6	0.16
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	5	0.16
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	7	0.16
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	8	0.16
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	17	0.16
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	18	0.16
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	20	0.16
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	10	0.16
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	10	0.16
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	10	0.16
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	10	0.16
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	10	0.16
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	10	0.16
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	10	0.16
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	10	0.16
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	19	0.16
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	19	0.16
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	19	0.16
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	19	0.16
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	19	0.16
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	19	0.16
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	19	0.16
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	19	0.16
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	19	0.16
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	10	0.16
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	10	0.16
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	10	0.16
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	12	0.16
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	12	0.16
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	12	0.16
(1,2261)	1:1906:A:GLN:H	1:1906:A:GLN:HB2	15	0.16
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	20	0.16
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD11	10	0.16
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD12	10	0.16
(1,2227)	1:1923:A:GLY:H	1:1922:A:ILE:HD13	10	0.16
(1,2165)	1:1841:A:GLY:H	1:1876:A:PHE:HE1	20	0.16
(1,2165)	1:1841:A:GLY:H	1:1876:A:PHE:HE2	20	0.16
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	16	0.16
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	16	0.16
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	16	0.16
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	1	0.16
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	12	0.16
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	15	0.16
(1,2037)	1:1843:A:LYS:HE3	1:1844:A:GLU:HG3	2	0.16
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	1	0.16
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	1	0.16
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	4	0.16
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	4	0.16
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	6	0.16
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	6	0.16
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	8	0.16
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	8	0.16
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	10	0.16
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	10	0.16
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	12	0.16
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	14	0.16
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	14	0.16
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	15	0.16
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	15	0.16
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD11	20	0.16
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD12	20	0.16
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD13	20	0.16
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG21	19	0.16
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG22	19	0.16
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG23	19	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	1	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	1	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	2	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	2	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	3	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	3	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	4	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	4	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	5	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	5	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	7	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	7	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	9	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	9	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	11	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	11	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	12	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	12	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	13	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	13	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	15	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	15	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	16	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	16	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	18	0.16
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	18	0.16
(1,1858)	1:1934:A:VAL:HA	1:1937:A:GLU:H	17	0.16
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD21	4	0.16
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD22	4	0.16
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD23	4	0.16
(1,1770)	1:1914:A:THR:HB	1:1915:A:PRO:HD2	11	0.16
(1,1755)	1:1907:A:MET:H	1:1906:A:GLN:HB2	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1689)	1:1928:A:GLU:H	1:1927:A:GLY:HA2	17	0.16
(1,1664)	1:1847:A:LYS:HD2	1:1847:A:LYS:HE2	1	0.16
(1,1664)	1:1847:A:LYS:HD2	1:1847:A:LYS:HE3	1	0.16
(1,1664)	1:1847:A:LYS:HD3	1:1847:A:LYS:HE2	1	0.16
(1,1664)	1:1847:A:LYS:HD3	1:1847:A:LYS:HE3	1	0.16
(1,1664)	1:1847:A:LYS:HD2	1:1847:A:LYS:HE2	2	0.16
(1,1664)	1:1847:A:LYS:HD2	1:1847:A:LYS:HE3	2	0.16
(1,1664)	1:1847:A:LYS:HD3	1:1847:A:LYS:HE2	2	0.16
(1,1664)	1:1847:A:LYS:HD3	1:1847:A:LYS:HE3	2	0.16
(1,1664)	1:1847:A:LYS:HD2	1:1847:A:LYS:HE2	14	0.16
(1,1664)	1:1847:A:LYS:HD2	1:1847:A:LYS:HE3	14	0.16
(1,1664)	1:1847:A:LYS:HD3	1:1847:A:LYS:HE2	14	0.16
(1,1664)	1:1847:A:LYS:HD3	1:1847:A:LYS:HE3	14	0.16
(1,1664)	1:1847:A:LYS:HD2	1:1847:A:LYS:HE2	16	0.16
(1,1664)	1:1847:A:LYS:HD2	1:1847:A:LYS:HE3	16	0.16
(1,1664)	1:1847:A:LYS:HD3	1:1847:A:LYS:HE2	16	0.16
(1,1664)	1:1847:A:LYS:HD3	1:1847:A:LYS:HE3	16	0.16
(1,1664)	1:1847:A:LYS:HD2	1:1847:A:LYS:HE2	17	0.16
(1,1664)	1:1847:A:LYS:HD2	1:1847:A:LYS:HE3	17	0.16
(1,1664)	1:1847:A:LYS:HD3	1:1847:A:LYS:HE2	17	0.16
(1,1664)	1:1847:A:LYS:HD3	1:1847:A:LYS:HE3	17	0.16
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD11	20	0.16
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD12	20	0.16
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD13	20	0.16
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD11	20	0.16
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD12	20	0.16
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD13	20	0.16
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD11	20	0.16
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD12	20	0.16
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD13	20	0.16
(1,1604)	1:1930:A:VAL:H	1:1931:A:GLY:H	9	0.16
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE2	1	0.16
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE3	1	0.16
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE2	14	0.16
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE3	14	0.16
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE2	15	0.16
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE3	15	0.16
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE2	17	0.16
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE3	17	0.16
(1,1470)	1:1824:A:SER:H	1:1827:A:ALA:H	14	0.16
(1,1458)	1:1955:A:ASP:H	1:1954:A:ASP:HA	1	0.16
(1,1458)	1:1955:A:ASP:H	1:1954:A:ASP:HA	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1458)	1:1955:A:ASP:H	1:1954:A:ASP:HA	15	0.16
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	8	0.16
(1,1439)	1:1928:A:GLU:HA	1:1928:A:GLU:HB3	12	0.16
(1,1439)	1:1928:A:GLU:HA	1:1928:A:GLU:HB3	16	0.16
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	3	0.16
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	3	0.16
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	4	0.16
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	4	0.16
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	13	0.16
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	13	0.16
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	15	0.16
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	15	0.16
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	17	0.16
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	17	0.16
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	19	0.16
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	19	0.16
(1,1345)	1:1821:A:ASP:H	1:1821:A:ASP:HB3	10	0.16
(1,1307)	1:1821:A:ASP:HA	1:1823:A:LYS:H	8	0.16
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG21	15	0.16
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG22	15	0.16
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG23	15	0.16
(1,1244)	1:1926:A:ASN:H	1:1926:A:ASN:HB2	14	0.16
(1,1244)	1:1926:A:ASN:H	1:1926:A:ASN:HB2	19	0.16
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	1	0.16
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	6	0.16
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	7	0.16
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	10	0.16
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	13	0.16
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	4	0.16
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	4	0.16
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	8	0.16
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	8	0.16
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	20	0.16
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	20	0.16
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE2	1	0.16
(1,1201)	1:1952:A:LYS:HG2	1:1952:A:LYS:HE3	1	0.16
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	1	0.16
(1,1201)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	1	0.16
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG11	16	0.16
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG12	16	0.16
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG13	16	0.16
(1,1121)	1:1820:A:ILE:H	1:1820:A:ILE:HG12	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1121)	1:1820:A:ILE:H	1:1820:A:ILE:HG12	13	0.16
(1,1120)	1:1941:A:ILE:HD11	1:1944:A:GLN:HE22	12	0.16
(1,1120)	1:1941:A:ILE:HD12	1:1944:A:GLN:HE22	12	0.16
(1,1120)	1:1941:A:ILE:HD13	1:1944:A:GLN:HE22	12	0.16
(1,1105)	1:1838:A:LYS:HD2	1:1943:A:ARG:HA	9	0.16
(1,1105)	1:1838:A:LYS:HD3	1:1943:A:ARG:HA	9	0.16
(1,1089)	1:1948:A:LEU:H	1:1948:A:LEU:HD11	13	0.16
(1,1089)	1:1948:A:LEU:H	1:1948:A:LEU:HD12	13	0.16
(1,1089)	1:1948:A:LEU:H	1:1948:A:LEU:HD13	13	0.16
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	1	0.16
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	1	0.16
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	2	0.16
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	2	0.16
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	3	0.16
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	3	0.16
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	7	0.16
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	7	0.16
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	10	0.16
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	10	0.16
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	13	0.16
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	13	0.16
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	14	0.16
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	14	0.16
(1,1032)	1:1829:A:VAL:H	1:1829:A:VAL:HG21	9	0.16
(1,1032)	1:1829:A:VAL:H	1:1829:A:VAL:HG22	9	0.16
(1,1032)	1:1829:A:VAL:H	1:1829:A:VAL:HG23	9	0.16
(1,1018)	1:1861:A:SER:HA	1:1862:A:ASP:H	11	0.16
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	7	0.16
(1,1000)	1:1917:A:SER:HA	1:1918:A:THR:H	1	0.16
(1,995)	1:1953:A:GLN:H	1:1953:A:GLN:HB3	9	0.16
(1,994)	1:1889:A:MET:HE1	1:1885:A:ARG:HG2	1	0.16
(1,994)	1:1889:A:MET:HE2	1:1885:A:ARG:HG2	1	0.16
(1,994)	1:1889:A:MET:HE3	1:1885:A:ARG:HG2	1	0.16
(1,982)	1:1858:A:LYS:H	1:1858:A:LYS:HG3	16	0.16
(1,981)	1:1818:A:SER:HB2	1:1820:A:ILE:H	12	0.16
(1,981)	1:1818:A:SER:HB3	1:1820:A:ILE:H	12	0.16
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	7	0.16
(1,957)	1:1936:A:LEU:H	1:1935:A:TYR:HB2	9	0.16
(1,957)	1:1936:A:LEU:H	1:1935:A:TYR:HB3	9	0.16
(1,954)	1:1863:A:ALA:H	1:1863:A:ALA:HA	17	0.16
(1,897)	1:1946:A:CYS:H	1:1945:A:ARG:HB2	2	0.16
(1,889)	1:1889:A:MET:H	1:1892:A:GLU:HG3	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	6	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	6	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	6	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	6	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	6	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	6	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	6	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	6	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	6	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	7	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	7	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	7	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	7	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	7	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	7	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	7	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	7	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	7	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	8	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	8	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	8	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	8	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	8	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	8	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	8	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	8	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	8	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	9	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	9	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	9	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	9	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	9	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	9	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	9	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	9	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	9	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	11	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	11	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	11	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	11	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	11	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	11	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	11	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	11	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	20	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	20	0.16
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	20	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	20	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	20	0.16
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	20	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	20	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	20	0.16
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	20	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	1	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	1	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	2	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	2	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	5	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	5	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	7	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	7	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	9	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	9	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	13	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	13	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	14	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	14	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	16	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	16	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	18	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	18	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	19	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	19	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	20	0.16
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	20	0.16
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	16	0.16
(1,828)	1:1851:A:ALA:HB1	1:1852:A:GLU:HG2	12	0.16
(1,828)	1:1851:A:ALA:HB2	1:1852:A:GLU:HG2	12	0.16
(1,828)	1:1851:A:ALA:HB3	1:1852:A:GLU:HG2	12	0.16
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	14	0.16
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	14	0.16
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	14	0.16
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	4	0.16
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	7	0.16
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	12	0.16
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	17	0.16
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG21	5	0.16
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG22	5	0.16
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG23	5	0.16
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG21	5	0.16
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG22	5	0.16
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG23	5	0.16
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG21	5	0.16
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG22	5	0.16
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG23	5	0.16
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	1	0.16
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	1	0.16
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	1	0.16
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	1	0.16
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	1	0.16
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	1	0.16
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	2	0.16
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	2	0.16
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	2	0.16
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	2	0.16
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	2	0.16
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	2	0.16
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	4	0.16
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	4	0.16
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	4	0.16
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	4	0.16
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	4	0.16
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	4	0.16
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	12	0.16
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	12	0.16
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	12	0.16
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	12	0.16
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	12	0.16
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	12	0.16
(1,736)	1:1898:A:SER:H	1:1897:A:ILE:H	12	0.16
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG21	11	0.16
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG22	11	0.16
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG23	11	0.16
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	7	0.16
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	7	0.16
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	7	0.16
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	16	0.16
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	16	0.16
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	16	0.16
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	4	0.16
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	6	0.16
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	13	0.16
(1,612)	1:1900:A:SER:HB3	1:1901:A:THR:H	7	0.16
(1,601)	1:1923:A:GLY:H	1:1922:A:ILE:HG13	1	0.16
(1,601)	1:1923:A:GLY:H	1:1922:A:ILE:HG13	13	0.16
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	13	0.16
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	9	0.16
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	3	0.16
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	4	0.16
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	9	0.16
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	10	0.16
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	15	0.16
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	17	0.16
(1,573)	1:1817:A:ALA:HB1	1:1819:A:ARG:H	2	0.16
(1,573)	1:1817:A:ALA:HB2	1:1819:A:ARG:H	2	0.16
(1,573)	1:1817:A:ALA:HB3	1:1819:A:ARG:H	2	0.16
(1,573)	1:1817:A:ALA:HB1	1:1819:A:ARG:H	12	0.16
(1,573)	1:1817:A:ALA:HB2	1:1819:A:ARG:H	12	0.16
(1,573)	1:1817:A:ALA:HB3	1:1819:A:ARG:H	12	0.16
(1,558)	1:1929:A:GLU:H	1:1928:A:GLU:HA	16	0.16
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	3	0.16
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	3	0.16
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	3	0.16
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	8	0.16
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	8	0.16
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	8	0.16
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	9	0.16
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	9	0.16
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	9	0.16
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	10	0.16
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	10	0.16
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	10	0.16
(1,525)	1:1924:A:ASN:H	1:1923:A:GLY:H	19	0.16
(1,509)	1:1865:A:ILE:HG21	1:1866:A:GLU:H	16	0.16
(1,509)	1:1865:A:ILE:HG22	1:1866:A:GLU:H	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,509)	1:1865:A:ILE:HG23	1:1866:A:GLU:H	16	0.16
(1,481)	1:1819:A:ARG:HB2	1:1820:A:ILE:H	11	0.16
(1,474)	1:1877:A:GLN:HG2	1:1874:A:GLN:HA	4	0.16
(1,474)	1:1877:A:GLN:HG2	1:1874:A:GLN:HA	8	0.16
(1,474)	1:1877:A:GLN:HG2	1:1874:A:GLN:HA	16	0.16
(1,466)	1:1917:A:SER:H	1:1917:A:SER:HB2	17	0.16
(1,450)	1:1896:A:ARG:HB2	1:1890:A:GLU:HG2	17	0.16
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	2	0.16
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	8	0.16
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	15	0.16
(1,416)	1:1955:A:ASP:H	1:1954:A:ASP:H	8	0.16
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	15	0.16
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	15	0.16
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	14	0.16
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	19	0.16
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	20	0.16
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	1	0.16
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	2	0.16
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	6	0.16
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	12	0.16
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	16	0.16
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	19	0.16
(1,330)	1:1827:A:ALA:H	1:1826:A:LYS:HB3	7	0.16
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	8	0.16
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	16	0.16
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD11	4	0.16
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD12	4	0.16
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD13	4	0.16
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD11	17	0.16
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD12	17	0.16
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD13	17	0.16
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD11	11	0.16
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD12	11	0.16
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD13	11	0.16
(1,229)	1:1823:A:LYS:HA	1:1826:A:LYS:HE2	3	0.16
(1,229)	1:1823:A:LYS:HA	1:1826:A:LYS:HE3	3	0.16
(1,186)	1:1884:A:LEU:HD11	1:1857:A:LYS:HD3	16	0.16
(1,186)	1:1884:A:LEU:HD12	1:1857:A:LYS:HD3	16	0.16
(1,186)	1:1884:A:LEU:HD13	1:1857:A:LYS:HD3	16	0.16
(1,104)	1:1951:A:THR:H	1:1951:A:THR:HB	19	0.16
(1,102)	1:1940:A:LYS:HA	1:1940:A:LYS:HD3	8	0.16
(1,102)	1:1940:A:LYS:HA	1:1940:A:LYS:HD3	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:1927:A:GLY:H	1:1929:A:GLU:H	3	0.16
(1,96)	1:1828:A:LYS:HA	1:1831:A:ASP:HB3	2	0.16
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD2	12	0.16
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD3	12	0.16
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD2	12	0.16
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD3	12	0.16
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD2	12	0.16
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD3	12	0.16
(1,61)	1:1948:A:LEU:HD11	1:1949:A:ASP:H	16	0.16
(1,61)	1:1948:A:LEU:HD12	1:1949:A:ASP:H	16	0.16
(1,61)	1:1948:A:LEU:HD13	1:1949:A:ASP:H	16	0.16
(1,61)	1:1948:A:LEU:HD11	1:1949:A:ASP:H	18	0.16
(1,61)	1:1948:A:LEU:HD12	1:1949:A:ASP:H	18	0.16
(1,61)	1:1948:A:LEU:HD13	1:1949:A:ASP:H	18	0.16
(1,28)	1:1909:A:VAL:HG11	1:1910:A:THR:H	7	0.16
(1,28)	1:1909:A:VAL:HG12	1:1910:A:THR:H	7	0.16
(1,28)	1:1909:A:VAL:HG13	1:1910:A:THR:H	7	0.16
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	7	0.16
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	7	0.16
(3,56)	1:1945:A:ARG:N	1:1941:A:ILE:O	2	0.15
(3,45)	1:1934:A:VAL:N	1:1930:A:VAL:O	5	0.15
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	4	0.15
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	5	0.15
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	9	0.15
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	18	0.15
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	20	0.15
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG21	9	0.15
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG22	9	0.15
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG23	9	0.15
(1,3278)	1:1942:A:LEU:HD11	1:1838:A:LYS:HG3	7	0.15
(1,3278)	1:1942:A:LEU:HD12	1:1838:A:LYS:HG3	7	0.15
(1,3278)	1:1942:A:LEU:HD13	1:1838:A:LYS:HG3	7	0.15
(1,3258)	1:1862:A:ASP:HA	1:1865:A:ILE:HB	7	0.15
(1,3246)	1:1904:A:SER:H	1:1905:A:PRO:HD2	19	0.15
(1,3245)	1:1891:A:ARG:HG3	1:1891:A:ARG:HE	16	0.15
(1,3168)	1:1874:A:GLN:HB2	1:1874:A:GLN:HG2	1	0.15
(1,3168)	1:1874:A:GLN:HB2	1:1874:A:GLN:HG2	2	0.15
(1,3168)	1:1874:A:GLN:HB2	1:1874:A:GLN:HG2	3	0.15
(1,3168)	1:1874:A:GLN:HB2	1:1874:A:GLN:HG2	10	0.15
(1,3168)	1:1874:A:GLN:HB2	1:1874:A:GLN:HG2	14	0.15
(1,3168)	1:1874:A:GLN:HB2	1:1874:A:GLN:HG2	20	0.15
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	12	0.15
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	14	0.15
(1,3142)	1:1900:A:SER:H	1:1900:A:SER:HA	2	0.15
(1,3142)	1:1900:A:SER:H	1:1900:A:SER:HA	11	0.15
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	1	0.15
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	1	0.15
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	1	0.15
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	9	0.15
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	9	0.15
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	9	0.15
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	12	0.15
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	12	0.15
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	12	0.15
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	13	0.15
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	13	0.15
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	13	0.15
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	20	0.15
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	20	0.15
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	20	0.15
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	10	0.15
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	13	0.15
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	14	0.15
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	14	0.15
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	19	0.15
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	19	0.15
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	9	0.15
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	9	0.15
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	18	0.15
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	18	0.15
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	3	0.15
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	8	0.15
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	12	0.15
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	13	0.15
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	14	0.15
(1,3020)	1:1948:A:LEU:HA	1:1949:A:ASP:H	11	0.15
(1,3020)	1:1948:A:LEU:HA	1:1949:A:ASP:H	16	0.15
(1,3015)	1:1938:A:ARG:HB2	1:1845:A:ASN:HD21	17	0.15
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	4	0.15
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	6	0.15
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	11	0.15
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	18	0.15
(1,2960)	1:1858:A:LYS:HB2	1:1855:A:GLU:H	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2924)	1:1900:A:SER:HB2	1:1903:A:ILE:HB	5	0.15
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	1	0.15
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	2	0.15
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	8	0.15
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	11	0.15
(1,2907)	1:1894:A:LYS:H	1:1894:A:LYS:HE3	4	0.15
(1,2893)	1:1887:A:ILE:HA	1:1890:A:GLU:HB2	3	0.15
(1,2893)	1:1887:A:ILE:HA	1:1890:A:GLU:HB2	8	0.15
(1,2893)	1:1887:A:ILE:HA	1:1890:A:GLU:HB2	9	0.15
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD21	10	0.15
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD22	10	0.15
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD23	10	0.15
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD21	12	0.15
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD22	12	0.15
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD23	12	0.15
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD21	17	0.15
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD22	17	0.15
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD23	17	0.15
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	11	0.15
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	11	0.15
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	11	0.15
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	11	0.15
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	11	0.15
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	11	0.15
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	11	0.15
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	11	0.15
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	11	0.15
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	16	0.15
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	16	0.15
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	16	0.15
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	16	0.15
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	16	0.15
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	16	0.15
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	16	0.15
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	16	0.15
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	16	0.15
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	3	0.15
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	4	0.15
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	4	0.15
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	11	0.15
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	3	0.15
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	5	0.15
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	6	0.15
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	11	0.15
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	14	0.15
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	15	0.15
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	16	0.15
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	2	0.15
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	2	0.15
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	2	0.15
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	3	0.15
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	3	0.15
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	3	0.15
(1,2733)	1:1885:A:ARG:HA	1:1889:A:MET:H	17	0.15
(1,2731)	1:1916:A:THR:HG21	1:1914:A:THR:HB	2	0.15
(1,2731)	1:1916:A:THR:HG22	1:1914:A:THR:HB	2	0.15
(1,2731)	1:1916:A:THR:HG23	1:1914:A:THR:HB	2	0.15
(1,2731)	1:1916:A:THR:HG21	1:1914:A:THR:HB	4	0.15
(1,2731)	1:1916:A:THR:HG22	1:1914:A:THR:HB	4	0.15
(1,2731)	1:1916:A:THR:HG23	1:1914:A:THR:HB	4	0.15
(1,2731)	1:1916:A:THR:HG21	1:1914:A:THR:HB	6	0.15
(1,2731)	1:1916:A:THR:HG22	1:1914:A:THR:HB	6	0.15
(1,2731)	1:1916:A:THR:HG23	1:1914:A:THR:HB	6	0.15
(1,2709)	1:1824:A:SER:HA	1:1825:A:SER:H	16	0.15
(1,2709)	1:1824:A:SER:HA	1:1825:A:SER:H	18	0.15
(1,2701)	1:1924:A:ASN:H	1:1923:A:GLY:HA2	8	0.15
(1,2701)	1:1924:A:ASN:H	1:1923:A:GLY:HA3	8	0.15
(1,2688)	1:1938:A:ARG:HD2	1:1934:A:VAL:HG21	4	0.15
(1,2688)	1:1938:A:ARG:HD2	1:1934:A:VAL:HG22	4	0.15
(1,2688)	1:1938:A:ARG:HD2	1:1934:A:VAL:HG23	4	0.15
(1,2688)	1:1938:A:ARG:HD3	1:1934:A:VAL:HG21	4	0.15
(1,2688)	1:1938:A:ARG:HD3	1:1934:A:VAL:HG22	4	0.15
(1,2688)	1:1938:A:ARG:HD3	1:1934:A:VAL:HG23	4	0.15
(1,2688)	1:1938:A:ARG:HD2	1:1934:A:VAL:HG21	8	0.15
(1,2688)	1:1938:A:ARG:HD2	1:1934:A:VAL:HG22	8	0.15
(1,2688)	1:1938:A:ARG:HD2	1:1934:A:VAL:HG23	8	0.15
(1,2688)	1:1938:A:ARG:HD3	1:1934:A:VAL:HG21	8	0.15
(1,2688)	1:1938:A:ARG:HD3	1:1934:A:VAL:HG22	8	0.15
(1,2688)	1:1938:A:ARG:HD3	1:1934:A:VAL:HG23	8	0.15
(1,2682)	1:1826:A:LYS:HB2	1:1871:A:ASN:HD22	9	0.15
(1,2672)	1:1906:A:GLN:HA	1:1906:A:GLN:HG2	11	0.15
(1,2672)	1:1906:A:GLN:HA	1:1906:A:GLN:HG3	11	0.15
(1,2672)	1:1906:A:GLN:HA	1:1906:A:GLN:HG2	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2672)	1:1906:A:GLN:HA	1:1906:A:GLN:HG3	16	0.15
(1,2672)	1:1906:A:GLN:HA	1:1906:A:GLN:HG2	19	0.15
(1,2672)	1:1906:A:GLN:HA	1:1906:A:GLN:HG3	19	0.15
(1,2672)	1:1906:A:GLN:HA	1:1906:A:GLN:HG2	20	0.15
(1,2672)	1:1906:A:GLN:HA	1:1906:A:GLN:HG3	20	0.15
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	2	0.15
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	2	0.15
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	2	0.15
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	6	0.15
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	6	0.15
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	6	0.15
(1,2606)	1:1840:A:ILE:HD11	1:1850:A:LEU:HA	4	0.15
(1,2606)	1:1840:A:ILE:HD12	1:1850:A:LEU:HA	4	0.15
(1,2606)	1:1840:A:ILE:HD13	1:1850:A:LEU:HA	4	0.15
(1,2606)	1:1840:A:ILE:HD11	1:1850:A:LEU:HA	13	0.15
(1,2606)	1:1840:A:ILE:HD12	1:1850:A:LEU:HA	13	0.15
(1,2606)	1:1840:A:ILE:HD13	1:1850:A:LEU:HA	13	0.15
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	2	0.15
(1,2581)	1:1920:A:SER:H	1:1919:A:VAL:HB	14	0.15
(1,2580)	1:1929:A:GLU:H	1:1928:A:GLU:HG2	2	0.15
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	2	0.15
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	13	0.15
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	19	0.15
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	1	0.15
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	2	0.15
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	3	0.15
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	5	0.15
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	6	0.15
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	7	0.15
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	8	0.15
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	11	0.15
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	12	0.15
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	17	0.15
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	20	0.15
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	3	0.15
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	12	0.15
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	13	0.15
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	3	0.15
(1,2504)	1:1867:A:PRO:HA	1:1871:A:ASN:HD21	4	0.15
(1,2490)	1:1820:A:ILE:HD11	1:1821:A:ASP:H	11	0.15
(1,2490)	1:1820:A:ILE:HD12	1:1821:A:ASP:H	11	0.15
(1,2490)	1:1820:A:ILE:HD13	1:1821:A:ASP:H	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2489)	1:1893:A:GLY:H	1:1891:A:ARG:HB2	5	0.15
(1,2489)	1:1893:A:GLY:H	1:1891:A:ARG:HB2	17	0.15
(1,2489)	1:1893:A:GLY:H	1:1891:A:ARG:HB2	20	0.15
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE1	14	0.15
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE2	14	0.15
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE1	19	0.15
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE2	19	0.15
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	1	0.15
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	5	0.15
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	13	0.15
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	16	0.15
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	18	0.15
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	19	0.15
(1,2424)	1:1950:A:ASN:HB2	1:1950:A:ASN:HA	2	0.15
(1,2424)	1:1950:A:ASN:HB2	1:1950:A:ASN:HA	14	0.15
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	5	0.15
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	8	0.15
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	16	0.15
(1,2380)	1:1897:A:ILE:H	1:1896:A:ARG:HA	3	0.15
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	2	0.15
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	1	0.15
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	2	0.15
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	4	0.15
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	9	0.15
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	1	0.15
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	4	0.15
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	9	0.15
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	11	0.15
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	13	0.15
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	15	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	2	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	2	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	2	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	2	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	2	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	2	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	2	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	2	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	2	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	6	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	6	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	6	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	6	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	6	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	6	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	6	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	6	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	9	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	9	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	9	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	9	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	9	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	9	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	9	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	9	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	9	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	11	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	11	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	11	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	11	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	11	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	11	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	11	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	11	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	11	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	12	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	12	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	12	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	12	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	12	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	12	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	12	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	12	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	12	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	15	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	15	0.15
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	15	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	15	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	15	0.15
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	15	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	15	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	15	0.15
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	3	0.15
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	3	0.15
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	3	0.15
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	18	0.15
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	18	0.15
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	18	0.15
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	19	0.15
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	19	0.15
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	19	0.15
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG21	7	0.15
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG22	7	0.15
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG23	7	0.15
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG21	12	0.15
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG22	12	0.15
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG23	12	0.15
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG21	20	0.15
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG22	20	0.15
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG23	20	0.15
(1,2265)	1:1824:A:SER:H	1:1823:A:LYS:HB2	2	0.15
(1,2265)	1:1824:A:SER:H	1:1823:A:LYS:HB2	11	0.15
(1,2261)	1:1906:A:GLN:H	1:1906:A:GLN:HB2	1	0.15
(1,2261)	1:1906:A:GLN:H	1:1906:A:GLN:HB2	10	0.15
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	12	0.15
(1,2234)	1:1924:A:ASN:H	1:1922:A:ILE:HA	20	0.15
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	20	0.15
(1,2179)	1:1940:A:LYS:HA	1:1943:A:ARG:HB2	12	0.15
(1,2162)	1:1858:A:LYS:HE3	1:1854:A:TYR:HE1	8	0.15
(1,2162)	1:1858:A:LYS:HE3	1:1854:A:TYR:HE2	8	0.15
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	19	0.15
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	20	0.15
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	11	0.15
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	11	0.15
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	11	0.15
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	18	0.15
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	18	0.15
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	18	0.15
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	17	0.15
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	17	0.15
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	16	0.15
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	16	0.15
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	16	0.15
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	17	0.15
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	17	0.15
(1,2100)	1:1822:A:GLU:H	1:1824:A:SER:H	14	0.15
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	19	0.15
(1,2037)	1:1843:A:LYS:HE3	1:1844:A:GLU:HG3	5	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	2	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	2	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	3	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	3	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	7	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	7	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	9	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	9	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	11	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	11	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	13	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	13	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	16	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	16	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	17	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	17	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	18	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	18	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	19	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	19	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG2	20	0.15
(1,1987)	1:1952:A:LYS:HA	1:1952:A:LYS:HG3	20	0.15
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD11	6	0.15
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD12	6	0.15
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD13	6	0.15
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD11	17	0.15
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD12	17	0.15
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD13	17	0.15
(1,1963)	1:1942:A:LEU:H	1:1941:A:ILE:HG12	17	0.15
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	1	0.15
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	5	0.15
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	13	0.15
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	14	0.15
(1,1932)	1:1830:A:ASN:HD21	1:1826:A:LYS:HA	9	0.15
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	1	0.15
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	4	0.15
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	8	0.15
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	11	0.15
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	12	0.15
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	14	0.15
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	15	0.15
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	17	0.15
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	18	0.15
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	20	0.15
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG21	15	0.15
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG22	15	0.15
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG23	15	0.15
(1,1898)	1:1928:A:GLU:H	1:1928:A:GLU:HB2	3	0.15
(1,1898)	1:1928:A:GLU:H	1:1928:A:GLU:HB2	12	0.15
(1,1876)	1:1863:A:ALA:HB1	1:1860:A:TYR:HB2	1	0.15
(1,1876)	1:1863:A:ALA:HB2	1:1860:A:TYR:HB2	1	0.15
(1,1876)	1:1863:A:ALA:HB3	1:1860:A:TYR:HB2	1	0.15
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	6	0.15
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	6	0.15
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	8	0.15
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	8	0.15
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	17	0.15
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	17	0.15
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	19	0.15
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	19	0.15
(1,1858)	1:1934:A:VAL:HA	1:1937:A:GLU:H	13	0.15
(1,1858)	1:1934:A:VAL:HA	1:1937:A:GLU:H	18	0.15
(1,1858)	1:1934:A:VAL:HA	1:1937:A:GLU:H	20	0.15
(1,1806)	1:1840:A:ILE:HB	1:1876:A:PHE:HZ	12	0.15
(1,1790)	1:1927:A:GLY:H	1:1925:A:THR:HB	14	0.15
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD21	1	0.15
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD22	1	0.15
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD23	1	0.15
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD21	3	0.15
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD22	3	0.15
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD23	3	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD11	2	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD12	2	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD13	2	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD11	2	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD12	2	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD13	2	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD11	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD12	2	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD13	2	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD11	5	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD12	5	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD13	5	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD11	5	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD12	5	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD13	5	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD11	5	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD12	5	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD13	5	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD11	13	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD12	13	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD13	13	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD11	13	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD12	13	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD13	13	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD11	13	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD12	13	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD13	13	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD11	16	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD12	16	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD13	16	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD11	16	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD12	16	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD13	16	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD11	16	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD12	16	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD13	16	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD11	18	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD12	18	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD13	18	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD11	18	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD12	18	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD13	18	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD11	18	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD12	18	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD13	18	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD11	20	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD12	20	0.15
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD13	20	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD11	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD12	20	0.15
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD13	20	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD11	20	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD12	20	0.15
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD13	20	0.15
(1,1689)	1:1928:A:GLU:H	1:1927:A:GLY:HA2	14	0.15
(1,1683)	1:1933:A:SER:H	1:1932:A:PRO:HB2	20	0.15
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE2	7	0.15
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE3	7	0.15
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE2	7	0.15
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE3	7	0.15
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE2	13	0.15
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE3	13	0.15
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE2	13	0.15
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE3	13	0.15
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE2	16	0.15
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE3	16	0.15
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE2	16	0.15
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE3	16	0.15
(1,1619)	1:1887:A:ILE:HG21	1:1890:A:GLU:HB2	18	0.15
(1,1619)	1:1887:A:ILE:HG22	1:1890:A:GLU:HB2	18	0.15
(1,1619)	1:1887:A:ILE:HG23	1:1890:A:GLU:HB2	18	0.15
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG21	7	0.15
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG22	7	0.15
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG23	7	0.15
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG21	15	0.15
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG22	15	0.15
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG23	15	0.15
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG21	18	0.15
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG22	18	0.15
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG23	18	0.15
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD11	1	0.15
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD12	1	0.15
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD13	1	0.15
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD11	1	0.15
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD12	1	0.15
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD13	1	0.15
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD11	3	0.15
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD12	3	0.15
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD13	3	0.15
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD11	3	0.15
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD12	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD13	3	0.15
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD11	19	0.15
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD12	19	0.15
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD13	19	0.15
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD11	19	0.15
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD12	19	0.15
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD13	19	0.15
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE2	20	0.15
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE3	20	0.15
(1,1567)	1:1894:A:LYS:H	1:1894:A:LYS:HD2	4	0.15
(1,1567)	1:1894:A:LYS:H	1:1894:A:LYS:HD2	11	0.15
(1,1556)	1:1853:A:LEU:HD11	1:1857:A:LYS:HD2	13	0.15
(1,1556)	1:1853:A:LEU:HD12	1:1857:A:LYS:HD2	13	0.15
(1,1556)	1:1853:A:LEU:HD13	1:1857:A:LYS:HD2	13	0.15
(1,1556)	1:1853:A:LEU:HD11	1:1857:A:LYS:HD2	14	0.15
(1,1556)	1:1853:A:LEU:HD12	1:1857:A:LYS:HD2	14	0.15
(1,1556)	1:1853:A:LEU:HD13	1:1857:A:LYS:HD2	14	0.15
(1,1532)	1:1822:A:GLU:HG3	1:1823:A:LYS:H	2	0.15
(1,1479)	1:1867:A:PRO:HD2	1:1868:A:PHE:H	3	0.15
(1,1439)	1:1928:A:GLU:HA	1:1928:A:GLU:HB3	14	0.15
(1,1439)	1:1928:A:GLU:HA	1:1928:A:GLU:HB3	19	0.15
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	14	0.15
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	14	0.15
(1,1379)	1:1939:A:LEU:HD11	1:1839:A:LYS:HB2	1	0.15
(1,1379)	1:1939:A:LEU:HD12	1:1839:A:LYS:HB2	1	0.15
(1,1379)	1:1939:A:LEU:HD13	1:1839:A:LYS:HB2	1	0.15
(1,1361)	1:1862:A:ASP:H	1:1861:A:SER:HB3	20	0.15
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	2	0.15
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	2	0.15
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	5	0.15
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	5	0.15
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	6	0.15
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	6	0.15
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	12	0.15
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	12	0.15
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD21	4	0.15
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD22	4	0.15
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD23	4	0.15
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD21	4	0.15
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD22	4	0.15
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD23	4	0.15
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD21	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD22	4	0.15
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD23	4	0.15
(1,1345)	1:1821:A:ASP:H	1:1821:A:ASP:HB3	15	0.15
(1,1342)	1:1859:A:LYS:H	1:1858:A:LYS:HG3	2	0.15
(1,1312)	1:1859:A:LYS:HE2	1:1859:A:LYS:HD2	12	0.15
(1,1312)	1:1859:A:LYS:HE3	1:1859:A:LYS:HD2	12	0.15
(1,1261)	1:1927:A:GLY:H	1:1925:A:THR:HG21	1	0.15
(1,1261)	1:1927:A:GLY:H	1:1925:A:THR:HG22	1	0.15
(1,1261)	1:1927:A:GLY:H	1:1925:A:THR:HG23	1	0.15
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	2	0.15
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	3	0.15
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	14	0.15
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	15	0.15
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	16	0.15
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	20	0.15
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	3	0.15
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	4	0.15
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	7	0.15
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	8	0.15
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	9	0.15
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	11	0.15
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	12	0.15
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	17	0.15
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	19	0.15
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	20	0.15
(1,1212)	1:1950:A:ASN:HB3	1:1950:A:ASN:HA	14	0.15
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	10	0.15
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	10	0.15
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	19	0.15
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	19	0.15
(1,1194)	1:1918:A:THR:HA	1:1918:A:THR:HB	3	0.15
(1,1121)	1:1820:A:ILE:H	1:1820:A:ILE:HG12	9	0.15
(1,1121)	1:1820:A:ILE:H	1:1820:A:ILE:HG12	10	0.15
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	20	0.15
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	20	0.15
(1,1081)	1:1826:A:LYS:HB2	1:1826:A:LYS:HD2	12	0.15
(1,1081)	1:1826:A:LYS:HB2	1:1826:A:LYS:HD3	12	0.15
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	8	0.15
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	16	0.15
(1,1000)	1:1917:A:SER:HA	1:1918:A:THR:H	13	0.15
(1,994)	1:1889:A:MET:HE1	1:1885:A:ARG:HG2	16	0.15
(1,994)	1:1889:A:MET:HE2	1:1885:A:ARG:HG2	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:1889:A:MET:HE3	1:1885:A:ARG:HG2	16	0.15
(1,985)	1:1877:A:GLN:HE21	1:1869:A:LEU:HD21	17	0.15
(1,985)	1:1877:A:GLN:HE21	1:1869:A:LEU:HD22	17	0.15
(1,985)	1:1877:A:GLN:HE21	1:1869:A:LEU:HD23	17	0.15
(1,982)	1:1858:A:LYS:H	1:1858:A:LYS:HG3	17	0.15
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	14	0.15
(1,957)	1:1936:A:LEU:H	1:1935:A:TYR:HB2	20	0.15
(1,957)	1:1936:A:LEU:H	1:1935:A:TYR:HB3	20	0.15
(1,929)	1:1922:A:ILE:HG13	1:1922:A:ILE:H	9	0.15
(1,897)	1:1946:A:CYS:H	1:1945:A:ARG:HB2	6	0.15
(1,897)	1:1946:A:CYS:H	1:1945:A:ARG:HB2	19	0.15
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	2	0.15
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	2	0.15
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	2	0.15
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	2	0.15
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	2	0.15
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	2	0.15
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	2	0.15
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	2	0.15
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	2	0.15
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	10	0.15
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	10	0.15
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	10	0.15
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	10	0.15
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	10	0.15
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	10	0.15
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	10	0.15
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	10	0.15
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	10	0.15
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	4	0.15
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	4	0.15
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	10	0.15
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	10	0.15
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	12	0.15
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	12	0.15
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	1	0.15
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	2	0.15
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	5	0.15
(1,828)	1:1851:A:ALA:HB1	1:1852:A:GLU:HG2	8	0.15
(1,828)	1:1851:A:ALA:HB2	1:1852:A:GLU:HG2	8	0.15
(1,828)	1:1851:A:ALA:HB3	1:1852:A:GLU:HG2	8	0.15
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	11	0.15
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	17	0.15
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	18	0.15
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	16	0.15
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	16	0.15
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	16	0.15
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	18	0.15
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	18	0.15
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	18	0.15
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	2	0.15
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	3	0.15
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	15	0.15
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	16	0.15
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	19	0.15
(1,807)	1:1907:A:MET:H	1:1906:A:GLN:HG2	8	0.15
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG21	20	0.15
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG22	20	0.15
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG23	20	0.15
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG21	20	0.15
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG22	20	0.15
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG23	20	0.15
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG21	20	0.15
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG22	20	0.15
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG23	20	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	6	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	6	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	6	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	6	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	6	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	6	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	9	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	9	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	9	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	9	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	9	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	9	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	13	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	13	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	13	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	13	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	13	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	14	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	14	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	14	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	14	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	14	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	14	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	15	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	15	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	15	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	15	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	15	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	15	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	16	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	16	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	16	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	16	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	16	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	16	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	18	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	18	0.15
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	18	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	18	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	18	0.15
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	18	0.15
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG21	13	0.15
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG22	13	0.15
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG23	13	0.15
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	17	0.15
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	15	0.15
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	3	0.15
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	3	0.15
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	3	0.15
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	5	0.15
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	5	0.15
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	5	0.15
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	12	0.15
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	12	0.15
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	12	0.15
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	13	0.15
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	13	0.15
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	13	0.15
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	11	0.15
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	12	0.15
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	15	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	1	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	2	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	4	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	5	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	6	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	7	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	8	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	9	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	10	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	12	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	14	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	15	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	16	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	17	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	18	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	19	0.15
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	20	0.15
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	11	0.15
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	20	0.15
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	6	0.15
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	7	0.15
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	12	0.15
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	13	0.15
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	14	0.15
(1,573)	1:1817:A:ALA:HB1	1:1819:A:ARG:H	1	0.15
(1,573)	1:1817:A:ALA:HB2	1:1819:A:ARG:H	1	0.15
(1,573)	1:1817:A:ALA:HB3	1:1819:A:ARG:H	1	0.15
(1,558)	1:1929:A:GLU:H	1:1928:A:GLU:HA	13	0.15
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	4	0.15
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	4	0.15
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	4	0.15
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	6	0.15
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	6	0.15
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	6	0.15
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	7	0.15
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	7	0.15
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	7	0.15
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	18	0.15
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	18	0.15
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE2	3	0.15
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE3	3	0.15
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE2	3	0.15
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE3	3	0.15
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE2	3	0.15
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE3	3	0.15
(1,526)	1:1885:A:ARG:HA	1:1888:A:GLU:HG2	2	0.15
(1,526)	1:1885:A:ARG:HA	1:1888:A:GLU:HG2	15	0.15
(1,509)	1:1865:A:ILE:HG21	1:1866:A:GLU:H	20	0.15
(1,509)	1:1865:A:ILE:HG22	1:1866:A:GLU:H	20	0.15
(1,509)	1:1865:A:ILE:HG23	1:1866:A:GLU:H	20	0.15
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	5	0.15
(1,489)	1:1854:A:TYR:H	1:1884:A:LEU:HB3	7	0.15
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	2	0.15
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	10	0.15
(1,450)	1:1896:A:ARG:HB2	1:1890:A:GLU:HG2	16	0.15
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	20	0.15
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	2	0.15
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	2	0.15
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	5	0.15
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	5	0.15
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	9	0.15
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	9	0.15
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	1	0.15
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	2	0.15
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	3	0.15
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	4	0.15
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	5	0.15
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	7	0.15
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	9	0.15
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	10	0.15
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	11	0.15
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	13	0.15
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	15	0.15
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	18	0.15
(1,377)	1:1820:A:ILE:HB	1:1823:A:LYS:HG2	12	0.15
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	3	0.15
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	4	0.15
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	8	0.15
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	9	0.15
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	8	0.15
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	17	0.15
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	17	0.15
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	4	0.15
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	11	0.15
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	17	0.15
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	2	0.15
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	10	0.15
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	14	0.15
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	20	0.15
(1,325)	1:1936:A:LEU:HB2	1:1933:A:SER:HA	15	0.15
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD11	2	0.15
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD12	2	0.15
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD13	2	0.15
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD11	14	0.15
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD12	14	0.15
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD13	14	0.15
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD11	20	0.15
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD12	20	0.15
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD13	20	0.15
(1,311)	1:1930:A:VAL:H	1:1930:A:VAL:HG21	10	0.15
(1,311)	1:1930:A:VAL:H	1:1930:A:VAL:HG22	10	0.15
(1,311)	1:1930:A:VAL:H	1:1930:A:VAL:HG23	10	0.15
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	6	0.15
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG11	2	0.15
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG12	2	0.15
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG13	2	0.15
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	2	0.15
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	2	0.15
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	11	0.15
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	11	0.15
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD11	8	0.15
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD12	8	0.15
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD13	8	0.15
(1,186)	1:1884:A:LEU:HD11	1:1857:A:LYS:HD3	8	0.15
(1,186)	1:1884:A:LEU:HD12	1:1857:A:LYS:HD3	8	0.15
(1,186)	1:1884:A:LEU:HD13	1:1857:A:LYS:HD3	8	0.15
(1,135)	1:1939:A:LEU:HD11	1:1839:A:LYS:HD2	12	0.15
(1,135)	1:1939:A:LEU:HD12	1:1839:A:LYS:HD2	12	0.15
(1,135)	1:1939:A:LEU:HD13	1:1839:A:LYS:HD2	12	0.15
(1,125)	1:1822:A:GLU:HG2	1:1823:A:LYS:H	10	0.15
(1,109)	1:1929:A:GLU:H	1:1927:A:GLY:HA2	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:1940:A:LYS:HA	1:1940:A:LYS:HD3	4	0.15
(1,97)	1:1927:A:GLY:H	1:1929:A:GLU:H	8	0.15
(1,89)	1:1924:A:ASN:H	1:1922:A:ILE:HG21	7	0.15
(1,89)	1:1924:A:ASN:H	1:1922:A:ILE:HG22	7	0.15
(1,89)	1:1924:A:ASN:H	1:1922:A:ILE:HG23	7	0.15
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD2	3	0.15
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD3	3	0.15
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD2	3	0.15
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD3	3	0.15
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD2	3	0.15
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD3	3	0.15
(1,61)	1:1948:A:LEU:HD11	1:1949:A:ASP:H	4	0.15
(1,61)	1:1948:A:LEU:HD12	1:1949:A:ASP:H	4	0.15
(1,61)	1:1948:A:LEU:HD13	1:1949:A:ASP:H	4	0.15
(1,31)	1:1827:A:ALA:H	1:1826:A:LYS:HB2	2	0.15
(1,31)	1:1827:A:ALA:H	1:1826:A:LYS:HB2	12	0.15
(1,31)	1:1827:A:ALA:H	1:1826:A:LYS:HB2	13	0.15
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	8	0.15
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	8	0.15
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	16	0.15
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	16	0.15
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	19	0.15
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	19	0.15
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	9	0.15
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	9	0.15
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	9	0.15
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	12	0.15
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	12	0.15
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	12	0.15
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	19	0.15
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	19	0.15
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	19	0.15
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	16	0.14
(1,3321)	1:1954:A:ASP:HA	1:1954:A:ASP:HB3	10	0.14
(1,3312)	1:1906:A:GLN:H	1:1906:A:GLN:HB3	11	0.14
(1,3312)	1:1906:A:GLN:H	1:1906:A:GLN:HB3	20	0.14
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG21	3	0.14
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG22	3	0.14
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG23	3	0.14
(1,3303)	1:1898:A:SER:H	1:1897:A:ILE:HG13	2	0.14
(1,3303)	1:1898:A:SER:H	1:1897:A:ILE:HG13	8	0.14
(1,3258)	1:1862:A:ASP:HA	1:1865:A:ILE:HB	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3258)	1:1862:A:ASP:HA	1:1865:A:ILE:HB	5	0.14
(1,3258)	1:1862:A:ASP:HA	1:1865:A:ILE:HB	14	0.14
(1,3255)	1:1926:A:ASN:H	1:1925:A:THR:HA	15	0.14
(1,3246)	1:1904:A:SER:H	1:1905:A:PRO:HD2	13	0.14
(1,3245)	1:1891:A:ARG:HG3	1:1891:A:ARG:HE	5	0.14
(1,3245)	1:1891:A:ARG:HG3	1:1891:A:ARG:HE	6	0.14
(1,3245)	1:1891:A:ARG:HG3	1:1891:A:ARG:HE	12	0.14
(1,3245)	1:1891:A:ARG:HG3	1:1891:A:ARG:HE	20	0.14
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	14	0.14
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	1	0.14
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	3	0.14
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	6	0.14
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	11	0.14
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	12	0.14
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	13	0.14
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	14	0.14
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	15	0.14
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	19	0.14
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	20	0.14
(1,3190)	1:1923:A:GLY:H	1:1922:A:ILE:H	13	0.14
(1,3190)	1:1923:A:GLY:H	1:1922:A:ILE:H	18	0.14
(1,3186)	1:1903:A:ILE:H	1:1902:A:GLY:H	7	0.14
(1,3172)	1:1902:A:GLY:H	1:1901:A:THR:HB	1	0.14
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG2	14	0.14
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG3	14	0.14
(1,3168)	1:1874:A:GLN:HB2	1:1874:A:GLN:HG2	7	0.14
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	19	0.14
(1,3159)	1:1822:A:GLU:H	1:1822:A:GLU:HG2	9	0.14
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD1	1	0.14
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD2	1	0.14
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD1	7	0.14
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD2	7	0.14
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD1	14	0.14
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD2	14	0.14
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG21	5	0.14
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG22	5	0.14
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG23	5	0.14
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG21	18	0.14
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG22	18	0.14
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG23	18	0.14
(1,3142)	1:1900:A:SER:H	1:1900:A:SER:HA	13	0.14
(1,3142)	1:1900:A:SER:H	1:1900:A:SER:HA	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3135)	1:1950:A:ASN:HB3	1:1950:A:ASN:HD21	11	0.14
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	18	0.14
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	18	0.14
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	18	0.14
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	11	0.14
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	16	0.14
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	12	0.14
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	12	0.14
(1,3086)	1:1903:A:ILE:H	1:1900:A:SER:HB3	3	0.14
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	9	0.14
(1,3062)	1:1872:A:SER:H	1:1870:A:LYS:HB2	14	0.14
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	6	0.14
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	9	0.14
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	11	0.14
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	19	0.14
(1,3020)	1:1948:A:LEU:HA	1:1949:A:ASP:H	5	0.14
(1,3015)	1:1938:A:ARG:HB2	1:1845:A:ASN:HD21	19	0.14
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	7	0.14
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	15	0.14
(1,3004)	1:1915:A:PRO:HD2	1:1914:A:THR:HG21	7	0.14
(1,3004)	1:1915:A:PRO:HD2	1:1914:A:THR:HG22	7	0.14
(1,3004)	1:1915:A:PRO:HD2	1:1914:A:THR:HG23	7	0.14
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD11	2	0.14
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD12	2	0.14
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD13	2	0.14
(1,2955)	1:1905:A:PRO:HD2	1:1904:A:SER:HA	11	0.14
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	16	0.14
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	16	0.14
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	16	0.14
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	4	0.14
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	15	0.14
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	18	0.14
(1,2893)	1:1887:A:ILE:HA	1:1890:A:GLU:HB2	14	0.14
(1,2893)	1:1887:A:ILE:HA	1:1890:A:GLU:HB2	18	0.14
(1,2886)	1:1905:A:PRO:HD2	1:1905:A:PRO:HB2	5	0.14
(1,2886)	1:1905:A:PRO:HD2	1:1905:A:PRO:HB2	6	0.14
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	4	0.14
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	4	0.14
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	4	0.14
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	4	0.14
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	4	0.14
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	4	0.14
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	4	0.14
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	4	0.14
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	14	0.14
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	14	0.14
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	14	0.14
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	14	0.14
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	14	0.14
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	14	0.14
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	14	0.14
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	14	0.14
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	14	0.14
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	3	0.14
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	12	0.14
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	2	0.14
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	12	0.14
(1,2858)	1:1883:A:GLY:HA2	1:1850:A:LEU:HD11	20	0.14
(1,2858)	1:1883:A:GLY:HA2	1:1850:A:LEU:HD12	20	0.14
(1,2858)	1:1883:A:GLY:HA2	1:1850:A:LEU:HD13	20	0.14
(1,2852)	1:1941:A:ILE:H	1:1941:A:ILE:HG13	6	0.14
(1,2807)	1:1889:A:MET:H	1:1888:A:GLU:HB2	17	0.14
(1,2807)	1:1889:A:MET:H	1:1888:A:GLU:HB2	19	0.14
(1,2805)	1:1846:A:THR:H	1:1846:A:THR:HG21	12	0.14
(1,2805)	1:1846:A:THR:H	1:1846:A:THR:HG22	12	0.14
(1,2805)	1:1846:A:THR:H	1:1846:A:THR:HG23	12	0.14
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	9	0.14
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	10	0.14
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	7	0.14
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	9	0.14
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	13	0.14
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	17	0.14
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	18	0.14
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	19	0.14
(1,2765)	1:1878:A:SER:HA	1:1881:A:GLU:HG3	7	0.14
(1,2731)	1:1916:A:THR:HG21	1:1914:A:THR:HB	3	0.14
(1,2731)	1:1916:A:THR:HG22	1:1914:A:THR:HB	3	0.14
(1,2731)	1:1916:A:THR:HG23	1:1914:A:THR:HB	3	0.14
(1,2672)	1:1906:A:GLN:HA	1:1906:A:GLN:HG2	18	0.14
(1,2672)	1:1906:A:GLN:HA	1:1906:A:GLN:HG3	18	0.14
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE1	15	0.14
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE2	15	0.14
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE1	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE2	15	0.14
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE1	15	0.14
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE2	15	0.14
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE1	18	0.14
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE2	18	0.14
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE1	18	0.14
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE2	18	0.14
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE1	18	0.14
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE2	18	0.14
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	1	0.14
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	1	0.14
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	1	0.14
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	3	0.14
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	3	0.14
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	3	0.14
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	5	0.14
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	5	0.14
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	5	0.14
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	13	0.14
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	13	0.14
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	13	0.14
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	17	0.14
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	17	0.14
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	17	0.14
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	18	0.14
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	18	0.14
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	18	0.14
(1,2616)	1:1919:A:VAL:H	1:1918:A:THR:HB	18	0.14
(1,2606)	1:1840:A:ILE:HD11	1:1850:A:LEU:HA	14	0.14
(1,2606)	1:1840:A:ILE:HD12	1:1850:A:LEU:HA	14	0.14
(1,2606)	1:1840:A:ILE:HD13	1:1850:A:LEU:HA	14	0.14
(1,2606)	1:1840:A:ILE:HD11	1:1850:A:LEU:HA	17	0.14
(1,2606)	1:1840:A:ILE:HD12	1:1850:A:LEU:HA	17	0.14
(1,2606)	1:1840:A:ILE:HD13	1:1850:A:LEU:HA	17	0.14
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	7	0.14
(1,2559)	1:1892:A:GLU:H	1:1890:A:GLU:HA	1	0.14
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	1	0.14
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	6	0.14
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	4	0.14
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	9	0.14
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	10	0.14
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	14	0.14
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	15	0.14
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	16	0.14
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	18	0.14
(1,2546)	1:1891:A:ARG:HG2	1:1891:A:ARG:HD2	19	0.14
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	9	0.14
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	15	0.14
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	17	0.14
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	19	0.14
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	11	0.14
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	13	0.14
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	20	0.14
(1,2518)	1:1848:A:GLU:HB2	1:1839:A:LYS:HD2	13	0.14
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	17	0.14
(1,2504)	1:1867:A:PRO:HA	1:1871:A:ASN:HD21	5	0.14
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	2	0.14
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	4	0.14
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	6	0.14
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	8	0.14
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	15	0.14
(1,2426)	1:1907:A:MET:HA	1:1908:A:GLU:H	7	0.14
(1,2410)	1:1898:A:SER:H	1:1898:A:SER:HB2	8	0.14
(1,2410)	1:1898:A:SER:H	1:1898:A:SER:HB2	10	0.14
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	4	0.14
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	6	0.14
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	13	0.14
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	6	0.14
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	7	0.14
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	8	0.14
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	18	0.14
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	20	0.14
(1,2339)	1:1840:A:ILE:H	1:1849:A:GLY:H	12	0.14
(1,2330)	1:1922:A:ILE:HG21	1:1922:A:ILE:H	1	0.14
(1,2330)	1:1922:A:ILE:HG22	1:1922:A:ILE:H	1	0.14
(1,2330)	1:1922:A:ILE:HG23	1:1922:A:ILE:H	1	0.14
(1,2328)	1:1950:A:ASN:H	1:1951:A:THR:H	4	0.14
(1,2298)	1:1891:A:ARG:H	1:1891:A:ARG:HB2	11	0.14
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	14	0.14
(1,2293)	1:1894:A:LYS:HA	1:1894:A:LYS:HB3	19	0.14
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	4	0.14
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	4	0.14
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	4	0.14
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	4	0.14
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	4	0.14
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	4	0.14
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	4	0.14
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	4	0.14
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	17	0.14
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	17	0.14
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	17	0.14
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	17	0.14
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	17	0.14
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	17	0.14
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	17	0.14
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	17	0.14
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	17	0.14
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	14	0.14
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	14	0.14
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	14	0.14
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG21	1	0.14
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG22	1	0.14
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG23	1	0.14
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG21	2	0.14
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG22	2	0.14
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG23	2	0.14
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG21	19	0.14
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG22	19	0.14
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG23	19	0.14
(1,2265)	1:1824:A:SER:H	1:1823:A:LYS:HB2	7	0.14
(1,2261)	1:1906:A:GLN:H	1:1906:A:GLN:HB2	3	0.14
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	9	0.14
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	10	0.14
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	15	0.14
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	16	0.14
(1,2243)	1:1862:A:ASP:HB2	1:1862:A:ASP:H	17	0.14
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	1	0.14
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	2	0.14
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	3	0.14
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	4	0.14
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	5	0.14
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	8	0.14
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	9	0.14
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	11	0.14
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	12	0.14
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	13	0.14
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	14	0.14
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	15	0.14
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	17	0.14
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	18	0.14
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	19	0.14
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG21	14	0.14
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG22	14	0.14
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG23	14	0.14
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG21	8	0.14
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG22	8	0.14
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG23	8	0.14
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG21	8	0.14
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG22	8	0.14
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG23	8	0.14
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG21	8	0.14
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG22	8	0.14
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG23	8	0.14
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG21	2	0.14
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG22	2	0.14
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG23	2	0.14
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG21	2	0.14
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG22	2	0.14
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG23	2	0.14
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG21	2	0.14
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG22	2	0.14
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG23	2	0.14
(1,2179)	1:1940:A:LYS:HA	1:1943:A:ARG:HB2	1	0.14
(1,2179)	1:1940:A:LYS:HA	1:1943:A:ARG:HB2	10	0.14
(1,2179)	1:1940:A:LYS:HA	1:1943:A:ARG:HB2	19	0.14
(1,2165)	1:1841:A:GLY:H	1:1876:A:PHE:HE1	14	0.14
(1,2165)	1:1841:A:GLY:H	1:1876:A:PHE:HE2	14	0.14
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	3	0.14
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	13	0.14
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	15	0.14
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	17	0.14
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	2	0.14
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	2	0.14
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	2	0.14
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	7	0.14
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	7	0.14
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	18	0.14
(1,2070)	1:1820:A:ILE:HG12	1:1821:A:ASP:H	20	0.14
(1,2048)	1:1838:A:LYS:HD2	1:1838:A:LYS:HE3	1	0.14
(1,2048)	1:1838:A:LYS:HD3	1:1838:A:LYS:HE3	1	0.14
(1,2048)	1:1838:A:LYS:HD2	1:1838:A:LYS:HE3	18	0.14
(1,2048)	1:1838:A:LYS:HD3	1:1838:A:LYS:HE3	18	0.14
(1,2037)	1:1843:A:LYS:HE3	1:1844:A:GLU:HG3	13	0.14
(1,1978)	1:1941:A:ILE:H	1:1940:A:LYS:H	9	0.14
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD11	7	0.14
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD12	7	0.14
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD13	7	0.14
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD11	13	0.14
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD12	13	0.14
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD13	13	0.14
(1,1952)	1:1840:A:ILE:HG21	1:1846:A:THR:HB	20	0.14
(1,1952)	1:1840:A:ILE:HG22	1:1846:A:THR:HB	20	0.14
(1,1952)	1:1840:A:ILE:HG23	1:1846:A:THR:HB	20	0.14
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	3	0.14
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	7	0.14
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	8	0.14
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	12	0.14
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	15	0.14
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	19	0.14
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	2	0.14
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	4	0.14
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	5	0.14
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	8	0.14
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	9	0.14
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	17	0.14
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	19	0.14
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	2	0.14
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	5	0.14
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	7	0.14
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	10	0.14
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	16	0.14
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	19	0.14
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE1	10	0.14
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE2	10	0.14
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE1	10	0.14
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE2	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE1	10	0.14
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE2	10	0.14
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG2	20	0.14
(1,1865)	1:1844:A:GLU:HB2	1:1844:A:GLU:HG3	20	0.14
(1,1858)	1:1934:A:VAL:HA	1:1937:A:GLU:H	5	0.14
(1,1858)	1:1934:A:VAL:HA	1:1937:A:GLU:H	7	0.14
(1,1853)	1:1827:A:ALA:H	1:1826:A:LYS:HG2	18	0.14
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	3	0.14
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	7	0.14
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	11	0.14
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	13	0.14
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	14	0.14
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	19	0.14
(1,1806)	1:1840:A:ILE:HB	1:1876:A:PHE:HZ	19	0.14
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD21	15	0.14
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD22	15	0.14
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD23	15	0.14
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD21	16	0.14
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD22	16	0.14
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD23	16	0.14
(1,1770)	1:1914:A:THR:HB	1:1915:A:PRO:HD2	17	0.14
(1,1770)	1:1914:A:THR:HB	1:1915:A:PRO:HD2	18	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD11	3	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD12	3	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD13	3	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD11	3	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD12	3	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD13	3	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD11	3	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD12	3	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD13	3	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD11	4	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD12	4	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD13	4	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD11	4	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD12	4	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD13	4	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD11	4	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD12	4	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD13	4	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD11	11	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD12	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD13	11	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD11	11	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD12	11	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD13	11	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD11	11	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD12	11	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD13	11	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD11	14	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD12	14	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD13	14	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD11	14	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD12	14	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD13	14	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD11	14	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD12	14	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD13	14	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD11	15	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD12	15	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD13	15	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD11	15	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD12	15	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD13	15	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD11	15	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD12	15	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD13	15	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD11	19	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD12	19	0.14
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD13	19	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD11	19	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD12	19	0.14
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD13	19	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD11	19	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD12	19	0.14
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD13	19	0.14
(1,1718)	1:1902:A:GLY:H	1:1901:A:THR:HA	3	0.14
(1,1718)	1:1902:A:GLY:H	1:1901:A:THR:HA	14	0.14
(1,1718)	1:1902:A:GLY:H	1:1901:A:THR:HA	15	0.14
(1,1666)	1:1907:A:MET:HG2	1:1908:A:GLU:H	13	0.14
(1,1641)	1:1862:A:ASP:HB2	1:1865:A:ILE:HD11	11	0.14
(1,1641)	1:1862:A:ASP:HB2	1:1865:A:ILE:HD12	11	0.14
(1,1641)	1:1862:A:ASP:HB2	1:1865:A:ILE:HD13	11	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE2	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE3	1	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE2	1	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE3	1	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE2	3	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE3	3	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE2	3	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE3	3	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE2	4	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE3	4	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE2	4	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE3	4	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE2	6	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE3	6	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE2	6	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE3	6	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE2	8	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE3	8	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE2	8	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE3	8	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE2	11	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE3	11	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE2	11	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE3	11	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE2	12	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE3	12	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE2	12	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE3	12	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE2	17	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE3	17	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE2	17	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE3	17	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE2	18	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE3	18	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE2	18	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE3	18	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE2	19	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE3	19	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE2	19	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE3	19	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE2	20	0.14
(1,1626)	1:1843:A:LYS:HD2	1:1843:A:LYS:HE3	20	0.14
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE2	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1626)	1:1843:A:LYS:HD3	1:1843:A:LYS:HE3	20	0.14
(1,1619)	1:1887:A:ILE:HG21	1:1890:A:GLU:HB2	3	0.14
(1,1619)	1:1887:A:ILE:HG22	1:1890:A:GLU:HB2	3	0.14
(1,1619)	1:1887:A:ILE:HG23	1:1890:A:GLU:HB2	3	0.14
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD11	9	0.14
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD12	9	0.14
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD13	9	0.14
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD11	9	0.14
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD12	9	0.14
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD13	9	0.14
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD11	9	0.14
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD12	9	0.14
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD13	9	0.14
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE2	4	0.14
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE3	4	0.14
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE2	7	0.14
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE3	7	0.14
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE2	12	0.14
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE3	12	0.14
(1,1567)	1:1894:A:LYS:H	1:1894:A:LYS:HD2	1	0.14
(1,1556)	1:1853:A:LEU:HD11	1:1857:A:LYS:HD2	3	0.14
(1,1556)	1:1853:A:LEU:HD12	1:1857:A:LYS:HD2	3	0.14
(1,1556)	1:1853:A:LEU:HD13	1:1857:A:LYS:HD2	3	0.14
(1,1556)	1:1853:A:LEU:HD11	1:1857:A:LYS:HD2	10	0.14
(1,1556)	1:1853:A:LEU:HD12	1:1857:A:LYS:HD2	10	0.14
(1,1556)	1:1853:A:LEU:HD13	1:1857:A:LYS:HD2	10	0.14
(1,1556)	1:1853:A:LEU:HD11	1:1857:A:LYS:HD2	20	0.14
(1,1556)	1:1853:A:LEU:HD12	1:1857:A:LYS:HD2	20	0.14
(1,1556)	1:1853:A:LEU:HD13	1:1857:A:LYS:HD2	20	0.14
(1,1470)	1:1824:A:SER:H	1:1827:A:ALA:H	12	0.14
(1,1462)	1:1924:A:ASN:HB3	1:1924:A:ASN:HA	12	0.14
(1,1458)	1:1955:A:ASP:H	1:1954:A:ASP:HA	12	0.14
(1,1458)	1:1955:A:ASP:H	1:1954:A:ASP:HA	17	0.14
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	2	0.14
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	2	0.14
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	16	0.14
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	16	0.14
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	20	0.14
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	20	0.14
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	8	0.14
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	8	0.14
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	11	0.14
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	12	0.14
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	12	0.14
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	18	0.14
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	18	0.14
(1,1379)	1:1939:A:LEU:HD11	1:1839:A:LYS:HB2	10	0.14
(1,1379)	1:1939:A:LEU:HD12	1:1839:A:LYS:HB2	10	0.14
(1,1379)	1:1939:A:LEU:HD13	1:1839:A:LYS:HB2	10	0.14
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	1	0.14
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	1	0.14
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	11	0.14
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	11	0.14
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	14	0.14
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	14	0.14
(1,1352)	1:1860:A:TYR:HD1	1:1861:A:SER:H	20	0.14
(1,1352)	1:1860:A:TYR:HD2	1:1861:A:SER:H	20	0.14
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD21	19	0.14
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD22	19	0.14
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD23	19	0.14
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD21	19	0.14
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD22	19	0.14
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD23	19	0.14
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD21	19	0.14
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD22	19	0.14
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD23	19	0.14
(1,1312)	1:1859:A:LYS:HE2	1:1859:A:LYS:HD2	1	0.14
(1,1312)	1:1859:A:LYS:HE3	1:1859:A:LYS:HD2	1	0.14
(1,1312)	1:1859:A:LYS:HE2	1:1859:A:LYS:HD2	3	0.14
(1,1312)	1:1859:A:LYS:HE3	1:1859:A:LYS:HD2	3	0.14
(1,1312)	1:1859:A:LYS:HE2	1:1859:A:LYS:HD2	7	0.14
(1,1312)	1:1859:A:LYS:HE3	1:1859:A:LYS:HD2	7	0.14
(1,1312)	1:1859:A:LYS:HE2	1:1859:A:LYS:HD2	8	0.14
(1,1312)	1:1859:A:LYS:HE3	1:1859:A:LYS:HD2	8	0.14
(1,1312)	1:1859:A:LYS:HE2	1:1859:A:LYS:HD2	9	0.14
(1,1312)	1:1859:A:LYS:HE3	1:1859:A:LYS:HD2	9	0.14
(1,1312)	1:1859:A:LYS:HE2	1:1859:A:LYS:HD2	10	0.14
(1,1312)	1:1859:A:LYS:HE3	1:1859:A:LYS:HD2	10	0.14
(1,1312)	1:1859:A:LYS:HE2	1:1859:A:LYS:HD2	11	0.14
(1,1312)	1:1859:A:LYS:HE3	1:1859:A:LYS:HD2	11	0.14
(1,1312)	1:1859:A:LYS:HE2	1:1859:A:LYS:HD2	13	0.14
(1,1312)	1:1859:A:LYS:HE3	1:1859:A:LYS:HD2	13	0.14
(1,1312)	1:1859:A:LYS:HE2	1:1859:A:LYS:HD2	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1312)	1:1859:A:LYS:HE3	1:1859:A:LYS:HD2	17	0.14
(1,1312)	1:1859:A:LYS:HE2	1:1859:A:LYS:HD2	18	0.14
(1,1312)	1:1859:A:LYS:HE3	1:1859:A:LYS:HD2	18	0.14
(1,1312)	1:1859:A:LYS:HE2	1:1859:A:LYS:HD2	19	0.14
(1,1312)	1:1859:A:LYS:HE3	1:1859:A:LYS:HD2	19	0.14
(1,1312)	1:1859:A:LYS:HE2	1:1859:A:LYS:HD2	20	0.14
(1,1312)	1:1859:A:LYS:HE3	1:1859:A:LYS:HD2	20	0.14
(1,1272)	1:1895:A:GLY:H	1:1893:A:GLY:H	1	0.14
(1,1272)	1:1895:A:GLY:H	1:1893:A:GLY:H	10	0.14
(1,1272)	1:1895:A:GLY:H	1:1893:A:GLY:H	13	0.14
(1,1272)	1:1895:A:GLY:H	1:1893:A:GLY:H	17	0.14
(1,1270)	1:1893:A:GLY:H	1:1894:A:LYS:HD2	18	0.14
(1,1244)	1:1926:A:ASN:H	1:1926:A:ASN:HB2	16	0.14
(1,1241)	1:1877:A:GLN:HG2	1:1877:A:GLN:HA	4	0.14
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	1	0.14
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	2	0.14
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	5	0.14
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	6	0.14
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	10	0.14
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	13	0.14
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	14	0.14
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	15	0.14
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	16	0.14
(1,1225)	1:1836:A:ILE:H	1:1835:A:GLU:HA	18	0.14
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	13	0.14
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	13	0.14
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	13	0.14
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	14	0.14
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	14	0.14
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	14	0.14
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	20	0.14
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	20	0.14
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	20	0.14
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	2	0.14
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	2	0.14
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	14	0.14
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	14	0.14
(1,1200)	1:1922:A:ILE:HB	1:1922:A:ILE:H	2	0.14
(1,1200)	1:1922:A:ILE:HB	1:1922:A:ILE:H	5	0.14
(1,1200)	1:1922:A:ILE:HB	1:1922:A:ILE:H	12	0.14
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD11	12	0.14
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD12	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD13	12	0.14
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD11	13	0.14
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD12	13	0.14
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD13	13	0.14
(1,1131)	1:1824:A:SER:H	1:1827:A:ALA:HB1	10	0.14
(1,1131)	1:1824:A:SER:H	1:1827:A:ALA:HB2	10	0.14
(1,1131)	1:1824:A:SER:H	1:1827:A:ALA:HB3	10	0.14
(1,1121)	1:1820:A:ILE:H	1:1820:A:ILE:HG12	2	0.14
(1,1121)	1:1820:A:ILE:H	1:1820:A:ILE:HG12	6	0.14
(1,1098)	1:1905:A:PRO:HD2	1:1904:A:SER:HB2	14	0.14
(1,1098)	1:1905:A:PRO:HD2	1:1904:A:SER:HB3	14	0.14
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	8	0.14
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	8	0.14
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	9	0.14
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	9	0.14
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	11	0.14
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	11	0.14
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	12	0.14
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	12	0.14
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	16	0.14
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	16	0.14
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	17	0.14
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	17	0.14
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	18	0.14
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	18	0.14
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	19	0.14
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	19	0.14
(1,1081)	1:1826:A:LYS:HB2	1:1826:A:LYS:HD2	2	0.14
(1,1081)	1:1826:A:LYS:HB2	1:1826:A:LYS:HD3	2	0.14
(1,1081)	1:1826:A:LYS:HB2	1:1826:A:LYS:HD2	17	0.14
(1,1081)	1:1826:A:LYS:HB2	1:1826:A:LYS:HD3	17	0.14
(1,1080)	1:1847:A:LYS:HA	1:1850:A:LEU:HB2	12	0.14
(1,1056)	1:1927:A:GLY:H	1:1926:A:ASN:HA	13	0.14
(1,1032)	1:1829:A:VAL:H	1:1829:A:VAL:HG21	5	0.14
(1,1032)	1:1829:A:VAL:H	1:1829:A:VAL:HG22	5	0.14
(1,1032)	1:1829:A:VAL:H	1:1829:A:VAL:HG23	5	0.14
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	4	0.14
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	5	0.14
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	11	0.14
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	13	0.14
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	19	0.14
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	5	0.14
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	5	0.14
(1,994)	1:1889:A:MET:HE1	1:1885:A:ARG:HG2	14	0.14
(1,994)	1:1889:A:MET:HE2	1:1885:A:ARG:HG2	14	0.14
(1,994)	1:1889:A:MET:HE3	1:1885:A:ARG:HG2	14	0.14
(1,994)	1:1889:A:MET:HE1	1:1885:A:ARG:HG2	20	0.14
(1,994)	1:1889:A:MET:HE2	1:1885:A:ARG:HG2	20	0.14
(1,994)	1:1889:A:MET:HE3	1:1885:A:ARG:HG2	20	0.14
(1,974)	1:1856:A:TYR:HD1	1:1833:A:LEU:HD11	9	0.14
(1,974)	1:1856:A:TYR:HD1	1:1833:A:LEU:HD12	9	0.14
(1,974)	1:1856:A:TYR:HD1	1:1833:A:LEU:HD13	9	0.14
(1,974)	1:1856:A:TYR:HD2	1:1833:A:LEU:HD11	9	0.14
(1,974)	1:1856:A:TYR:HD2	1:1833:A:LEU:HD12	9	0.14
(1,974)	1:1856:A:TYR:HD2	1:1833:A:LEU:HD13	9	0.14
(1,937)	1:1894:A:LYS:H	1:1894:A:LYS:HG3	8	0.14
(1,929)	1:1922:A:ILE:HG13	1:1922:A:ILE:H	7	0.14
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB2	14	0.14
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB3	14	0.14
(1,888)	1:1887:A:ILE:HA	1:1890:A:GLU:HG2	18	0.14
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	4	0.14
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	4	0.14
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	4	0.14
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	4	0.14
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	4	0.14
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	4	0.14
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	4	0.14
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	4	0.14
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	4	0.14
(1,844)	1:1890:A:GLU:HA	1:1890:A:GLU:HG2	19	0.14
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD2	6	0.14
(1,842)	1:1896:A:ARG:HA	1:1896:A:ARG:HD3	6	0.14
(1,841)	1:1845:A:ASN:HB3	1:1839:A:LYS:HG3	10	0.14
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	4	0.14
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	14	0.14
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	15	0.14
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	18	0.14
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	19	0.14
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	20	0.14
(1,828)	1:1851:A:ALA:HB1	1:1852:A:GLU:HG2	10	0.14
(1,828)	1:1851:A:ALA:HB2	1:1852:A:GLU:HG2	10	0.14
(1,828)	1:1851:A:ALA:HB3	1:1852:A:GLU:HG2	10	0.14
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	9	0.14
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	7	0.14
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	7	0.14
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	7	0.14
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	9	0.14
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	9	0.14
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	9	0.14
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	19	0.14
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	19	0.14
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	19	0.14
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	6	0.14
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	10	0.14
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	11	0.14
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	13	0.14
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	14	0.14
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	18	0.14
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	20	0.14
(1,801)	1:1955:A:ASP:H	1:1955:A:ASP:HB2	3	0.14
(1,801)	1:1955:A:ASP:H	1:1955:A:ASP:HB3	3	0.14
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	5	0.14
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	5	0.14
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	5	0.14
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	5	0.14
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	5	0.14
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	5	0.14
(1,736)	1:1898:A:SER:H	1:1897:A:ILE:H	6	0.14
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG21	9	0.14
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG22	9	0.14
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG23	9	0.14
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG21	16	0.14
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG22	16	0.14
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG23	16	0.14
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	4	0.14
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	9	0.14
(1,679)	1:1954:A:ASP:H	1:1953:A:GLN:HB2	19	0.14
(1,653)	1:1898:A:SER:H	1:1898:A:SER:HB3	13	0.14
(1,632)	1:1949:A:ASP:H	1:1949:A:ASP:HB3	16	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	4	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	4	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	4	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	6	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	6	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	8	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	8	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	8	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	9	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	9	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	9	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	11	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	11	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	11	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	15	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	15	0.14
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	15	0.14
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	13	0.14
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	16	0.14
(1,601)	1:1923:A:GLY:H	1:1922:A:ILE:HG13	11	0.14
(1,601)	1:1923:A:GLY:H	1:1922:A:ILE:HG13	18	0.14
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	3	0.14
(1,597)	1:1891:A:ARG:HD3	1:1891:A:ARG:HG3	11	0.14
(1,595)	1:1823:A:LYS:HA	1:1823:A:LYS:HB2	7	0.14
(1,595)	1:1823:A:LYS:HA	1:1823:A:LYS:HB2	9	0.14
(1,593)	1:1920:A:SER:HA	1:1915:A:PRO:HB3	1	0.14
(1,585)	1:1923:A:GLY:H	1:1922:A:ILE:HB	16	0.14
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	1	0.14
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	5	0.14
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	8	0.14
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	18	0.14
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	11	0.14
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	11	0.14
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	11	0.14
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	14	0.14
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	14	0.14
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	14	0.14
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	20	0.14
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	20	0.14
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	20	0.14
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE2	13	0.14
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE3	13	0.14
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE2	13	0.14
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE3	13	0.14
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE2	13	0.14
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE3	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE2	14	0.14
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE3	14	0.14
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE2	14	0.14
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE3	14	0.14
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE2	14	0.14
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE3	14	0.14
(1,526)	1:1885:A:ARG:HA	1:1888:A:GLU:HG2	14	0.14
(1,489)	1:1854:A:TYR:H	1:1884:A:LEU:HB3	20	0.14
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	5	0.14
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	6	0.14
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	15	0.14
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	16	0.14
(1,461)	1:1845:A:ASN:HD21	1:1839:A:LYS:HG3	9	0.14
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	6	0.14
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	7	0.14
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	11	0.14
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	14	0.14
(1,416)	1:1955:A:ASP:H	1:1954:A:ASP:H	16	0.14
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	10	0.14
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	10	0.14
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	14	0.14
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	14	0.14
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	6	0.14
(1,389)	1:1858:A:LYS:H	1:1858:A:LYS:HG2	12	0.14
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	14	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	1	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	1	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	2	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	2	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	3	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	3	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	4	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	4	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	5	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	5	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	6	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	6	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	7	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	7	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	9	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	9	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	10	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	11	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	11	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	12	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	12	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	14	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	14	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	15	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	15	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	16	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	16	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	18	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	18	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	20	0.14
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	20	0.14
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	5	0.14
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	7	0.14
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	8	0.14
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	13	0.14
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	14	0.14
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	15	0.14
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	18	0.14
(1,330)	1:1827:A:ALA:H	1:1826:A:LYS:HB3	1	0.14
(1,330)	1:1827:A:ALA:H	1:1826:A:LYS:HB3	6	0.14
(1,330)	1:1827:A:ALA:H	1:1826:A:LYS:HB3	15	0.14
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	1	0.14
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	3	0.14
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	4	0.14
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	5	0.14
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	6	0.14
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	7	0.14
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	11	0.14
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	12	0.14
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	13	0.14
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	15	0.14
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	17	0.14
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	18	0.14
(1,328)	1:1830:A:ASN:H	1:1829:A:VAL:HA	19	0.14
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD11	6	0.14
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD12	6	0.14
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD13	6	0.14
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD11	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD12	7	0.14
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD13	7	0.14
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	8	0.14
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	10	0.14
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	12	0.14
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	15	0.14
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	15	0.14
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	17	0.14
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	17	0.14
(1,265)	1:1904:A:SER:HB2	1:1913:A:PRO:HG3	5	0.14
(1,265)	1:1904:A:SER:HB2	1:1913:A:PRO:HG3	14	0.14
(1,258)	1:1941:A:ILE:HA	1:1941:A:ILE:HG13	2	0.14
(1,258)	1:1941:A:ILE:HA	1:1941:A:ILE:HG13	7	0.14
(1,258)	1:1941:A:ILE:HA	1:1941:A:ILE:HG13	13	0.14
(1,258)	1:1941:A:ILE:HA	1:1941:A:ILE:HG13	18	0.14
(1,239)	1:1896:A:ARG:H	1:1897:A:ILE:HB	4	0.14
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG21	17	0.14
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG22	17	0.14
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG23	17	0.14
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	2	0.14
(1,135)	1:1939:A:LEU:HD11	1:1839:A:LYS:HD2	15	0.14
(1,135)	1:1939:A:LEU:HD12	1:1839:A:LYS:HD2	15	0.14
(1,135)	1:1939:A:LEU:HD13	1:1839:A:LYS:HD2	15	0.14
(1,135)	1:1939:A:LEU:HD11	1:1839:A:LYS:HD2	20	0.14
(1,135)	1:1939:A:LEU:HD12	1:1839:A:LYS:HD2	20	0.14
(1,135)	1:1939:A:LEU:HD13	1:1839:A:LYS:HD2	20	0.14
(1,125)	1:1822:A:GLU:HG2	1:1823:A:LYS:H	14	0.14
(1,96)	1:1828:A:LYS:HA	1:1831:A:ASP:HB3	1	0.14
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD2	17	0.14
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD3	17	0.14
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD2	17	0.14
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD3	17	0.14
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD2	17	0.14
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD3	17	0.14
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	1	0.14
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	1	0.14
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	2	0.14
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	2	0.14
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	3	0.14
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	3	0.14
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	5	0.14
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	12	0.14
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	12	0.14
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	15	0.14
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	15	0.14
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE2	20	0.14
(1,5)	1:1952:A:LYS:HG3	1:1952:A:LYS:HE3	20	0.14
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	4	0.14
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	4	0.14
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	4	0.14
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	5	0.14
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	5	0.14
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	5	0.14
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	18	0.14
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	18	0.14
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	18	0.14
(3,32)	1:1880:A:VAL:N	1:1876:A:PHE:O	8	0.13
(1,3312)	1:1906:A:GLN:H	1:1906:A:GLN:HB3	8	0.13
(1,3258)	1:1862:A:ASP:HA	1:1865:A:ILE:HB	19	0.13
(1,3248)	1:1840:A:ILE:HD11	1:1837:A:PHE:HE1	6	0.13
(1,3248)	1:1840:A:ILE:HD11	1:1837:A:PHE:HE2	6	0.13
(1,3248)	1:1840:A:ILE:HD12	1:1837:A:PHE:HE1	6	0.13
(1,3248)	1:1840:A:ILE:HD12	1:1837:A:PHE:HE2	6	0.13
(1,3248)	1:1840:A:ILE:HD13	1:1837:A:PHE:HE1	6	0.13
(1,3248)	1:1840:A:ILE:HD13	1:1837:A:PHE:HE2	6	0.13
(1,3246)	1:1904:A:SER:H	1:1905:A:PRO:HD2	4	0.13
(1,3245)	1:1891:A:ARG:HG3	1:1891:A:ARG:HE	1	0.13
(1,3245)	1:1891:A:ARG:HG3	1:1891:A:ARG:HE	14	0.13
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	2	0.13
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	14	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	1	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	2	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	3	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	4	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	6	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	7	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	8	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	10	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	11	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	12	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	13	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	15	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	17	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	18	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	19	0.13
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	20	0.13
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	7	0.13
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	10	0.13
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	16	0.13
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	18	0.13
(1,3190)	1:1923:A:GLY:H	1:1922:A:ILE:H	10	0.13
(1,3190)	1:1923:A:GLY:H	1:1922:A:ILE:H	11	0.13
(1,3172)	1:1902:A:GLY:H	1:1901:A:THR:HB	2	0.13
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG2	10	0.13
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG3	10	0.13
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	15	0.13
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	20	0.13
(1,3159)	1:1822:A:GLU:H	1:1822:A:GLU:HG2	15	0.13
(1,3159)	1:1822:A:GLU:H	1:1822:A:GLU:HG2	19	0.13
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD1	6	0.13
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD2	6	0.13
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD1	8	0.13
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD2	8	0.13
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD1	11	0.13
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD2	11	0.13
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG21	16	0.13
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG22	16	0.13
(1,3145)	1:1931:A:GLY:H	1:1930:A:VAL:HG23	16	0.13
(1,3126)	1:1818:A:SER:H	1:1818:A:SER:HB2	2	0.13
(1,3126)	1:1818:A:SER:H	1:1818:A:SER:HB3	2	0.13
(1,3126)	1:1818:A:SER:H	1:1818:A:SER:HB2	5	0.13
(1,3126)	1:1818:A:SER:H	1:1818:A:SER:HB3	5	0.13
(1,3111)	1:1931:A:GLY:H	1:1930:A:VAL:HB	3	0.13
(1,3111)	1:1931:A:GLY:H	1:1930:A:VAL:HB	15	0.13
(1,3098)	1:1920:A:SER:H	1:1920:A:SER:HB3	1	0.13
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	7	0.13
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	7	0.13
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	17	0.13
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	17	0.13
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	18	0.13
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	19	0.13
(1,3075)	1:1942:A:LEU:HB3	1:1838:A:LYS:HG3	7	0.13
(1,3062)	1:1872:A:SER:H	1:1870:A:LYS:HB2	4	0.13
(1,3062)	1:1872:A:SER:H	1:1870:A:LYS:HB2	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3032)	1:1835:A:GLU:H	1:1833:A:LEU:HB2	16	0.13
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG21	3	0.13
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG22	3	0.13
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG23	3	0.13
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG21	3	0.13
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG22	3	0.13
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG23	3	0.13
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG21	3	0.13
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG22	3	0.13
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG23	3	0.13
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG21	15	0.13
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG22	15	0.13
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG23	15	0.13
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG21	15	0.13
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG22	15	0.13
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG23	15	0.13
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG21	15	0.13
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG22	15	0.13
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG23	15	0.13
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	3	0.13
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	12	0.13
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	13	0.13
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD11	10	0.13
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD12	10	0.13
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD13	10	0.13
(1,2975)	1:1892:A:GLU:H	1:1891:A:ARG:HG3	6	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	1	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	1	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	1	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	2	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	2	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	2	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	3	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	3	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	3	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	4	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	4	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	4	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	6	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	6	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	6	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	7	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	7	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	9	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	9	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	9	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	10	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	10	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	10	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	12	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	12	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	12	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	13	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	13	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	13	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	15	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	15	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	15	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	17	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	17	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	17	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	19	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	19	0.13
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	19	0.13
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	19	0.13
(1,2907)	1:1894:A:LYS:H	1:1894:A:LYS:HE3	2	0.13
(1,2907)	1:1894:A:LYS:H	1:1894:A:LYS:HE3	15	0.13
(1,2907)	1:1894:A:LYS:H	1:1894:A:LYS:HE3	20	0.13
(1,2886)	1:1905:A:PRO:HD2	1:1905:A:PRO:HB2	19	0.13
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	13	0.13
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	16	0.13
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	18	0.13
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	20	0.13
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	9	0.13
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	10	0.13
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	13	0.13
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	16	0.13
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	19	0.13
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	20	0.13
(1,2842)	1:1950:A:ASN:HB2	1:1951:A:THR:H	3	0.13
(1,2842)	1:1950:A:ASN:HB2	1:1951:A:THR:H	20	0.13
(1,2807)	1:1889:A:MET:H	1:1888:A:GLU:HB2	16	0.13
(1,2801)	1:1874:A:GLN:HA	1:1874:A:GLN:HG2	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2793)	1:1849:A:GLY:H	1:1848:A:GLU:HG2	20	0.13
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	10	0.13
(1,2788)	1:1937:A:GLU:HA	1:1938:A:ARG:H	20	0.13
(1,2737)	1:1823:A:LYS:HA	1:1824:A:SER:H	1	0.13
(1,2737)	1:1823:A:LYS:HA	1:1824:A:SER:H	3	0.13
(1,2737)	1:1823:A:LYS:HA	1:1824:A:SER:H	4	0.13
(1,2737)	1:1823:A:LYS:HA	1:1824:A:SER:H	19	0.13
(1,2731)	1:1916:A:THR:HG21	1:1914:A:THR:HB	8	0.13
(1,2731)	1:1916:A:THR:HG22	1:1914:A:THR:HB	8	0.13
(1,2731)	1:1916:A:THR:HG23	1:1914:A:THR:HB	8	0.13
(1,2731)	1:1916:A:THR:HG21	1:1914:A:THR:HB	11	0.13
(1,2731)	1:1916:A:THR:HG22	1:1914:A:THR:HB	11	0.13
(1,2731)	1:1916:A:THR:HG23	1:1914:A:THR:HB	11	0.13
(1,2731)	1:1916:A:THR:HG21	1:1914:A:THR:HB	16	0.13
(1,2731)	1:1916:A:THR:HG22	1:1914:A:THR:HB	16	0.13
(1,2731)	1:1916:A:THR:HG23	1:1914:A:THR:HB	16	0.13
(1,2724)	1:1864:A:ASP:H	1:1864:A:ASP:HB2	7	0.13
(1,2710)	1:1899:A:THR:H	1:1898:A:SER:HA	10	0.13
(1,2709)	1:1824:A:SER:HA	1:1825:A:SER:H	20	0.13
(1,2705)	1:1889:A:MET:HA	1:1894:A:LYS:HB3	15	0.13
(1,2685)	1:1859:A:LYS:HA	1:1859:A:LYS:HG3	20	0.13
(1,2672)	1:1906:A:GLN:HA	1:1906:A:GLN:HG2	9	0.13
(1,2672)	1:1906:A:GLN:HA	1:1906:A:GLN:HG3	9	0.13
(1,2668)	1:1925:A:THR:H	1:1924:A:ASN:HB2	10	0.13
(1,2648)	1:1853:A:LEU:HA	1:1856:A:TYR:HB3	3	0.13
(1,2648)	1:1853:A:LEU:HA	1:1856:A:TYR:HB3	7	0.13
(1,2648)	1:1853:A:LEU:HA	1:1856:A:TYR:HB3	18	0.13
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE1	5	0.13
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE2	5	0.13
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE1	5	0.13
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE2	5	0.13
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE1	5	0.13
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE2	5	0.13
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE1	12	0.13
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE2	12	0.13
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE1	12	0.13
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE2	12	0.13
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE1	12	0.13
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE2	12	0.13
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE1	14	0.13
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE2	14	0.13
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE1	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE2	14	0.13
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE1	14	0.13
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE2	14	0.13
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	8	0.13
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	8	0.13
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	8	0.13
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	9	0.13
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	9	0.13
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	9	0.13
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	11	0.13
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	11	0.13
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	11	0.13
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	14	0.13
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	14	0.13
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	14	0.13
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	15	0.13
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	15	0.13
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	15	0.13
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	19	0.13
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	19	0.13
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	19	0.13
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	20	0.13
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	20	0.13
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	20	0.13
(1,2616)	1:1919:A:VAL:H	1:1918:A:THR:HB	3	0.13
(1,2606)	1:1840:A:ILE:HD11	1:1850:A:LEU:HA	19	0.13
(1,2606)	1:1840:A:ILE:HD12	1:1850:A:LEU:HA	19	0.13
(1,2606)	1:1840:A:ILE:HD13	1:1850:A:LEU:HA	19	0.13
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	3	0.13
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	4	0.13
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	11	0.13
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	12	0.13
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	14	0.13
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	16	0.13
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	20	0.13
(1,2564)	1:1909:A:VAL:H	1:1910:A:THR:H	6	0.13
(1,2558)	1:1891:A:ARG:H	1:1890:A:GLU:HG3	13	0.13
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	3	0.13
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	4	0.13
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	8	0.13
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	8	0.13
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2518)	1:1848:A:GLU:HB2	1:1839:A:LYS:HD2	8	0.13
(1,2518)	1:1848:A:GLU:HB2	1:1839:A:LYS:HD2	11	0.13
(1,2517)	1:1882:A:ARG:HA	1:1881:A:GLU:HG3	17	0.13
(1,2515)	1:1898:A:SER:H	1:1897:A:ILE:HB	2	0.13
(1,2515)	1:1898:A:SER:H	1:1897:A:ILE:HB	7	0.13
(1,2515)	1:1898:A:SER:H	1:1897:A:ILE:HB	8	0.13
(1,2515)	1:1898:A:SER:H	1:1897:A:ILE:HB	16	0.13
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	9	0.13
(1,2504)	1:1867:A:PRO:HA	1:1871:A:ASN:HD21	2	0.13
(1,2504)	1:1867:A:PRO:HA	1:1871:A:ASN:HD21	9	0.13
(1,2489)	1:1893:A:GLY:H	1:1891:A:ARG:HB2	10	0.13
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	6	0.13
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	16	0.13
(1,2483)	1:1908:A:GLU:H	1:1908:A:GLU:HG2	10	0.13
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE1	2	0.13
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE2	2	0.13
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE1	17	0.13
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE2	17	0.13
(1,2471)	1:1865:A:ILE:HD11	1:1857:A:LYS:HE2	16	0.13
(1,2471)	1:1865:A:ILE:HD11	1:1857:A:LYS:HE3	16	0.13
(1,2471)	1:1865:A:ILE:HD12	1:1857:A:LYS:HE2	16	0.13
(1,2471)	1:1865:A:ILE:HD12	1:1857:A:LYS:HE3	16	0.13
(1,2471)	1:1865:A:ILE:HD13	1:1857:A:LYS:HE2	16	0.13
(1,2471)	1:1865:A:ILE:HD13	1:1857:A:LYS:HE3	16	0.13
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	9	0.13
(1,2426)	1:1907:A:MET:HA	1:1908:A:GLU:H	5	0.13
(1,2426)	1:1907:A:MET:HA	1:1908:A:GLU:H	8	0.13
(1,2426)	1:1907:A:MET:HA	1:1908:A:GLU:H	20	0.13
(1,2424)	1:1950:A:ASN:HB2	1:1950:A:ASN:HA	1	0.13
(1,2424)	1:1950:A:ASN:HB2	1:1950:A:ASN:HA	9	0.13
(1,2415)	1:1857:A:LYS:HA	1:1857:A:LYS:HG2	17	0.13
(1,2415)	1:1857:A:LYS:HA	1:1857:A:LYS:HG2	20	0.13
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	19	0.13
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	10	0.13
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	16	0.13
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	17	0.13
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	8	0.13
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	20	0.13
(1,2345)	1:1930:A:VAL:H	1:1930:A:VAL:HG11	16	0.13
(1,2345)	1:1930:A:VAL:H	1:1930:A:VAL:HG12	16	0.13
(1,2345)	1:1930:A:VAL:H	1:1930:A:VAL:HG13	16	0.13
(1,2330)	1:1922:A:ILE:HG21	1:1922:A:ILE:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2330)	1:1922:A:ILE:HG22	1:1922:A:ILE:H	3	0.13
(1,2330)	1:1922:A:ILE:HG23	1:1922:A:ILE:H	3	0.13
(1,2330)	1:1922:A:ILE:HG21	1:1922:A:ILE:H	10	0.13
(1,2330)	1:1922:A:ILE:HG22	1:1922:A:ILE:H	10	0.13
(1,2330)	1:1922:A:ILE:HG23	1:1922:A:ILE:H	10	0.13
(1,2330)	1:1922:A:ILE:HG21	1:1922:A:ILE:H	11	0.13
(1,2330)	1:1922:A:ILE:HG22	1:1922:A:ILE:H	11	0.13
(1,2330)	1:1922:A:ILE:HG23	1:1922:A:ILE:H	11	0.13
(1,2330)	1:1922:A:ILE:HG21	1:1922:A:ILE:H	18	0.13
(1,2330)	1:1922:A:ILE:HG22	1:1922:A:ILE:H	18	0.13
(1,2330)	1:1922:A:ILE:HG23	1:1922:A:ILE:H	18	0.13
(1,2321)	1:1903:A:ILE:H	1:1902:A:GLY:HA2	4	0.13
(1,2321)	1:1903:A:ILE:H	1:1902:A:GLY:HA3	4	0.13
(1,2298)	1:1891:A:ARG:H	1:1891:A:ARG:HB2	17	0.13
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	7	0.13
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	7	0.13
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	7	0.13
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	7	0.13
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	7	0.13
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	7	0.13
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	7	0.13
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	7	0.13
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	7	0.13
(1,2287)	1:1863:A:ALA:H	1:1862:A:ASP:HA	6	0.13
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	4	0.13
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	4	0.13
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	4	0.13
(1,2261)	1:1906:A:GLN:H	1:1906:A:GLN:HB2	12	0.13
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD21	3	0.13
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD22	3	0.13
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD23	3	0.13
(1,2245)	1:1954:A:ASP:HA	1:1954:A:ASP:HB2	17	0.13
(1,2245)	1:1954:A:ASP:HA	1:1954:A:ASP:HB2	19	0.13
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	2	0.13
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	3	0.13
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	5	0.13
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	8	0.13
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	17	0.13
(1,2243)	1:1862:A:ASP:HB2	1:1862:A:ASP:H	16	0.13
(1,2238)	1:1840:A:ILE:H	1:1838:A:LYS:HA	12	0.13
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	12	0.13
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	6	0.13
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	7	0.13
(1,2228)	1:1857:A:LYS:HA	1:1857:A:LYS:HB3	16	0.13
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG21	11	0.13
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG22	11	0.13
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG23	11	0.13
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG21	11	0.13
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG22	11	0.13
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG23	11	0.13
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG21	11	0.13
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG22	11	0.13
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG23	11	0.13
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG21	15	0.13
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG22	15	0.13
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG23	15	0.13
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG21	15	0.13
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG22	15	0.13
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG23	15	0.13
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG21	15	0.13
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG22	15	0.13
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG23	15	0.13
(1,2193)	1:1889:A:MET:HB2	1:1894:A:LYS:HE2	16	0.13
(1,2179)	1:1940:A:LYS:HA	1:1943:A:ARG:HB2	15	0.13
(1,2179)	1:1940:A:LYS:HA	1:1943:A:ARG:HB2	17	0.13
(1,2162)	1:1858:A:LYS:HE3	1:1854:A:TYR:HE1	16	0.13
(1,2162)	1:1858:A:LYS:HE3	1:1854:A:TYR:HE2	16	0.13
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	6	0.13
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	11	0.13
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	12	0.13
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	16	0.13
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	3	0.13
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	3	0.13
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	3	0.13
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	14	0.13
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	14	0.13
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	14	0.13
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	15	0.13
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	15	0.13
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	15	0.13
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	8	0.13
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	7	0.13
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	9	0.13
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	9	0.13
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	16	0.13
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	16	0.13
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	9	0.13
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	9	0.13
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	9	0.13
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	11	0.13
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	11	0.13
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	11	0.13
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	14	0.13
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	14	0.13
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	14	0.13
(1,2089)	1:1916:A:THR:H	1:1915:A:PRO:HB2	5	0.13
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	15	0.13
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	4	0.13
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	11	0.13
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	13	0.13
(1,2055)	1:1922:A:ILE:HA	1:1922:A:ILE:HG12	1	0.13
(1,2048)	1:1838:A:LYS:HD2	1:1838:A:LYS:HE3	7	0.13
(1,2048)	1:1838:A:LYS:HD3	1:1838:A:LYS:HE3	7	0.13
(1,2048)	1:1838:A:LYS:HD2	1:1838:A:LYS:HE3	15	0.13
(1,2048)	1:1838:A:LYS:HD3	1:1838:A:LYS:HE3	15	0.13
(1,1979)	1:1941:A:ILE:HG21	1:1942:A:LEU:HG	17	0.13
(1,1979)	1:1941:A:ILE:HG22	1:1942:A:LEU:HG	17	0.13
(1,1979)	1:1941:A:ILE:HG23	1:1942:A:LEU:HG	17	0.13
(1,1978)	1:1941:A:ILE:H	1:1940:A:LYS:H	11	0.13
(1,1963)	1:1942:A:LEU:H	1:1941:A:ILE:HG12	6	0.13
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	2	0.13
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	4	0.13
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	6	0.13
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	16	0.13
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	17	0.13
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	18	0.13
(1,1931)	1:1821:A:ASP:H	1:1821:A:ASP:HB2	13	0.13
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	1	0.13
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	3	0.13
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	7	0.13
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	11	0.13
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	13	0.13
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	14	0.13
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	16	0.13
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	18	0.13
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	20	0.13
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	3	0.13
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	9	0.13
(1,1911)	1:1884:A:LEU:HA	1:1885:A:ARG:H	13	0.13
(1,1907)	1:1858:A:LYS:HA	1:1861:A:SER:HA	2	0.13
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE1	11	0.13
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE2	11	0.13
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE1	11	0.13
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE2	11	0.13
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE1	11	0.13
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE2	11	0.13
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE1	17	0.13
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE2	17	0.13
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE1	17	0.13
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE2	17	0.13
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE1	17	0.13
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE2	17	0.13
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE1	20	0.13
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE2	20	0.13
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE1	20	0.13
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE2	20	0.13
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE1	20	0.13
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE2	20	0.13
(1,1858)	1:1934:A:VAL:HA	1:1937:A:GLU:H	1	0.13
(1,1858)	1:1934:A:VAL:HA	1:1937:A:GLU:H	10	0.13
(1,1858)	1:1934:A:VAL:HA	1:1937:A:GLU:H	11	0.13
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	1	0.13
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	2	0.13
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	4	0.13
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	5	0.13
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	6	0.13
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	12	0.13
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	15	0.13
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	16	0.13
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	17	0.13
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	18	0.13
(1,1806)	1:1840:A:ILE:HB	1:1876:A:PHE:HZ	1	0.13
(1,1806)	1:1840:A:ILE:HB	1:1876:A:PHE:HZ	2	0.13
(1,1806)	1:1840:A:ILE:HB	1:1876:A:PHE:HZ	3	0.13
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD21	6	0.13
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD22	6	0.13
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD23	6	0.13
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD21	8	0.13
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD22	8	0.13
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD23	8	0.13
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD21	13	0.13
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD22	13	0.13
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD23	13	0.13
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD11	7	0.13
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD12	7	0.13
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD13	7	0.13
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD11	7	0.13
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD12	7	0.13
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD13	7	0.13
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD11	7	0.13
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD12	7	0.13
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD13	7	0.13
(1,1747)	1:1853:A:LEU:HD11	1:1856:A:TYR:HB2	8	0.13
(1,1747)	1:1853:A:LEU:HD12	1:1856:A:TYR:HB2	8	0.13
(1,1747)	1:1853:A:LEU:HD13	1:1856:A:TYR:HB2	8	0.13
(1,1747)	1:1853:A:LEU:HD11	1:1856:A:TYR:HB2	20	0.13
(1,1747)	1:1853:A:LEU:HD12	1:1856:A:TYR:HB2	20	0.13
(1,1747)	1:1853:A:LEU:HD13	1:1856:A:TYR:HB2	20	0.13
(1,1718)	1:1902:A:GLY:H	1:1901:A:THR:HA	16	0.13
(1,1700)	1:1922:A:ILE:HG12	1:1922:A:ILE:H	13	0.13
(1,1689)	1:1928:A:GLU:H	1:1927:A:GLY:HA2	10	0.13
(1,1689)	1:1928:A:GLU:H	1:1927:A:GLY:HA2	16	0.13
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	2	0.13
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	2	0.13
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	8	0.13
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	8	0.13
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	9	0.13
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	9	0.13
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	11	0.13
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	11	0.13
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	16	0.13
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	16	0.13
(1,1624)	1:1941:A:ILE:HA	1:1944:A:GLN:HB2	4	0.13
(1,1624)	1:1941:A:ILE:HA	1:1944:A:GLN:HB3	4	0.13
(1,1619)	1:1887:A:ILE:HG21	1:1890:A:GLU:HB2	5	0.13
(1,1619)	1:1887:A:ILE:HG22	1:1890:A:GLU:HB2	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1619)	1:1887:A:ILE:HG23	1:1890:A:GLU:HB2	5	0.13
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG21	8	0.13
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG22	8	0.13
(1,1600)	1:1925:A:THR:H	1:1925:A:THR:HG23	8	0.13
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD11	18	0.13
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD12	18	0.13
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD13	18	0.13
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD11	18	0.13
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD12	18	0.13
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD13	18	0.13
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE2	19	0.13
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE3	19	0.13
(1,1582)	1:1884:A:LEU:HD11	1:1853:A:LEU:HA	7	0.13
(1,1582)	1:1884:A:LEU:HD12	1:1853:A:LEU:HA	7	0.13
(1,1582)	1:1884:A:LEU:HD13	1:1853:A:LEU:HA	7	0.13
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	14	0.13
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	14	0.13
(1,1567)	1:1894:A:LYS:H	1:1894:A:LYS:HD2	12	0.13
(1,1556)	1:1853:A:LEU:HD11	1:1857:A:LYS:HD2	9	0.13
(1,1556)	1:1853:A:LEU:HD12	1:1857:A:LYS:HD2	9	0.13
(1,1556)	1:1853:A:LEU:HD13	1:1857:A:LYS:HD2	9	0.13
(1,1532)	1:1822:A:GLU:HG3	1:1823:A:LYS:H	8	0.13
(1,1514)	1:1896:A:ARG:HB2	1:1889:A:MET:HE1	11	0.13
(1,1514)	1:1896:A:ARG:HB2	1:1889:A:MET:HE2	11	0.13
(1,1514)	1:1896:A:ARG:HB2	1:1889:A:MET:HE3	11	0.13
(1,1514)	1:1896:A:ARG:HB2	1:1889:A:MET:HE1	20	0.13
(1,1514)	1:1896:A:ARG:HB2	1:1889:A:MET:HE2	20	0.13
(1,1514)	1:1896:A:ARG:HB2	1:1889:A:MET:HE3	20	0.13
(1,1479)	1:1867:A:PRO:HD2	1:1868:A:PHE:H	16	0.13
(1,1479)	1:1867:A:PRO:HD2	1:1868:A:PHE:H	19	0.13
(1,1462)	1:1924:A:ASN:HB3	1:1924:A:ASN:HA	17	0.13
(1,1458)	1:1955:A:ASP:H	1:1954:A:ASP:HA	19	0.13
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	6	0.13
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	1	0.13
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	1	0.13
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	3	0.13
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	3	0.13
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	12	0.13
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	12	0.13
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	13	0.13
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	13	0.13
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	15	0.13
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	17	0.13
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	17	0.13
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	18	0.13
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	18	0.13
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	3	0.13
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	3	0.13
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	6	0.13
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	6	0.13
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	7	0.13
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	7	0.13
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	10	0.13
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	10	0.13
(1,1379)	1:1939:A:LEU:HD11	1:1839:A:LYS:HB2	20	0.13
(1,1379)	1:1939:A:LEU:HD12	1:1839:A:LYS:HB2	20	0.13
(1,1379)	1:1939:A:LEU:HD13	1:1839:A:LYS:HB2	20	0.13
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD21	6	0.13
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD22	6	0.13
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD23	6	0.13
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD21	6	0.13
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD22	6	0.13
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD23	6	0.13
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD21	6	0.13
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD22	6	0.13
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD23	6	0.13
(1,1342)	1:1859:A:LYS:H	1:1858:A:LYS:HG3	4	0.13
(1,1342)	1:1859:A:LYS:H	1:1858:A:LYS:HG3	14	0.13
(1,1308)	1:1882:A:ARG:H	1:1883:A:GLY:H	17	0.13
(1,1307)	1:1821:A:ASP:HA	1:1823:A:LYS:H	7	0.13
(1,1305)	1:1837:A:PHE:HE1	1:1876:A:PHE:HE1	10	0.13
(1,1305)	1:1837:A:PHE:HE1	1:1876:A:PHE:HE2	10	0.13
(1,1305)	1:1837:A:PHE:HE2	1:1876:A:PHE:HE1	10	0.13
(1,1305)	1:1837:A:PHE:HE2	1:1876:A:PHE:HE2	10	0.13
(1,1272)	1:1895:A:GLY:H	1:1893:A:GLY:H	9	0.13
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG21	19	0.13
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG22	19	0.13
(1,1265)	1:1822:A:GLU:H	1:1820:A:ILE:HG23	19	0.13
(1,1255)	1:1865:A:ILE:HD11	1:1857:A:LYS:HE2	18	0.13
(1,1255)	1:1865:A:ILE:HD12	1:1857:A:LYS:HE2	18	0.13
(1,1255)	1:1865:A:ILE:HD13	1:1857:A:LYS:HE2	18	0.13
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	1	0.13
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	1	0.13
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	6	0.13
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	6	0.13
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	6	0.13
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	7	0.13
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	7	0.13
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	7	0.13
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	9	0.13
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	9	0.13
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	9	0.13
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	10	0.13
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	10	0.13
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	10	0.13
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	5	0.13
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	5	0.13
(1,1206)	1:1845:A:ASN:HB2	1:1842:A:SER:HB3	9	0.13
(1,1206)	1:1845:A:ASN:HB3	1:1842:A:SER:HB3	9	0.13
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD11	2	0.13
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD12	2	0.13
(1,1196)	1:1900:A:SER:HB3	1:1903:A:ILE:HD13	2	0.13
(1,1131)	1:1824:A:SER:H	1:1827:A:ALA:HB1	11	0.13
(1,1131)	1:1824:A:SER:H	1:1827:A:ALA:HB2	11	0.13
(1,1131)	1:1824:A:SER:H	1:1827:A:ALA:HB3	11	0.13
(1,1098)	1:1905:A:PRO:HD2	1:1904:A:SER:HB2	3	0.13
(1,1098)	1:1905:A:PRO:HD2	1:1904:A:SER:HB3	3	0.13
(1,1098)	1:1905:A:PRO:HD2	1:1904:A:SER:HB2	20	0.13
(1,1098)	1:1905:A:PRO:HD2	1:1904:A:SER:HB3	20	0.13
(1,1090)	1:1852:A:GLU:H	1:1850:A:LEU:H	7	0.13
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB2	4	0.13
(1,1086)	1:1874:A:GLN:HA	1:1874:A:GLN:HB3	4	0.13
(1,1080)	1:1847:A:LYS:HA	1:1850:A:LEU:HB2	17	0.13
(1,1056)	1:1927:A:GLY:H	1:1926:A:ASN:HA	17	0.13
(1,1028)	1:1886:A:VAL:HA	1:1888:A:GLU:H	10	0.13
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	1	0.13
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	2	0.13
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	3	0.13
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	3	0.13
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	3	0.13
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	14	0.13
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	14	0.13
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	14	0.13
(1,1000)	1:1917:A:SER:HA	1:1918:A:THR:H	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:1889:A:MET:HE1	1:1885:A:ARG:HG2	5	0.13
(1,994)	1:1889:A:MET:HE2	1:1885:A:ARG:HG2	5	0.13
(1,994)	1:1889:A:MET:HE3	1:1885:A:ARG:HG2	5	0.13
(1,986)	1:1837:A:PHE:H	1:1840:A:ILE:H	10	0.13
(1,986)	1:1837:A:PHE:H	1:1840:A:ILE:H	15	0.13
(1,972)	1:1952:A:LYS:H	1:1951:A:THR:HB	19	0.13
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	1	0.13
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	3	0.13
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	4	0.13
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	5	0.13
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	6	0.13
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	8	0.13
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	9	0.13
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	12	0.13
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	13	0.13
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	15	0.13
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	17	0.13
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	18	0.13
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	20	0.13
(1,952)	1:1949:A:ASP:HA	1:1949:A:ASP:HB3	9	0.13
(1,952)	1:1949:A:ASP:HA	1:1949:A:ASP:HB3	20	0.13
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB2	5	0.13
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB3	5	0.13
(1,897)	1:1946:A:CYS:H	1:1945:A:ARG:HB2	16	0.13
(1,897)	1:1946:A:CYS:H	1:1945:A:ARG:HB2	17	0.13
(1,897)	1:1946:A:CYS:H	1:1945:A:ARG:HB2	18	0.13
(1,889)	1:1889:A:MET:H	1:1892:A:GLU:HG3	3	0.13
(1,889)	1:1889:A:MET:H	1:1892:A:GLU:HG3	9	0.13
(1,889)	1:1889:A:MET:H	1:1892:A:GLU:HG3	15	0.13
(1,888)	1:1887:A:ILE:HA	1:1890:A:GLU:HG2	9	0.13
(1,888)	1:1887:A:ILE:HA	1:1890:A:GLU:HG2	19	0.13
(1,874)	1:1823:A:LYS:H	1:1820:A:ILE:HG21	15	0.13
(1,874)	1:1823:A:LYS:H	1:1820:A:ILE:HG22	15	0.13
(1,874)	1:1823:A:LYS:H	1:1820:A:ILE:HG23	15	0.13
(1,871)	1:1866:A:GLU:HA	1:1868:A:PHE:H	20	0.13
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	14	0.13
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	14	0.13
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	14	0.13
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	14	0.13
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	14	0.13
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	14	0.13
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	14	0.13
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	14	0.13
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD11	15	0.13
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD12	15	0.13
(1,858)	1:1840:A:ILE:HD11	1:1850:A:LEU:HD13	15	0.13
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD11	15	0.13
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD12	15	0.13
(1,858)	1:1840:A:ILE:HD12	1:1850:A:LEU:HD13	15	0.13
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD11	15	0.13
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD12	15	0.13
(1,858)	1:1840:A:ILE:HD13	1:1850:A:LEU:HD13	15	0.13
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	3	0.13
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	6	0.13
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	7	0.13
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	10	0.13
(1,828)	1:1851:A:ALA:HB1	1:1852:A:GLU:HG2	1	0.13
(1,828)	1:1851:A:ALA:HB2	1:1852:A:GLU:HG2	1	0.13
(1,828)	1:1851:A:ALA:HB3	1:1852:A:GLU:HG2	1	0.13
(1,828)	1:1851:A:ALA:HB1	1:1852:A:GLU:HG2	4	0.13
(1,828)	1:1851:A:ALA:HB2	1:1852:A:GLU:HG2	4	0.13
(1,828)	1:1851:A:ALA:HB3	1:1852:A:GLU:HG2	4	0.13
(1,828)	1:1851:A:ALA:HB1	1:1852:A:GLU:HG2	5	0.13
(1,828)	1:1851:A:ALA:HB2	1:1852:A:GLU:HG2	5	0.13
(1,828)	1:1851:A:ALA:HB3	1:1852:A:GLU:HG2	5	0.13
(1,828)	1:1851:A:ALA:HB1	1:1852:A:GLU:HG2	13	0.13
(1,828)	1:1851:A:ALA:HB2	1:1852:A:GLU:HG2	13	0.13
(1,828)	1:1851:A:ALA:HB3	1:1852:A:GLU:HG2	13	0.13
(1,828)	1:1851:A:ALA:HB1	1:1852:A:GLU:HG2	17	0.13
(1,828)	1:1851:A:ALA:HB2	1:1852:A:GLU:HG2	17	0.13
(1,828)	1:1851:A:ALA:HB3	1:1852:A:GLU:HG2	17	0.13
(1,828)	1:1851:A:ALA:HB1	1:1852:A:GLU:HG2	19	0.13
(1,828)	1:1851:A:ALA:HB2	1:1852:A:GLU:HG2	19	0.13
(1,828)	1:1851:A:ALA:HB3	1:1852:A:GLU:HG2	19	0.13
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	3	0.13
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	14	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	1	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	1	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	1	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	2	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	2	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	2	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	8	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	8	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	12	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	12	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	12	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	15	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	15	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	15	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	17	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	17	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	17	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	20	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	20	0.13
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	20	0.13
(1,815)	1:1911:A:CYS:HA	1:1912:A:VAL:HG11	4	0.13
(1,815)	1:1911:A:CYS:HA	1:1912:A:VAL:HG12	4	0.13
(1,815)	1:1911:A:CYS:HA	1:1912:A:VAL:HG13	4	0.13
(1,781)	1:1819:A:ARG:HB2	1:1819:A:ARG:HA	17	0.13
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG21	2	0.13
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG22	2	0.13
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG23	2	0.13
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG21	2	0.13
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG22	2	0.13
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG23	2	0.13
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG21	2	0.13
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG22	2	0.13
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG23	2	0.13
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG21	9	0.13
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG22	9	0.13
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG23	9	0.13
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG21	9	0.13
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG22	9	0.13
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG23	9	0.13
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG21	9	0.13
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG22	9	0.13
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG23	9	0.13
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG21	11	0.13
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG22	11	0.13
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG23	11	0.13
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG21	11	0.13
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG22	11	0.13
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG23	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG21	11	0.13
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG22	11	0.13
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG23	11	0.13
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	7	0.13
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	7	0.13
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	7	0.13
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	7	0.13
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	7	0.13
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	7	0.13
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	8	0.13
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	8	0.13
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	8	0.13
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	8	0.13
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	8	0.13
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	8	0.13
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	11	0.13
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	11	0.13
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	11	0.13
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	11	0.13
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	11	0.13
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	11	0.13
(1,736)	1:1898:A:SER:H	1:1897:A:ILE:H	11	0.13
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG21	6	0.13
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG22	6	0.13
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG23	6	0.13
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG21	17	0.13
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG22	17	0.13
(1,730)	1:1910:A:THR:HB	1:1914:A:THR:HG23	17	0.13
(1,724)	1:1956:A:ARG:H	1:1955:A:ASP:HA	19	0.13
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	2	0.13
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	5	0.13
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	8	0.13
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	19	0.13
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	1	0.13
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	2	0.13
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	8	0.13
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	12	0.13
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	13	0.13
(1,669)	1:1890:A:GLU:H	1:1890:A:GLU:HG3	11	0.13
(1,632)	1:1949:A:ASP:H	1:1949:A:ASP:HB3	1	0.13
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	2	0.13
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	5	0.13
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	18	0.13
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	20	0.13
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	1	0.13
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	3	0.13
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	4	0.13
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	5	0.13
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	19	0.13
(1,610)	1:1950:A:ASN:HB2	1:1950:A:ASN:HD21	2	0.13
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	1	0.13
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	1	0.13
(1,595)	1:1823:A:LYS:HA	1:1823:A:LYS:HB2	13	0.13
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	2	0.13
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	12	0.13
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	11	0.13
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	16	0.13
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	16	0.13
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	16	0.13
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD11	19	0.13
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD12	19	0.13
(1,549)	1:1877:A:GLN:H	1:1869:A:LEU:HD13	19	0.13
(1,526)	1:1885:A:ARG:HA	1:1888:A:GLU:HG2	3	0.13
(1,526)	1:1885:A:ARG:HA	1:1888:A:GLU:HG2	7	0.13
(1,526)	1:1885:A:ARG:HA	1:1888:A:GLU:HG2	9	0.13
(1,526)	1:1885:A:ARG:HA	1:1888:A:GLU:HG2	16	0.13
(1,516)	1:1886:A:VAL:HG21	1:1882:A:ARG:HG3	1	0.13
(1,516)	1:1886:A:VAL:HG22	1:1882:A:ARG:HG3	1	0.13
(1,516)	1:1886:A:VAL:HG23	1:1882:A:ARG:HG3	1	0.13
(1,509)	1:1865:A:ILE:HG21	1:1866:A:GLU:H	11	0.13
(1,509)	1:1865:A:ILE:HG22	1:1866:A:GLU:H	11	0.13
(1,509)	1:1865:A:ILE:HG23	1:1866:A:GLU:H	11	0.13
(1,509)	1:1865:A:ILE:HG21	1:1866:A:GLU:H	17	0.13
(1,509)	1:1865:A:ILE:HG22	1:1866:A:GLU:H	17	0.13
(1,509)	1:1865:A:ILE:HG23	1:1866:A:GLU:H	17	0.13
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	3	0.13
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	8	0.13
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	13	0.13
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	1	0.13
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	8	0.13
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	13	0.13
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	14	0.13
(1,461)	1:1845:A:ASN:HD21	1:1839:A:LYS:HG3	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:1896:A:ARG:HB2	1:1890:A:GLU:HG2	12	0.13
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	16	0.13
(1,416)	1:1955:A:ASP:H	1:1954:A:ASP:H	7	0.13
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	6	0.13
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	6	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	1	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	1	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	1	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	2	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	2	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	2	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	3	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	3	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	3	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	4	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	4	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	4	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	5	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	5	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	5	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	7	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	7	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	7	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	8	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	8	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	8	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	9	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	9	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	9	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	10	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	10	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	10	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	11	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	11	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	11	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	12	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	12	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	12	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	13	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	13	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	13	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	14	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	14	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	15	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	15	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	15	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	16	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	16	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	16	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	17	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	17	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	17	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	18	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	18	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	18	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	19	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	19	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	19	0.13
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	20	0.13
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	20	0.13
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	20	0.13
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	1	0.13
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	2	0.13
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	5	0.13
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	17	0.13
(1,375)	1:1896:A:ARG:HG2	1:1896:A:ARG:HD2	6	0.13
(1,375)	1:1896:A:ARG:HG2	1:1896:A:ARG:HD3	6	0.13
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	13	0.13
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	13	0.13
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD2	19	0.13
(1,355)	1:1858:A:LYS:HG2	1:1858:A:LYS:HD3	19	0.13
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	3	0.13
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	9	0.13
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	10	0.13
(1,346)	1:1835:A:GLU:H	1:1833:A:LEU:HB3	20	0.13
(1,336)	1:1932:A:PRO:HD2	1:1930:A:VAL:HA	17	0.13
(1,330)	1:1827:A:ALA:H	1:1826:A:LYS:HB3	9	0.13
(1,330)	1:1827:A:ALA:H	1:1826:A:LYS:HB3	11	0.13
(1,324)	1:1889:A:MET:HE1	1:1896:A:ARG:HD2	10	0.13
(1,324)	1:1889:A:MET:HE2	1:1896:A:ARG:HD2	10	0.13
(1,324)	1:1889:A:MET:HE3	1:1896:A:ARG:HD2	10	0.13
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	1	0.13
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	15	0.13
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	16	0.13
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	17	0.13
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG11	8	0.13
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG12	8	0.13
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG13	8	0.13
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	7	0.13
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	7	0.13
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	10	0.13
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	10	0.13
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	12	0.13
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	12	0.13
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	20	0.13
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	20	0.13
(1,258)	1:1941:A:ILE:HA	1:1941:A:ILE:HG13	3	0.13
(1,258)	1:1941:A:ILE:HA	1:1941:A:ILE:HG13	4	0.13
(1,258)	1:1941:A:ILE:HA	1:1941:A:ILE:HG13	5	0.13
(1,258)	1:1941:A:ILE:HA	1:1941:A:ILE:HG13	14	0.13
(1,258)	1:1941:A:ILE:HA	1:1941:A:ILE:HG13	15	0.13
(1,258)	1:1941:A:ILE:HA	1:1941:A:ILE:HG13	16	0.13
(1,258)	1:1941:A:ILE:HA	1:1941:A:ILE:HG13	19	0.13
(1,258)	1:1941:A:ILE:HA	1:1941:A:ILE:HG13	20	0.13
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	8	0.13
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	8	0.13
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	9	0.13
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	9	0.13
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	10	0.13
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	10	0.13
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	14	0.13
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	14	0.13
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD11	9	0.13
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD12	9	0.13
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD13	9	0.13
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD11	19	0.13
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD12	19	0.13
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD13	19	0.13
(1,239)	1:1896:A:ARG:H	1:1897:A:ILE:HB	9	0.13
(1,239)	1:1896:A:ARG:H	1:1897:A:ILE:HB	14	0.13
(1,229)	1:1823:A:LYS:HA	1:1826:A:LYS:HE2	10	0.13
(1,229)	1:1823:A:LYS:HA	1:1826:A:LYS:HE3	10	0.13
(1,215)	1:1828:A:LYS:HA	1:1831:A:ASP:HB2	16	0.13
(1,195)	1:1844:A:GLU:HA	1:1846:A:THR:HG21	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,195)	1:1844:A:GLU:HA	1:1846:A:THR:HG22	15	0.13
(1,195)	1:1844:A:GLU:HA	1:1846:A:THR:HG23	15	0.13
(1,178)	1:1851:A:ALA:HB1	1:1887:A:ILE:HD11	7	0.13
(1,178)	1:1851:A:ALA:HB1	1:1887:A:ILE:HD12	7	0.13
(1,178)	1:1851:A:ALA:HB1	1:1887:A:ILE:HD13	7	0.13
(1,178)	1:1851:A:ALA:HB2	1:1887:A:ILE:HD11	7	0.13
(1,178)	1:1851:A:ALA:HB2	1:1887:A:ILE:HD12	7	0.13
(1,178)	1:1851:A:ALA:HB2	1:1887:A:ILE:HD13	7	0.13
(1,178)	1:1851:A:ALA:HB3	1:1887:A:ILE:HD11	7	0.13
(1,178)	1:1851:A:ALA:HB3	1:1887:A:ILE:HD12	7	0.13
(1,178)	1:1851:A:ALA:HB3	1:1887:A:ILE:HD13	7	0.13
(1,116)	1:1948:A:LEU:H	1:1949:A:ASP:H	12	0.13
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	11	0.13
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	16	0.13
(1,96)	1:1828:A:LYS:HA	1:1831:A:ASP:HB3	17	0.13
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	1	0.13
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	6	0.13
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	7	0.13
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	19	0.13
(3,46)	1:1935:A:TYR:N	1:1931:A:GLY:O	4	0.12
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG21	8	0.12
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG22	8	0.12
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG23	8	0.12
(1,3258)	1:1862:A:ASP:HA	1:1865:A:ILE:HB	1	0.12
(1,3258)	1:1862:A:ASP:HA	1:1865:A:ILE:HB	15	0.12
(1,3255)	1:1926:A:ASN:H	1:1925:A:THR:HA	4	0.12
(1,3246)	1:1904:A:SER:H	1:1905:A:PRO:HD2	6	0.12
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	3	0.12
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	4	0.12
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	7	0.12
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	8	0.12
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	20	0.12
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	5	0.12
(1,3234)	1:1877:A:GLN:HG3	1:1877:A:GLN:HE22	9	0.12
(1,3186)	1:1903:A:ILE:H	1:1902:A:GLY:H	4	0.12
(1,3186)	1:1903:A:ILE:H	1:1902:A:GLY:H	16	0.12
(1,3172)	1:1902:A:GLY:H	1:1901:A:THR:HB	5	0.12
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG2	1	0.12
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG3	1	0.12
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG2	2	0.12
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG3	2	0.12
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG2	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG3	3	0.12
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG2	5	0.12
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG3	5	0.12
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG2	6	0.12
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG3	6	0.12
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG2	12	0.12
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG3	12	0.12
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG2	13	0.12
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG3	13	0.12
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG2	15	0.12
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG3	15	0.12
(1,3168)	1:1874:A:GLN:HB2	1:1874:A:GLN:HG2	4	0.12
(1,3168)	1:1874:A:GLN:HB2	1:1874:A:GLN:HG2	16	0.12
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	7	0.12
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	17	0.12
(1,3159)	1:1822:A:GLU:H	1:1822:A:GLU:HG2	1	0.12
(1,3159)	1:1822:A:GLU:H	1:1822:A:GLU:HG2	11	0.12
(1,3159)	1:1822:A:GLU:H	1:1822:A:GLU:HG2	14	0.12
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD1	4	0.12
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD2	4	0.12
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD1	19	0.12
(1,3157)	1:1875:A:PHE:HA	1:1875:A:PHE:HD2	19	0.12
(1,3142)	1:1900:A:SER:H	1:1900:A:SER:HA	6	0.12
(1,3134)	1:1852:A:GLU:HG2	1:1852:A:GLU:HB3	7	0.12
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	2	0.12
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	2	0.12
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	2	0.12
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	2	0.12
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	6	0.12
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	8	0.12
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	15	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	1	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	1	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	1	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	1	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	2	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	2	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	2	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	2	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	3	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	3	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	3	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	4	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	4	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	4	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	4	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	5	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	5	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	5	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	5	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	6	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	6	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	6	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	6	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	7	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	7	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	7	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	7	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	8	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	8	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	8	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	8	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	9	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	9	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	9	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	9	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	10	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	10	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	10	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	10	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	11	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	11	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	11	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	11	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	12	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	12	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	12	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	12	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	13	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	13	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	13	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	13	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	14	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	14	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	14	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	15	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	15	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	15	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	15	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	16	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	16	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	16	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	16	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	17	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	17	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	17	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	17	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	18	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	18	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	18	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	18	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	19	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	19	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	19	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	19	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB2	20	0.12
(1,3113)	1:1835:A:GLU:HG2	1:1835:A:GLU:HB3	20	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB2	20	0.12
(1,3113)	1:1835:A:GLU:HG3	1:1835:A:GLU:HB3	20	0.12
(1,3111)	1:1931:A:GLY:H	1:1930:A:VAL:HB	5	0.12
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	20	0.12
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	3	0.12
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	3	0.12
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	10	0.12
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	10	0.12
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	8	0.12
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	8	0.12
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	11	0.12
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	11	0.12
(1,3077)	1:1884:A:LEU:HA	1:1888:A:GLU:H	11	0.12
(1,3075)	1:1942:A:LEU:HB3	1:1838:A:LYS:HG3	3	0.12
(1,3075)	1:1942:A:LEU:HB3	1:1838:A:LYS:HG3	18	0.12
(1,3032)	1:1835:A:GLU:H	1:1833:A:LEU:HB2	2	0.12
(1,3032)	1:1835:A:GLU:H	1:1833:A:LEU:HB2	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3022)	1:1885:A:ARG:HB3	1:1885:A:ARG:HD3	1	0.12
(1,3020)	1:1948:A:LEU:HA	1:1949:A:ASP:H	1	0.12
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG21	1	0.12
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG22	1	0.12
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG23	1	0.12
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG21	1	0.12
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG22	1	0.12
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG23	1	0.12
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG21	1	0.12
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG22	1	0.12
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG23	1	0.12
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG21	9	0.12
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG22	9	0.12
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG23	9	0.12
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG21	9	0.12
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG22	9	0.12
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG23	9	0.12
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG21	9	0.12
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG22	9	0.12
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG23	9	0.12
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG21	10	0.12
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG22	10	0.12
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG23	10	0.12
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG21	10	0.12
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG22	10	0.12
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG23	10	0.12
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG21	10	0.12
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG22	10	0.12
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG23	10	0.12
(1,3015)	1:1938:A:ARG:HB2	1:1845:A:ASN:HD21	6	0.12
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD11	1	0.12
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD12	1	0.12
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD13	1	0.12
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD11	3	0.12
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD12	3	0.12
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD13	3	0.12
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD11	13	0.12
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD12	13	0.12
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD13	13	0.12
(1,2975)	1:1892:A:GLU:H	1:1891:A:ARG:HG3	2	0.12
(1,2975)	1:1892:A:GLU:H	1:1891:A:ARG:HG3	16	0.12
(1,2974)	1:1930:A:VAL:H	1:1929:A:GLU:HB3	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2973)	1:1870:A:LYS:HA	1:1874:A:GLN:HE21	7	0.12
(1,2973)	1:1870:A:LYS:HA	1:1874:A:GLN:HE21	17	0.12
(1,2940)	1:1857:A:LYS:HB2	1:1865:A:ILE:HD11	2	0.12
(1,2940)	1:1857:A:LYS:HB2	1:1865:A:ILE:HD12	2	0.12
(1,2940)	1:1857:A:LYS:HB2	1:1865:A:ILE:HD13	2	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	5	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	5	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	5	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	8	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	8	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	8	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	11	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	11	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	11	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	14	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	14	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	14	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	18	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	18	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	18	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD21	20	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD22	20	0.12
(1,2939)	1:1937:A:GLU:H	1:1936:A:LEU:HD23	20	0.12
(1,2929)	1:1922:A:ILE:HA	1:1922:A:ILE:HB	2	0.12
(1,2929)	1:1922:A:ILE:HA	1:1922:A:ILE:HB	4	0.12
(1,2929)	1:1922:A:ILE:HA	1:1922:A:ILE:HB	5	0.12
(1,2929)	1:1922:A:ILE:HA	1:1922:A:ILE:HB	6	0.12
(1,2929)	1:1922:A:ILE:HA	1:1922:A:ILE:HB	12	0.12
(1,2929)	1:1922:A:ILE:HA	1:1922:A:ILE:HB	16	0.12
(1,2929)	1:1922:A:ILE:HA	1:1922:A:ILE:HB	17	0.12
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	6	0.12
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	14	0.12
(1,2918)	1:1858:A:LYS:H	1:1857:A:LYS:HB3	20	0.12
(1,2907)	1:1894:A:LYS:H	1:1894:A:LYS:HE3	1	0.12
(1,2893)	1:1887:A:ILE:HA	1:1890:A:GLU:HB2	7	0.12
(1,2893)	1:1887:A:ILE:HA	1:1890:A:GLU:HB2	11	0.12
(1,2893)	1:1887:A:ILE:HA	1:1890:A:GLU:HB2	12	0.12
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD21	2	0.12
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD22	2	0.12
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD23	2	0.12
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD21	13	0.12
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD22	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2892)	1:1839:A:LYS:HA	1:1942:A:LEU:HD23	13	0.12
(1,2886)	1:1905:A:PRO:HD2	1:1905:A:PRO:HB2	13	0.12
(1,2886)	1:1905:A:PRO:HD2	1:1905:A:PRO:HB2	16	0.12
(1,2877)	1:1897:A:ILE:H	1:1895:A:GLY:HA2	2	0.12
(1,2877)	1:1897:A:ILE:H	1:1895:A:GLY:HA3	2	0.12
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	1	0.12
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	1	0.12
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	1	0.12
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	1	0.12
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	1	0.12
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	1	0.12
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	1	0.12
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	1	0.12
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	1	0.12
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	5	0.12
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	5	0.12
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	5	0.12
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	5	0.12
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	5	0.12
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	5	0.12
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	5	0.12
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	5	0.12
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	5	0.12
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	4	0.12
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	5	0.12
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	7	0.12
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	9	0.12
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	11	0.12
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	19	0.12
(1,2859)	1:1943:A:ARG:HA	1:1838:A:LYS:HE2	15	0.12
(1,2842)	1:1950:A:ASN:HB2	1:1951:A:THR:H	18	0.12
(1,2818)	1:1886:A:VAL:H	1:1885:A:ARG:HG3	7	0.12
(1,2818)	1:1886:A:VAL:H	1:1885:A:ARG:HG3	17	0.12
(1,2807)	1:1889:A:MET:H	1:1888:A:GLU:HB2	9	0.12
(1,2807)	1:1889:A:MET:H	1:1888:A:GLU:HB2	11	0.12
(1,2807)	1:1889:A:MET:H	1:1888:A:GLU:HB2	15	0.12
(1,2801)	1:1874:A:GLN:HA	1:1874:A:GLN:HG2	8	0.12
(1,2801)	1:1874:A:GLN:HA	1:1874:A:GLN:HG2	11	0.12
(1,2801)	1:1874:A:GLN:HA	1:1874:A:GLN:HG2	17	0.12
(1,2801)	1:1874:A:GLN:HA	1:1874:A:GLN:HG2	18	0.12
(1,2801)	1:1874:A:GLN:HA	1:1874:A:GLN:HG2	19	0.12
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	4	0.12
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	4	0.12
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	14	0.12
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	14	0.12
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	14	0.12
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD21	20	0.12
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD22	20	0.12
(1,2781)	1:1836:A:ILE:H	1:1939:A:LEU:HD23	20	0.12
(1,2765)	1:1878:A:SER:HA	1:1881:A:GLU:HG3	6	0.12
(1,2765)	1:1878:A:SER:HA	1:1881:A:GLU:HG3	17	0.12
(1,2760)	1:1903:A:ILE:HA	1:1903:A:ILE:HG12	14	0.12
(1,2737)	1:1823:A:LYS:HA	1:1824:A:SER:H	17	0.12
(1,2731)	1:1916:A:THR:HG21	1:1914:A:THR:HB	13	0.12
(1,2731)	1:1916:A:THR:HG22	1:1914:A:THR:HB	13	0.12
(1,2731)	1:1916:A:THR:HG23	1:1914:A:THR:HB	13	0.12
(1,2710)	1:1899:A:THR:H	1:1898:A:SER:HA	11	0.12
(1,2710)	1:1899:A:THR:H	1:1898:A:SER:HA	19	0.12
(1,2685)	1:1859:A:LYS:HA	1:1859:A:LYS:HG3	7	0.12
(1,2685)	1:1859:A:LYS:HA	1:1859:A:LYS:HG3	8	0.12
(1,2685)	1:1859:A:LYS:HA	1:1859:A:LYS:HG3	11	0.12
(1,2685)	1:1859:A:LYS:HA	1:1859:A:LYS:HG3	12	0.12
(1,2685)	1:1859:A:LYS:HA	1:1859:A:LYS:HG3	17	0.12
(1,2685)	1:1859:A:LYS:HA	1:1859:A:LYS:HG3	19	0.12
(1,2682)	1:1826:A:LYS:HB2	1:1871:A:ASN:HD22	15	0.12
(1,2682)	1:1826:A:LYS:HB2	1:1871:A:ASN:HD22	19	0.12
(1,2648)	1:1853:A:LEU:HA	1:1856:A:TYR:HB3	2	0.12
(1,2648)	1:1853:A:LEU:HA	1:1856:A:TYR:HB3	5	0.12
(1,2648)	1:1853:A:LEU:HA	1:1856:A:TYR:HB3	20	0.12
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE1	10	0.12
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE2	10	0.12
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE1	10	0.12
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE2	10	0.12
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE1	10	0.12
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE2	10	0.12
(1,2631)	1:1929:A:GLU:HB2	1:1930:A:VAL:H	9	0.12
(1,2624)	1:1882:A:ARG:HG3	1:1882:A:ARG:HD2	2	0.12
(1,2624)	1:1882:A:ARG:HG3	1:1882:A:ARG:HD3	2	0.12
(1,2624)	1:1882:A:ARG:HG3	1:1882:A:ARG:HD2	6	0.12
(1,2624)	1:1882:A:ARG:HG3	1:1882:A:ARG:HD3	6	0.12
(1,2624)	1:1882:A:ARG:HG3	1:1882:A:ARG:HD2	8	0.12
(1,2624)	1:1882:A:ARG:HG3	1:1882:A:ARG:HD3	8	0.12
(1,2606)	1:1840:A:ILE:HD11	1:1850:A:LEU:HA	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:1840:A:ILE:HD12	1:1850:A:LEU:HA	2	0.12
(1,2606)	1:1840:A:ILE:HD13	1:1850:A:LEU:HA	2	0.12
(1,2606)	1:1840:A:ILE:HD11	1:1850:A:LEU:HA	18	0.12
(1,2606)	1:1840:A:ILE:HD12	1:1850:A:LEU:HA	18	0.12
(1,2606)	1:1840:A:ILE:HD13	1:1850:A:LEU:HA	18	0.12
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	5	0.12
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	8	0.12
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	9	0.12
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	15	0.12
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	19	0.12
(1,2580)	1:1929:A:GLU:H	1:1928:A:GLU:HG2	1	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	1	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	1	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	2	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	2	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	3	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	3	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	4	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	4	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	5	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	5	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	6	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	6	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	7	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	7	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	8	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	8	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	9	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	9	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	10	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	10	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	11	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	11	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	12	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	12	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	13	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	13	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	14	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	14	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	16	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	16	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	17	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	18	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	18	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	19	0.12
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	19	0.12
(1,2564)	1:1909:A:VAL:H	1:1910:A:THR:H	3	0.12
(1,2564)	1:1909:A:VAL:H	1:1910:A:THR:H	17	0.12
(1,2559)	1:1892:A:GLU:H	1:1890:A:GLU:HA	11	0.12
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	4	0.12
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	1	0.12
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	7	0.12
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	17	0.12
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	19	0.12
(1,2515)	1:1898:A:SER:H	1:1897:A:ILE:HB	3	0.12
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	1	0.12
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	3	0.12
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	5	0.12
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	6	0.12
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	7	0.12
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	10	0.12
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	16	0.12
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	18	0.12
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	19	0.12
(1,2502)	1:1892:A:GLU:HG3	1:1892:A:GLU:HB3	1	0.12
(1,2502)	1:1892:A:GLU:HG3	1:1892:A:GLU:HB3	15	0.12
(1,2490)	1:1820:A:ILE:HD11	1:1821:A:ASP:H	15	0.12
(1,2490)	1:1820:A:ILE:HD12	1:1821:A:ASP:H	15	0.12
(1,2490)	1:1820:A:ILE:HD13	1:1821:A:ASP:H	15	0.12
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	2	0.12
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	4	0.12
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	5	0.12
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	8	0.12
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	9	0.12
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	10	0.12
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	13	0.12
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	18	0.12
(1,2483)	1:1908:A:GLU:H	1:1908:A:GLU:HG2	2	0.12
(1,2483)	1:1908:A:GLU:H	1:1908:A:GLU:HG2	4	0.12
(1,2483)	1:1908:A:GLU:H	1:1908:A:GLU:HG2	9	0.12
(1,2483)	1:1908:A:GLU:H	1:1908:A:GLU:HG2	19	0.12
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE1	11	0.12
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE2	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE1	18	0.12
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE2	18	0.12
(1,2451)	1:1861:A:SER:H	1:1860:A:TYR:HB3	2	0.12
(1,2451)	1:1861:A:SER:H	1:1860:A:TYR:HB3	16	0.12
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	12	0.12
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	14	0.12
(1,2428)	1:1848:A:GLU:H	1:1847:A:LYS:HB2	20	0.12
(1,2426)	1:1907:A:MET:HA	1:1908:A:GLU:H	4	0.12
(1,2426)	1:1907:A:MET:HA	1:1908:A:GLU:H	9	0.12
(1,2426)	1:1907:A:MET:HA	1:1908:A:GLU:H	13	0.12
(1,2426)	1:1907:A:MET:HA	1:1908:A:GLU:H	14	0.12
(1,2426)	1:1907:A:MET:HA	1:1908:A:GLU:H	15	0.12
(1,2426)	1:1907:A:MET:HA	1:1908:A:GLU:H	17	0.12
(1,2426)	1:1907:A:MET:HA	1:1908:A:GLU:H	19	0.12
(1,2424)	1:1950:A:ASN:HB2	1:1950:A:ASN:HA	3	0.12
(1,2424)	1:1950:A:ASN:HB2	1:1950:A:ASN:HA	16	0.12
(1,2424)	1:1950:A:ASN:HB2	1:1950:A:ASN:HA	17	0.12
(1,2423)	1:1931:A:GLY:H	1:1930:A:VAL:HA	4	0.12
(1,2415)	1:1857:A:LYS:HA	1:1857:A:LYS:HG2	6	0.12
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	1	0.12
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	10	0.12
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	3	0.12
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	5	0.12
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	9	0.12
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	12	0.12
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	13	0.12
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	19	0.12
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	6	0.12
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	10	0.12
(1,2339)	1:1840:A:ILE:H	1:1849:A:GLY:H	8	0.12
(1,2339)	1:1840:A:ILE:H	1:1849:A:GLY:H	15	0.12
(1,2330)	1:1922:A:ILE:HG21	1:1922:A:ILE:H	13	0.12
(1,2330)	1:1922:A:ILE:HG22	1:1922:A:ILE:H	13	0.12
(1,2330)	1:1922:A:ILE:HG23	1:1922:A:ILE:H	13	0.12
(1,2328)	1:1950:A:ASN:H	1:1951:A:THR:H	1	0.12
(1,2298)	1:1891:A:ARG:H	1:1891:A:ARG:HB2	10	0.12
(1,2298)	1:1891:A:ARG:H	1:1891:A:ARG:HB2	12	0.12
(1,2298)	1:1891:A:ARG:H	1:1891:A:ARG:HB2	13	0.12
(1,2298)	1:1891:A:ARG:H	1:1891:A:ARG:HB2	18	0.12
(1,2298)	1:1891:A:ARG:H	1:1891:A:ARG:HB2	19	0.12
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD21	8	0.12
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD22	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2289)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD23	8	0.12
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD21	8	0.12
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD22	8	0.12
(1,2289)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD23	8	0.12
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD21	8	0.12
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD22	8	0.12
(1,2289)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD23	8	0.12
(1,2287)	1:1863:A:ALA:H	1:1862:A:ASP:HA	3	0.12
(1,2287)	1:1863:A:ALA:H	1:1862:A:ASP:HA	7	0.12
(1,2287)	1:1863:A:ALA:H	1:1862:A:ASP:HA	9	0.12
(1,2287)	1:1863:A:ALA:H	1:1862:A:ASP:HA	13	0.12
(1,2287)	1:1863:A:ALA:H	1:1862:A:ASP:HA	18	0.12
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG21	4	0.12
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG22	4	0.12
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG23	4	0.12
(1,2261)	1:1906:A:GLN:H	1:1906:A:GLN:HB2	2	0.12
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD21	4	0.12
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD22	4	0.12
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD23	4	0.12
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD21	10	0.12
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD22	10	0.12
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD23	10	0.12
(1,2245)	1:1954:A:ASP:HA	1:1954:A:ASP:HB2	12	0.12
(1,2245)	1:1954:A:ASP:HA	1:1954:A:ASP:HB2	15	0.12
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	6	0.12
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	19	0.12
(1,2234)	1:1924:A:ASN:H	1:1922:A:ILE:HA	11	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	1	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	2	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	3	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	4	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	5	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	6	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	7	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	8	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	9	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	10	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	11	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	13	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	15	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	16	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	18	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	19	0.12
(1,2230)	1:1835:A:GLU:HB2	1:1835:A:GLU:HA	20	0.12
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG21	11	0.12
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG22	11	0.12
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG23	11	0.12
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG21	16	0.12
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG22	16	0.12
(1,2220)	1:1914:A:THR:H	1:1914:A:THR:HG23	16	0.12
(1,2180)	1:1884:A:LEU:H	1:1850:A:LEU:HD11	16	0.12
(1,2180)	1:1884:A:LEU:H	1:1850:A:LEU:HD12	16	0.12
(1,2180)	1:1884:A:LEU:H	1:1850:A:LEU:HD13	16	0.12
(1,2179)	1:1940:A:LYS:HA	1:1943:A:ARG:HB2	2	0.12
(1,2179)	1:1940:A:LYS:HA	1:1943:A:ARG:HB2	5	0.12
(1,2165)	1:1841:A:GLY:H	1:1876:A:PHE:HE1	11	0.12
(1,2165)	1:1841:A:GLY:H	1:1876:A:PHE:HE2	11	0.12
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	1	0.12
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	2	0.12
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	10	0.12
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	18	0.12
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	9	0.12
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	9	0.12
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	9	0.12
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	10	0.12
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	10	0.12
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	10	0.12
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	17	0.12
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	17	0.12
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	17	0.12
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	19	0.12
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	19	0.12
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	19	0.12
(1,2156)	1:1892:A:GLU:HG3	1:1894:A:LYS:HD2	7	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	1	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	1	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	2	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	2	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	6	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	6	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	8	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	8	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	13	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	14	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	14	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	18	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	18	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	19	0.12
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	19	0.12
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	4	0.12
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	4	0.12
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	4	0.12
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	6	0.12
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	6	0.12
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	6	0.12
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	18	0.12
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	18	0.12
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	18	0.12
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	19	0.12
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	19	0.12
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	19	0.12
(1,2099)	1:1927:A:GLY:H	1:1928:A:GLU:H	9	0.12
(1,2089)	1:1916:A:THR:H	1:1915:A:PRO:HB2	16	0.12
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	4	0.12
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	5	0.12
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	7	0.12
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	9	0.12
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	11	0.12
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	12	0.12
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	13	0.12
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	14	0.12
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	17	0.12
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	19	0.12
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	17	0.12
(1,2070)	1:1820:A:ILE:HG12	1:1821:A:ASP:H	12	0.12
(1,2055)	1:1922:A:ILE:HA	1:1922:A:ILE:HG12	9	0.12
(1,2055)	1:1922:A:ILE:HA	1:1922:A:ILE:HG12	13	0.12
(1,2051)	1:1840:A:ILE:HA	1:1846:A:THR:HA	4	0.12
(1,2051)	1:1840:A:ILE:HA	1:1846:A:THR:HA	8	0.12
(1,2051)	1:1840:A:ILE:HA	1:1846:A:THR:HA	13	0.12
(1,2028)	1:1824:A:SER:H	1:1823:A:LYS:HG3	18	0.12
(1,1979)	1:1941:A:ILE:HG21	1:1942:A:LEU:HG	12	0.12
(1,1979)	1:1941:A:ILE:HG22	1:1942:A:LEU:HG	12	0.12
(1,1979)	1:1941:A:ILE:HG23	1:1942:A:LEU:HG	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1978)	1:1941:A:ILE:H	1:1940:A:LYS:H	4	0.12
(1,1978)	1:1941:A:ILE:H	1:1940:A:LYS:H	7	0.12
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD11	15	0.12
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD12	15	0.12
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD13	15	0.12
(1,1957)	1:1927:A:GLY:H	1:1926:A:ASN:HB2	1	0.12
(1,1956)	1:1953:A:GLN:HA	1:1953:A:GLN:HB3	4	0.12
(1,1952)	1:1840:A:ILE:HG21	1:1846:A:THR:HB	8	0.12
(1,1952)	1:1840:A:ILE:HG22	1:1846:A:THR:HB	8	0.12
(1,1952)	1:1840:A:ILE:HG23	1:1846:A:THR:HB	8	0.12
(1,1952)	1:1840:A:ILE:HG21	1:1846:A:THR:HB	9	0.12
(1,1952)	1:1840:A:ILE:HG22	1:1846:A:THR:HB	9	0.12
(1,1952)	1:1840:A:ILE:HG23	1:1846:A:THR:HB	9	0.12
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	9	0.12
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	10	0.12
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	11	0.12
(1,1944)	1:1885:A:ARG:HA	1:1885:A:ARG:HG3	20	0.12
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	6	0.12
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	10	0.12
(1,1915)	1:1871:A:ASN:HB3	1:1871:A:ASN:HA	12	0.12
(1,1895)	1:1855:A:GLU:H	1:1852:A:GLU:HG2	7	0.12
(1,1895)	1:1855:A:GLU:H	1:1852:A:GLU:HG2	9	0.12
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE1	3	0.12
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE2	3	0.12
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE1	3	0.12
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE2	3	0.12
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE1	3	0.12
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE2	3	0.12
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE1	4	0.12
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE2	4	0.12
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE1	4	0.12
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE2	4	0.12
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE1	4	0.12
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE2	4	0.12
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE1	8	0.12
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE2	8	0.12
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE1	8	0.12
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE2	8	0.12
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE1	8	0.12
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE2	8	0.12
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE1	9	0.12
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE2	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE1	9	0.12
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE2	9	0.12
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE1	9	0.12
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE2	9	0.12
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE1	14	0.12
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE2	14	0.12
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE1	14	0.12
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE2	14	0.12
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE1	14	0.12
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE2	14	0.12
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE1	15	0.12
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE2	15	0.12
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE1	15	0.12
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE2	15	0.12
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE1	15	0.12
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE2	15	0.12
(1,1871)	1:1832:A:PHE:HE1	1:1935:A:TYR:HE1	6	0.12
(1,1871)	1:1832:A:PHE:HE1	1:1935:A:TYR:HE2	6	0.12
(1,1871)	1:1832:A:PHE:HE2	1:1935:A:TYR:HE1	6	0.12
(1,1871)	1:1832:A:PHE:HE2	1:1935:A:TYR:HE2	6	0.12
(1,1858)	1:1934:A:VAL:HA	1:1937:A:GLU:H	2	0.12
(1,1858)	1:1934:A:VAL:HA	1:1937:A:GLU:H	19	0.12
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	8	0.12
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	9	0.12
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	10	0.12
(1,1833)	1:1941:A:ILE:H	1:1941:A:ILE:HA	11	0.12
(1,1806)	1:1840:A:ILE:HB	1:1876:A:PHE:HZ	6	0.12
(1,1806)	1:1840:A:ILE:HB	1:1876:A:PHE:HZ	16	0.12
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	16	0.12
(1,1790)	1:1927:A:GLY:H	1:1925:A:THR:HB	15	0.12
(1,1790)	1:1927:A:GLY:H	1:1925:A:THR:HB	20	0.12
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD21	12	0.12
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD22	12	0.12
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD23	12	0.12
(1,1761)	1:1909:A:VAL:H	1:1909:A:VAL:HB	16	0.12
(1,1755)	1:1907:A:MET:H	1:1906:A:GLN:HB2	4	0.12
(1,1752)	1:1899:A:THR:HG21	1:1899:A:THR:H	10	0.12
(1,1752)	1:1899:A:THR:HG22	1:1899:A:THR:H	10	0.12
(1,1752)	1:1899:A:THR:HG23	1:1899:A:THR:H	10	0.12
(1,1750)	1:1924:A:ASN:HB2	1:1924:A:ASN:HA	5	0.12
(1,1747)	1:1853:A:LEU:HD11	1:1856:A:TYR:HB2	6	0.12
(1,1747)	1:1853:A:LEU:HD12	1:1856:A:TYR:HB2	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1747)	1:1853:A:LEU:HD13	1:1856:A:TYR:HB2	6	0.12
(1,1718)	1:1902:A:GLY:H	1:1901:A:THR:HA	6	0.12
(1,1689)	1:1928:A:GLU:H	1:1927:A:GLY:HA2	4	0.12
(1,1683)	1:1933:A:SER:H	1:1932:A:PRO:HB2	10	0.12
(1,1678)	1:1832:A:PHE:HD1	1:1856:A:TYR:HE1	16	0.12
(1,1678)	1:1832:A:PHE:HD1	1:1856:A:TYR:HE2	16	0.12
(1,1678)	1:1832:A:PHE:HD2	1:1856:A:TYR:HE1	16	0.12
(1,1678)	1:1832:A:PHE:HD2	1:1856:A:TYR:HE2	16	0.12
(1,1666)	1:1907:A:MET:HG2	1:1908:A:GLU:H	16	0.12
(1,1666)	1:1907:A:MET:HG2	1:1908:A:GLU:H	19	0.12
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	1	0.12
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	1	0.12
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	3	0.12
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	3	0.12
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	4	0.12
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	4	0.12
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	5	0.12
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	5	0.12
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	6	0.12
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	6	0.12
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	10	0.12
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	10	0.12
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	13	0.12
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	13	0.12
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	15	0.12
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	15	0.12
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	17	0.12
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	17	0.12
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	18	0.12
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	18	0.12
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	19	0.12
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	19	0.12
(1,1642)	1:1939:A:LEU:HD21	1:1935:A:TYR:HE1	7	0.12
(1,1642)	1:1939:A:LEU:HD21	1:1935:A:TYR:HE2	7	0.12
(1,1642)	1:1939:A:LEU:HD22	1:1935:A:TYR:HE1	7	0.12
(1,1642)	1:1939:A:LEU:HD22	1:1935:A:TYR:HE2	7	0.12
(1,1642)	1:1939:A:LEU:HD23	1:1935:A:TYR:HE1	7	0.12
(1,1642)	1:1939:A:LEU:HD23	1:1935:A:TYR:HE2	7	0.12
(1,1619)	1:1887:A:ILE:HG21	1:1890:A:GLU:HB2	14	0.12
(1,1619)	1:1887:A:ILE:HG22	1:1890:A:GLU:HB2	14	0.12
(1,1619)	1:1887:A:ILE:HG23	1:1890:A:GLU:HB2	14	0.12
(1,1619)	1:1887:A:ILE:HG21	1:1890:A:GLU:HB2	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1619)	1:1887:A:ILE:HG22	1:1890:A:GLU:HB2	16	0.12
(1,1619)	1:1887:A:ILE:HG23	1:1890:A:GLU:HB2	16	0.12
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD11	6	0.12
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD12	6	0.12
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD13	6	0.12
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD11	6	0.12
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD12	6	0.12
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD13	6	0.12
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD11	6	0.12
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD12	6	0.12
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD13	6	0.12
(1,1604)	1:1930:A:VAL:H	1:1931:A:GLY:H	1	0.12
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD11	4	0.12
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD12	4	0.12
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD13	4	0.12
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD11	4	0.12
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD12	4	0.12
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD13	4	0.12
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD11	5	0.12
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD12	5	0.12
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD13	5	0.12
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD11	5	0.12
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD12	5	0.12
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD13	5	0.12
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD11	9	0.12
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD12	9	0.12
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD13	9	0.12
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD11	9	0.12
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD12	9	0.12
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD13	9	0.12
(1,1582)	1:1884:A:LEU:HD11	1:1853:A:LEU:HA	20	0.12
(1,1582)	1:1884:A:LEU:HD12	1:1853:A:LEU:HA	20	0.12
(1,1582)	1:1884:A:LEU:HD13	1:1853:A:LEU:HA	20	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	1	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	1	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	2	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	2	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	3	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	3	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	4	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	4	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	5	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	6	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	6	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	7	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	7	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	8	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	8	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	9	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	9	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	10	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	10	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	11	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	11	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	12	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	12	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	13	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	13	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	15	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	15	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	16	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	16	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	17	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	17	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	18	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	18	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	19	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	19	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG2	20	0.12
(1,1578)	1:1835:A:GLU:HB2	1:1835:A:GLU:HG3	20	0.12
(1,1564)	1:1904:A:SER:H	1:1903:A:ILE:HG21	14	0.12
(1,1564)	1:1904:A:SER:H	1:1903:A:ILE:HG22	14	0.12
(1,1564)	1:1904:A:SER:H	1:1903:A:ILE:HG23	14	0.12
(1,1554)	1:1926:A:ASN:H	1:1925:A:THR:HB	6	0.12
(1,1532)	1:1822:A:GLU:HG3	1:1823:A:LYS:H	16	0.12
(1,1504)	1:1855:A:GLU:HA	1:1858:A:LYS:HE2	9	0.12
(1,1504)	1:1855:A:GLU:HA	1:1858:A:LYS:HE2	10	0.12
(1,1479)	1:1867:A:PRO:HD2	1:1868:A:PHE:H	1	0.12
(1,1469)	1:1866:A:GLU:HB2	1:1866:A:GLU:HG3	4	0.12
(1,1469)	1:1866:A:GLU:HB3	1:1866:A:GLU:HG3	4	0.12
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	15	0.12
(1,1439)	1:1928:A:GLU:HA	1:1928:A:GLU:HB3	17	0.12
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	5	0.12
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	9	0.12
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	9	0.12
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	11	0.12
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	11	0.12
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	4	0.12
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	4	0.12
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	15	0.12
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	15	0.12
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	19	0.12
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	19	0.12
(1,1410)	1:1951:A:THR:HG21	1:1951:A:THR:H	2	0.12
(1,1410)	1:1951:A:THR:HG22	1:1951:A:THR:H	2	0.12
(1,1410)	1:1951:A:THR:HG23	1:1951:A:THR:H	2	0.12
(1,1409)	1:1944:A:GLN:H	1:1944:A:GLN:HG2	1	0.12
(1,1401)	1:1829:A:VAL:HG21	1:1864:A:ASP:HB3	2	0.12
(1,1401)	1:1829:A:VAL:HG22	1:1864:A:ASP:HB3	2	0.12
(1,1401)	1:1829:A:VAL:HG23	1:1864:A:ASP:HB3	2	0.12
(1,1401)	1:1829:A:VAL:HG21	1:1864:A:ASP:HB3	16	0.12
(1,1401)	1:1829:A:VAL:HG22	1:1864:A:ASP:HB3	16	0.12
(1,1401)	1:1829:A:VAL:HG23	1:1864:A:ASP:HB3	16	0.12
(1,1395)	1:1893:A:GLY:H	1:1892:A:GLU:HG3	2	0.12
(1,1395)	1:1893:A:GLY:H	1:1892:A:GLU:HG3	7	0.12
(1,1395)	1:1893:A:GLY:H	1:1892:A:GLU:HG3	14	0.12
(1,1381)	1:1922:A:ILE:H	1:1921:A:SER:HB2	7	0.12
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD21	9	0.12
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD22	9	0.12
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD23	9	0.12
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD21	9	0.12
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD22	9	0.12
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD23	9	0.12
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD21	9	0.12
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD22	9	0.12
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD23	9	0.12
(1,1342)	1:1859:A:LYS:H	1:1858:A:LYS:HG3	5	0.12
(1,1342)	1:1859:A:LYS:H	1:1858:A:LYS:HG3	6	0.12
(1,1342)	1:1859:A:LYS:H	1:1858:A:LYS:HG3	15	0.12
(1,1335)	1:1953:A:GLN:HA	1:1953:A:GLN:HG2	16	0.12
(1,1330)	1:1893:A:GLY:H	1:1892:A:GLU:HB2	10	0.12
(1,1305)	1:1837:A:PHE:HE1	1:1876:A:PHE:HE1	9	0.12
(1,1305)	1:1837:A:PHE:HE1	1:1876:A:PHE:HE2	9	0.12
(1,1305)	1:1837:A:PHE:HE2	1:1876:A:PHE:HE1	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1305)	1:1837:A:PHE:HE2	1:1876:A:PHE:HE2	9	0.12
(1,1305)	1:1837:A:PHE:HE1	1:1876:A:PHE:HE1	11	0.12
(1,1305)	1:1837:A:PHE:HE1	1:1876:A:PHE:HE2	11	0.12
(1,1305)	1:1837:A:PHE:HE2	1:1876:A:PHE:HE1	11	0.12
(1,1305)	1:1837:A:PHE:HE2	1:1876:A:PHE:HE2	11	0.12
(1,1305)	1:1837:A:PHE:HE1	1:1876:A:PHE:HE1	20	0.12
(1,1305)	1:1837:A:PHE:HE1	1:1876:A:PHE:HE2	20	0.12
(1,1305)	1:1837:A:PHE:HE2	1:1876:A:PHE:HE1	20	0.12
(1,1305)	1:1837:A:PHE:HE2	1:1876:A:PHE:HE2	20	0.12
(1,1239)	1:1890:A:GLU:HA	1:1896:A:ARG:HG3	2	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	3	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	3	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	3	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	4	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	4	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	4	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	8	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	8	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	8	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	12	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	12	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	12	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	17	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	17	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	17	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	18	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	18	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	18	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	19	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	19	0.12
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	19	0.12
(1,1200)	1:1922:A:ILE:HB	1:1922:A:ILE:H	6	0.12
(1,1200)	1:1922:A:ILE:HB	1:1922:A:ILE:H	19	0.12
(1,1200)	1:1922:A:ILE:HB	1:1922:A:ILE:H	20	0.12
(1,1194)	1:1918:A:THR:HA	1:1918:A:THR:HB	8	0.12
(1,1194)	1:1918:A:THR:HA	1:1918:A:THR:HB	18	0.12
(1,1189)	1:1956:A:ARG:HB2	1:1956:A:ARG:HD2	8	0.12
(1,1189)	1:1956:A:ARG:HB2	1:1956:A:ARG:HD3	8	0.12
(1,1187)	1:1838:A:LYS:H	1:1838:A:LYS:HG3	20	0.12
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG11	13	0.12
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG12	13	0.12
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG13	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1121)	1:1820:A:ILE:H	1:1820:A:ILE:HG12	11	0.12
(1,1121)	1:1820:A:ILE:H	1:1820:A:ILE:HG12	12	0.12
(1,1121)	1:1820:A:ILE:H	1:1820:A:ILE:HG12	20	0.12
(1,1113)	1:1887:A:ILE:HG21	1:1891:A:ARG:HG2	18	0.12
(1,1113)	1:1887:A:ILE:HG22	1:1891:A:ARG:HG2	18	0.12
(1,1113)	1:1887:A:ILE:HG23	1:1891:A:ARG:HG2	18	0.12
(1,1098)	1:1905:A:PRO:HD2	1:1904:A:SER:HB2	8	0.12
(1,1098)	1:1905:A:PRO:HD2	1:1904:A:SER:HB3	8	0.12
(1,1081)	1:1826:A:LYS:HB2	1:1826:A:LYS:HD2	16	0.12
(1,1081)	1:1826:A:LYS:HB2	1:1826:A:LYS:HD3	16	0.12
(1,1028)	1:1886:A:VAL:HA	1:1888:A:GLU:H	11	0.12
(1,1028)	1:1886:A:VAL:HA	1:1888:A:GLU:H	15	0.12
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	3	0.12
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	18	0.12
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	3	0.12
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	8	0.12
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	11	0.12
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	20	0.12
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	20	0.12
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	20	0.12
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	20	0.12
(1,1000)	1:1917:A:SER:HA	1:1918:A:THR:H	2	0.12
(1,1000)	1:1917:A:SER:HA	1:1918:A:THR:H	11	0.12
(1,1000)	1:1917:A:SER:HA	1:1918:A:THR:H	16	0.12
(1,994)	1:1889:A:MET:HE1	1:1885:A:ARG:HG2	6	0.12
(1,994)	1:1889:A:MET:HE2	1:1885:A:ARG:HG2	6	0.12
(1,994)	1:1889:A:MET:HE3	1:1885:A:ARG:HG2	6	0.12
(1,994)	1:1889:A:MET:HE1	1:1885:A:ARG:HG2	17	0.12
(1,994)	1:1889:A:MET:HE2	1:1885:A:ARG:HG2	17	0.12
(1,994)	1:1889:A:MET:HE3	1:1885:A:ARG:HG2	17	0.12
(1,986)	1:1837:A:PHE:H	1:1840:A:ILE:H	2	0.12
(1,974)	1:1856:A:TYR:HD1	1:1833:A:LEU:HD11	11	0.12
(1,974)	1:1856:A:TYR:HD1	1:1833:A:LEU:HD12	11	0.12
(1,974)	1:1856:A:TYR:HD1	1:1833:A:LEU:HD13	11	0.12
(1,974)	1:1856:A:TYR:HD2	1:1833:A:LEU:HD11	11	0.12
(1,974)	1:1856:A:TYR:HD2	1:1833:A:LEU:HD12	11	0.12
(1,974)	1:1856:A:TYR:HD2	1:1833:A:LEU:HD13	11	0.12
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	10	0.12
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	11	0.12
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	16	0.12
(1,959)	1:1898:A:SER:H	1:1897:A:ILE:HG12	17	0.12
(1,937)	1:1894:A:LYS:H	1:1894:A:LYS:HG3	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB2	3	0.12
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB3	3	0.12
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB2	6	0.12
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB3	6	0.12
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB2	11	0.12
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB3	11	0.12
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB2	13	0.12
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB3	13	0.12
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB2	17	0.12
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB3	17	0.12
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB2	20	0.12
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB3	20	0.12
(1,902)	1:1877:A:GLN:HG2	1:1872:A:SER:H	2	0.12
(1,897)	1:1946:A:CYS:H	1:1945:A:ARG:HB2	7	0.12
(1,897)	1:1946:A:CYS:H	1:1945:A:ARG:HB2	15	0.12
(1,888)	1:1887:A:ILE:HA	1:1890:A:GLU:HG2	4	0.12
(1,888)	1:1887:A:ILE:HA	1:1890:A:GLU:HG2	11	0.12
(1,878)	1:1820:A:ILE:H	1:1820:A:ILE:HB	4	0.12
(1,878)	1:1820:A:ILE:H	1:1820:A:ILE:HB	8	0.12
(1,866)	1:1896:A:ARG:H	1:1896:A:ARG:HG3	11	0.12
(1,844)	1:1890:A:GLU:HA	1:1890:A:GLU:HG2	8	0.12
(1,844)	1:1890:A:GLU:HA	1:1890:A:GLU:HG2	9	0.12
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	11	0.12
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	12	0.12
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	13	0.12
(1,828)	1:1851:A:ALA:HB1	1:1852:A:GLU:HG2	2	0.12
(1,828)	1:1851:A:ALA:HB2	1:1852:A:GLU:HG2	2	0.12
(1,828)	1:1851:A:ALA:HB3	1:1852:A:GLU:HG2	2	0.12
(1,828)	1:1851:A:ALA:HB1	1:1852:A:GLU:HG2	16	0.12
(1,828)	1:1851:A:ALA:HB2	1:1852:A:GLU:HG2	16	0.12
(1,828)	1:1851:A:ALA:HB3	1:1852:A:GLU:HG2	16	0.12
(1,822)	1:1857:A:LYS:HA	1:1861:A:SER:H	13	0.12
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	4	0.12
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	4	0.12
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	4	0.12
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	5	0.12
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	5	0.12
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	5	0.12
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	6	0.12
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	6	0.12
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	6	0.12
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	10	0.12
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	10	0.12
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	13	0.12
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	13	0.12
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	13	0.12
(1,818)	1:1861:A:SER:H	1:1862:A:ASP:H	16	0.12
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	5	0.12
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	8	0.12
(1,807)	1:1907:A:MET:H	1:1906:A:GLN:HG2	14	0.12
(1,781)	1:1819:A:ARG:HB2	1:1819:A:ARG:HA	3	0.12
(1,781)	1:1819:A:ARG:HB2	1:1819:A:ARG:HA	7	0.12
(1,781)	1:1819:A:ARG:HB2	1:1819:A:ARG:HA	16	0.12
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	3	0.12
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	3	0.12
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	3	0.12
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	3	0.12
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	3	0.12
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	3	0.12
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	17	0.12
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	17	0.12
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	17	0.12
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	17	0.12
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	17	0.12
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	17	0.12
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG21	20	0.12
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG22	20	0.12
(1,742)	1:1879:A:TYR:HE1	1:1886:A:VAL:HG23	20	0.12
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG21	20	0.12
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG22	20	0.12
(1,742)	1:1879:A:TYR:HE2	1:1886:A:VAL:HG23	20	0.12
(1,739)	1:1822:A:GLU:H	1:1822:A:GLU:HG3	3	0.12
(1,739)	1:1822:A:GLU:H	1:1822:A:GLU:HG3	5	0.12
(1,739)	1:1822:A:GLU:H	1:1822:A:GLU:HG3	18	0.12
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	6	0.12
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	7	0.12
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	11	0.12
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	12	0.12
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	14	0.12
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	15	0.12
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	18	0.12
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	16	0.12
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,675)	1:1890:A:GLU:HB3	1:1890:A:GLU:HG2	6	0.12
(1,669)	1:1890:A:GLU:H	1:1890:A:GLU:HG3	4	0.12
(1,669)	1:1890:A:GLU:H	1:1890:A:GLU:HG3	17	0.12
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	14	0.12
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	14	0.12
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	14	0.12
(1,630)	1:1926:A:ASN:HA	1:1926:A:ASN:HB2	6	0.12
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	9	0.12
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	10	0.12
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	11	0.12
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	2	0.12
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	11	0.12
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	13	0.12
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	14	0.12
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	15	0.12
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	18	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	5	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	5	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	6	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	6	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	7	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	7	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	8	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	8	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	9	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	9	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	12	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	12	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	14	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	14	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	17	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	17	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	20	0.12
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	20	0.12
(1,601)	1:1923:A:GLY:H	1:1922:A:ILE:HG13	10	0.12
(1,595)	1:1823:A:LYS:HA	1:1823:A:LYS:HB2	2	0.12
(1,595)	1:1823:A:LYS:HA	1:1823:A:LYS:HB2	10	0.12
(1,595)	1:1823:A:LYS:HA	1:1823:A:LYS:HB2	14	0.12
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	7	0.12
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	8	0.12
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	13	0.12
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,585)	1:1923:A:GLY:H	1:1922:A:ILE:HB	8	0.12
(1,578)	1:1857:A:LYS:H	1:1857:A:LYS:HB3	20	0.12
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE2	5	0.12
(1,548)	1:1884:A:LEU:HD11	1:1857:A:LYS:HE3	5	0.12
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE2	5	0.12
(1,548)	1:1884:A:LEU:HD12	1:1857:A:LYS:HE3	5	0.12
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE2	5	0.12
(1,548)	1:1884:A:LEU:HD13	1:1857:A:LYS:HE3	5	0.12
(1,526)	1:1885:A:ARG:HA	1:1888:A:GLU:HG2	13	0.12
(1,525)	1:1924:A:ASN:H	1:1923:A:GLY:H	12	0.12
(1,516)	1:1886:A:VAL:HG21	1:1882:A:ARG:HG3	14	0.12
(1,516)	1:1886:A:VAL:HG22	1:1882:A:ARG:HG3	14	0.12
(1,516)	1:1886:A:VAL:HG23	1:1882:A:ARG:HG3	14	0.12
(1,509)	1:1865:A:ILE:HG21	1:1866:A:GLU:H	1	0.12
(1,509)	1:1865:A:ILE:HG22	1:1866:A:GLU:H	1	0.12
(1,509)	1:1865:A:ILE:HG23	1:1866:A:GLU:H	1	0.12
(1,509)	1:1865:A:ILE:HG21	1:1866:A:GLU:H	5	0.12
(1,509)	1:1865:A:ILE:HG22	1:1866:A:GLU:H	5	0.12
(1,509)	1:1865:A:ILE:HG23	1:1866:A:GLU:H	5	0.12
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	1	0.12
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	9	0.12
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	10	0.12
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	11	0.12
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	14	0.12
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	15	0.12
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	20	0.12
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	3	0.12
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	12	0.12
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	17	0.12
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	18	0.12
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	19	0.12
(1,472)	1:1894:A:LYS:H	1:1894:A:LYS:HB3	1	0.12
(1,472)	1:1894:A:LYS:H	1:1894:A:LYS:HB3	4	0.12
(1,472)	1:1894:A:LYS:H	1:1894:A:LYS:HB3	17	0.12
(1,466)	1:1917:A:SER:H	1:1917:A:SER:HB2	13	0.12
(1,461)	1:1845:A:ASN:HD21	1:1839:A:LYS:HG3	2	0.12
(1,461)	1:1845:A:ASN:HD21	1:1839:A:LYS:HG3	3	0.12
(1,461)	1:1845:A:ASN:HD21	1:1839:A:LYS:HG3	5	0.12
(1,461)	1:1845:A:ASN:HD21	1:1839:A:LYS:HG3	11	0.12
(1,461)	1:1845:A:ASN:HD21	1:1839:A:LYS:HG3	16	0.12
(1,461)	1:1845:A:ASN:HD21	1:1839:A:LYS:HG3	17	0.12
(1,461)	1:1845:A:ASN:HD21	1:1839:A:LYS:HG3	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	1:1845:A:ASN:HD21	1:1839:A:LYS:HG3	19	0.12
(1,450)	1:1896:A:ARG:HB2	1:1890:A:GLU:HG2	5	0.12
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	1	0.12
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	5	0.12
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	19	0.12
(1,444)	1:1872:A:SER:H	1:1877:A:GLN:HG3	7	0.12
(1,442)	1:1948:A:LEU:HB2	1:1949:A:ASP:H	7	0.12
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	3	0.12
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	3	0.12
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	8	0.12
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	8	0.12
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	11	0.12
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	11	0.12
(1,379)	1:1853:A:LEU:HD11	1:1853:A:LEU:HB3	6	0.12
(1,379)	1:1853:A:LEU:HD12	1:1853:A:LEU:HB3	6	0.12
(1,379)	1:1853:A:LEU:HD13	1:1853:A:LEU:HB3	6	0.12
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	7	0.12
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	8	0.12
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	11	0.12
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	12	0.12
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	13	0.12
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	14	0.12
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	19	0.12
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	20	0.12
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	12	0.12
(1,357)	1:1926:A:ASN:HB3	1:1926:A:ASN:HA	6	0.12
(1,330)	1:1827:A:ALA:H	1:1826:A:LYS:HB3	17	0.12
(1,330)	1:1827:A:ALA:H	1:1826:A:LYS:HB3	19	0.12
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD11	1	0.12
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD12	1	0.12
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD13	1	0.12
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD11	12	0.12
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD12	12	0.12
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD13	12	0.12
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD11	15	0.12
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD12	15	0.12
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD13	15	0.12
(1,316)	1:1919:A:VAL:HG21	1:1918:A:THR:HG21	4	0.12
(1,316)	1:1919:A:VAL:HG21	1:1918:A:THR:HG22	4	0.12
(1,316)	1:1919:A:VAL:HG21	1:1918:A:THR:HG23	4	0.12
(1,316)	1:1919:A:VAL:HG22	1:1918:A:THR:HG21	4	0.12
(1,316)	1:1919:A:VAL:HG22	1:1918:A:THR:HG22	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,316)	1:1919:A:VAL:HG22	1:1918:A:THR:HG23	4	0.12
(1,316)	1:1919:A:VAL:HG23	1:1918:A:THR:HG21	4	0.12
(1,316)	1:1919:A:VAL:HG23	1:1918:A:THR:HG22	4	0.12
(1,316)	1:1919:A:VAL:HG23	1:1918:A:THR:HG23	4	0.12
(1,311)	1:1930:A:VAL:H	1:1930:A:VAL:HG21	12	0.12
(1,311)	1:1930:A:VAL:H	1:1930:A:VAL:HG22	12	0.12
(1,311)	1:1930:A:VAL:H	1:1930:A:VAL:HG23	12	0.12
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	2	0.12
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	3	0.12
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	4	0.12
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	5	0.12
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	7	0.12
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	13	0.12
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	18	0.12
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	19	0.12
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG11	6	0.12
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG12	6	0.12
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG13	6	0.12
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG11	17	0.12
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG12	17	0.12
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG13	17	0.12
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	1	0.12
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	1	0.12
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	4	0.12
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	4	0.12
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	19	0.12
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	19	0.12
(1,258)	1:1941:A:ILE:HA	1:1941:A:ILE:HG13	11	0.12
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	2	0.12
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	2	0.12
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	3	0.12
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	3	0.12
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	6	0.12
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	6	0.12
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	11	0.12
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	11	0.12
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	12	0.12
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	12	0.12
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	15	0.12
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	15	0.12
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	16	0.12
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,246)	1:1874:A:GLN:H	1:1874:A:GLN:HG2	4	0.12
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD11	13	0.12
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD12	13	0.12
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD13	13	0.12
(1,239)	1:1896:A:ARG:H	1:1897:A:ILE:HB	7	0.12
(1,239)	1:1896:A:ARG:H	1:1897:A:ILE:HB	17	0.12
(1,229)	1:1823:A:LYS:HA	1:1826:A:LYS:HE2	8	0.12
(1,229)	1:1823:A:LYS:HA	1:1826:A:LYS:HE3	8	0.12
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	5	0.12
(1,215)	1:1828:A:LYS:HA	1:1831:A:ASP:HB2	5	0.12
(1,215)	1:1828:A:LYS:HA	1:1831:A:ASP:HB2	7	0.12
(1,186)	1:1884:A:LEU:HD11	1:1857:A:LYS:HD3	20	0.12
(1,186)	1:1884:A:LEU:HD12	1:1857:A:LYS:HD3	20	0.12
(1,186)	1:1884:A:LEU:HD13	1:1857:A:LYS:HD3	20	0.12
(1,135)	1:1939:A:LEU:HD11	1:1839:A:LYS:HD2	1	0.12
(1,135)	1:1939:A:LEU:HD12	1:1839:A:LYS:HD2	1	0.12
(1,135)	1:1939:A:LEU:HD13	1:1839:A:LYS:HD2	1	0.12
(1,125)	1:1822:A:GLU:HG2	1:1823:A:LYS:H	3	0.12
(1,125)	1:1822:A:GLU:HG2	1:1823:A:LYS:H	17	0.12
(1,111)	1:1894:A:LYS:H	1:1892:A:GLU:HB3	18	0.12
(1,104)	1:1951:A:THR:H	1:1951:A:THR:HB	1	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	1	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	2	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	3	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	4	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	6	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	7	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	8	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	9	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	10	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	12	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	13	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	14	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	15	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	17	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	18	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	19	0.12
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	20	0.12
(1,96)	1:1828:A:LYS:HA	1:1831:A:ASP:HB3	10	0.12
(1,96)	1:1828:A:LYS:HA	1:1831:A:ASP:HB3	11	0.12
(1,93)	1:1857:A:LYS:HA	1:1865:A:ILE:HD11	8	0.12
(1,93)	1:1857:A:LYS:HA	1:1865:A:ILE:HD12	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:1857:A:LYS:HA	1:1865:A:ILE:HD13	8	0.12
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	10	0.12
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	13	0.12
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	16	0.12
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	17	0.12
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD2	2	0.12
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD3	2	0.12
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD2	2	0.12
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD3	2	0.12
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD2	2	0.12
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD3	2	0.12
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD2	5	0.12
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD3	5	0.12
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD2	5	0.12
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD3	5	0.12
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD2	5	0.12
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD3	5	0.12
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD2	10	0.12
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD3	10	0.12
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD2	10	0.12
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD3	10	0.12
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD2	10	0.12
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD3	10	0.12
(1,41)	1:1922:A:ILE:H	1:1921:A:SER:HB3	15	0.12
(1,12)	1:1928:A:GLU:H	1:1928:A:GLU:HG2	2	0.12
(1,12)	1:1928:A:GLU:H	1:1928:A:GLU:HG3	2	0.12
(1,12)	1:1928:A:GLU:H	1:1928:A:GLU:HG2	8	0.12
(1,12)	1:1928:A:GLU:H	1:1928:A:GLU:HG3	8	0.12
(1,12)	1:1928:A:GLU:H	1:1928:A:GLU:HG2	10	0.12
(1,12)	1:1928:A:GLU:H	1:1928:A:GLU:HG3	10	0.12
(1,12)	1:1928:A:GLU:H	1:1928:A:GLU:HG2	20	0.12
(1,12)	1:1928:A:GLU:H	1:1928:A:GLU:HG3	20	0.12
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD21	3	0.12
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD22	3	0.12
(1,2)	1:1842:A:SER:HB2	1:1942:A:LEU:HD23	3	0.12
(3,56)	1:1945:A:ARG:N	1:1941:A:ILE:O	13	0.11
(1,3312)	1:1906:A:GLN:H	1:1906:A:GLN:HB3	9	0.11
(1,3311)	1:1826:A:LYS:H	1:1825:A:SER:HB2	3	0.11
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG21	7	0.11
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG22	7	0.11
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG23	7	0.11
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG21	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG22	11	0.11
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG23	11	0.11
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG21	20	0.11
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG22	20	0.11
(1,3304)	1:1855:A:GLU:H	1:1887:A:ILE:HG23	20	0.11
(1,3274)	1:1884:A:LEU:HD11	1:1869:A:LEU:HD11	13	0.11
(1,3274)	1:1884:A:LEU:HD11	1:1869:A:LEU:HD12	13	0.11
(1,3274)	1:1884:A:LEU:HD11	1:1869:A:LEU:HD13	13	0.11
(1,3274)	1:1884:A:LEU:HD12	1:1869:A:LEU:HD11	13	0.11
(1,3274)	1:1884:A:LEU:HD12	1:1869:A:LEU:HD12	13	0.11
(1,3274)	1:1884:A:LEU:HD12	1:1869:A:LEU:HD13	13	0.11
(1,3274)	1:1884:A:LEU:HD13	1:1869:A:LEU:HD11	13	0.11
(1,3274)	1:1884:A:LEU:HD13	1:1869:A:LEU:HD12	13	0.11
(1,3274)	1:1884:A:LEU:HD13	1:1869:A:LEU:HD13	13	0.11
(1,3265)	1:1847:A:LYS:H	1:1846:A:THR:HB	13	0.11
(1,3246)	1:1904:A:SER:H	1:1905:A:PRO:HD2	14	0.11
(1,3242)	1:1823:A:LYS:H	1:1823:A:LYS:HE2	8	0.11
(1,3242)	1:1823:A:LYS:H	1:1823:A:LYS:HE3	8	0.11
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	1	0.11
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	9	0.11
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	10	0.11
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	11	0.11
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	12	0.11
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	13	0.11
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	15	0.11
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	17	0.11
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	18	0.11
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	19	0.11
(1,3238)	1:1920:A:SER:H	1:1919:A:VAL:H	6	0.11
(1,3238)	1:1920:A:SER:H	1:1919:A:VAL:H	9	0.11
(1,3238)	1:1920:A:SER:H	1:1919:A:VAL:H	11	0.11
(1,3238)	1:1920:A:SER:H	1:1919:A:VAL:H	15	0.11
(1,3238)	1:1920:A:SER:H	1:1919:A:VAL:H	20	0.11
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	2	0.11
(1,3212)	1:1902:A:GLY:H	1:1900:A:SER:HB2	17	0.11
(1,3203)	1:1903:A:ILE:H	1:1900:A:SER:HB2	8	0.11
(1,3172)	1:1902:A:GLY:H	1:1901:A:THR:HB	11	0.11
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG2	17	0.11
(1,3169)	1:1906:A:GLN:HB2	1:1906:A:GLN:HG3	17	0.11
(1,3168)	1:1874:A:GLN:HB2	1:1874:A:GLN:HG2	6	0.11
(1,3168)	1:1874:A:GLN:HB2	1:1874:A:GLN:HG2	15	0.11
(1,3166)	1:1889:A:MET:H	1:1889:A:MET:HG2	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3159)	1:1822:A:GLU:H	1:1822:A:GLU:HG2	17	0.11
(1,3144)	1:1845:A:ASN:HA	1:1845:A:ASN:HD21	13	0.11
(1,3142)	1:1900:A:SER:H	1:1900:A:SER:HA	5	0.11
(1,3142)	1:1900:A:SER:H	1:1900:A:SER:HA	16	0.11
(1,3134)	1:1852:A:GLU:HG2	1:1852:A:GLU:HB3	9	0.11
(1,3134)	1:1852:A:GLU:HG2	1:1852:A:GLU:HB3	13	0.11
(1,3134)	1:1852:A:GLU:HG2	1:1852:A:GLU:HB3	18	0.11
(1,3134)	1:1852:A:GLU:HG2	1:1852:A:GLU:HB3	20	0.11
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD21	17	0.11
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD22	17	0.11
(1,3130)	1:1854:A:TYR:HA	1:1884:A:LEU:HD23	17	0.11
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	7	0.11
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	12	0.11
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	17	0.11
(1,3115)	1:1956:A:ARG:HA	1:1957:A:PRO:HD2	19	0.11
(1,3107)	1:1825:A:SER:H	1:1825:A:SER:HB2	12	0.11
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	13	0.11
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	17	0.11
(1,3098)	1:1920:A:SER:H	1:1920:A:SER:HB3	4	0.11
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	9	0.11
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	9	0.11
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	20	0.11
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	20	0.11
(1,3086)	1:1903:A:ILE:H	1:1900:A:SER:HB3	14	0.11
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	3	0.11
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	3	0.11
(1,3075)	1:1942:A:LEU:HB3	1:1838:A:LYS:HG3	4	0.11
(1,3062)	1:1872:A:SER:H	1:1870:A:LYS:HB2	7	0.11
(1,3032)	1:1835:A:GLU:H	1:1833:A:LEU:HB2	1	0.11
(1,3032)	1:1835:A:GLU:H	1:1833:A:LEU:HB2	5	0.11
(1,3032)	1:1835:A:GLU:H	1:1833:A:LEU:HB2	6	0.11
(1,3032)	1:1835:A:GLU:H	1:1833:A:LEU:HB2	11	0.11
(1,3032)	1:1835:A:GLU:H	1:1833:A:LEU:HB2	18	0.11
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG21	5	0.11
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG22	5	0.11
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG23	5	0.11
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG21	5	0.11
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG22	5	0.11
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG23	5	0.11
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG21	5	0.11
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG22	5	0.11
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG23	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG21	8	0.11
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG22	8	0.11
(1,3016)	1:1887:A:ILE:HD11	1:1886:A:VAL:HG23	8	0.11
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG21	8	0.11
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG22	8	0.11
(1,3016)	1:1887:A:ILE:HD12	1:1886:A:VAL:HG23	8	0.11
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG21	8	0.11
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG22	8	0.11
(1,3016)	1:1887:A:ILE:HD13	1:1886:A:VAL:HG23	8	0.11
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	8	0.11
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	19	0.11
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD11	5	0.11
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD12	5	0.11
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD13	5	0.11
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD11	15	0.11
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD12	15	0.11
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD13	15	0.11
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD11	17	0.11
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD12	17	0.11
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD13	17	0.11
(1,2975)	1:1892:A:GLU:H	1:1891:A:ARG:HG3	9	0.11
(1,2975)	1:1892:A:GLU:H	1:1891:A:ARG:HG3	14	0.11
(1,2975)	1:1892:A:GLU:H	1:1891:A:ARG:HG3	17	0.11
(1,2975)	1:1892:A:GLU:H	1:1891:A:ARG:HG3	20	0.11
(1,2973)	1:1870:A:LYS:HA	1:1874:A:GLN:HE21	9	0.11
(1,2951)	1:1940:A:LYS:HD3	1:1940:A:LYS:HE2	2	0.11
(1,2951)	1:1940:A:LYS:HD3	1:1940:A:LYS:HE3	2	0.11
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG21	1	0.11
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG22	1	0.11
(1,2949)	1:1914:A:THR:H	1:1912:A:VAL:HG23	1	0.11
(1,2929)	1:1922:A:ILE:HA	1:1922:A:ILE:HB	14	0.11
(1,2929)	1:1922:A:ILE:HA	1:1922:A:ILE:HB	15	0.11
(1,2929)	1:1922:A:ILE:HA	1:1922:A:ILE:HB	19	0.11
(1,2929)	1:1922:A:ILE:HA	1:1922:A:ILE:HB	20	0.11
(1,2908)	1:1947:A:GLY:HA2	1:1949:A:ASP:H	4	0.11
(1,2908)	1:1947:A:GLY:HA3	1:1949:A:ASP:H	4	0.11
(1,2907)	1:1894:A:LYS:H	1:1894:A:LYS:HE3	6	0.11
(1,2907)	1:1894:A:LYS:H	1:1894:A:LYS:HE3	8	0.11
(1,2893)	1:1887:A:ILE:HA	1:1890:A:GLU:HB2	5	0.11
(1,2893)	1:1887:A:ILE:HA	1:1890:A:GLU:HB2	16	0.11
(1,2886)	1:1905:A:PRO:HD2	1:1905:A:PRO:HB2	4	0.11
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	2	0.11
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	2	0.11
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	2	0.11
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	2	0.11
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	2	0.11
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	2	0.11
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	2	0.11
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	2	0.11
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE1	18	0.11
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE2	18	0.11
(1,2866)	1:1886:A:VAL:HG21	1:1889:A:MET:HE3	18	0.11
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE1	18	0.11
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE2	18	0.11
(1,2866)	1:1886:A:VAL:HG22	1:1889:A:MET:HE3	18	0.11
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE1	18	0.11
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE2	18	0.11
(1,2866)	1:1886:A:VAL:HG23	1:1889:A:MET:HE3	18	0.11
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	1	0.11
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	2	0.11
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	6	0.11
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	8	0.11
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	10	0.11
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	14	0.11
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	15	0.11
(1,2863)	1:1836:A:ILE:HB	1:1835:A:GLU:HB2	17	0.11
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	1	0.11
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	6	0.11
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	8	0.11
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	14	0.11
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	15	0.11
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	17	0.11
(1,2860)	1:1908:A:GLU:H	1:1908:A:GLU:HB3	18	0.11
(1,2854)	1:1924:A:ASN:H	1:1924:A:ASN:HA	14	0.11
(1,2849)	1:1950:A:ASN:HB3	1:1951:A:THR:H	19	0.11
(1,2842)	1:1950:A:ASN:HB2	1:1951:A:THR:H	11	0.11
(1,2842)	1:1950:A:ASN:HB2	1:1951:A:THR:H	17	0.11
(1,2818)	1:1886:A:VAL:H	1:1885:A:ARG:HG3	2	0.11
(1,2818)	1:1886:A:VAL:H	1:1885:A:ARG:HG3	8	0.11
(1,2818)	1:1886:A:VAL:H	1:1885:A:ARG:HG3	13	0.11
(1,2818)	1:1886:A:VAL:H	1:1885:A:ARG:HG3	16	0.11
(1,2818)	1:1886:A:VAL:H	1:1885:A:ARG:HG3	18	0.11
(1,2818)	1:1886:A:VAL:H	1:1885:A:ARG:HG3	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2807)	1:1889:A:MET:H	1:1888:A:GLU:HB2	2	0.11
(1,2807)	1:1889:A:MET:H	1:1888:A:GLU:HB2	4	0.11
(1,2807)	1:1889:A:MET:H	1:1888:A:GLU:HB2	13	0.11
(1,2807)	1:1889:A:MET:H	1:1888:A:GLU:HB2	14	0.11
(1,2806)	1:1920:A:SER:HA	1:1915:A:PRO:HB2	9	0.11
(1,2801)	1:1874:A:GLN:HA	1:1874:A:GLN:HG2	12	0.11
(1,2776)	1:1916:A:THR:HB	1:1917:A:SER:H	17	0.11
(1,2760)	1:1903:A:ILE:HA	1:1903:A:ILE:HG12	4	0.11
(1,2760)	1:1903:A:ILE:HA	1:1903:A:ILE:HG12	15	0.11
(1,2760)	1:1903:A:ILE:HA	1:1903:A:ILE:HG12	16	0.11
(1,2737)	1:1823:A:LYS:HA	1:1824:A:SER:H	14	0.11
(1,2733)	1:1885:A:ARG:HA	1:1889:A:MET:H	3	0.11
(1,2731)	1:1916:A:THR:HG21	1:1914:A:THR:HB	19	0.11
(1,2731)	1:1916:A:THR:HG22	1:1914:A:THR:HB	19	0.11
(1,2731)	1:1916:A:THR:HG23	1:1914:A:THR:HB	19	0.11
(1,2729)	1:1856:A:TYR:H	1:1857:A:LYS:H	11	0.11
(1,2724)	1:1864:A:ASP:H	1:1864:A:ASP:HB2	13	0.11
(1,2710)	1:1899:A:THR:H	1:1898:A:SER:HA	1	0.11
(1,2710)	1:1899:A:THR:H	1:1898:A:SER:HA	12	0.11
(1,2705)	1:1889:A:MET:HA	1:1894:A:LYS:HB3	17	0.11
(1,2701)	1:1924:A:ASN:H	1:1923:A:GLY:HA2	10	0.11
(1,2701)	1:1924:A:ASN:H	1:1923:A:GLY:HA3	10	0.11
(1,2685)	1:1859:A:LYS:HA	1:1859:A:LYS:HG3	1	0.11
(1,2685)	1:1859:A:LYS:HA	1:1859:A:LYS:HG3	3	0.11
(1,2685)	1:1859:A:LYS:HA	1:1859:A:LYS:HG3	9	0.11
(1,2685)	1:1859:A:LYS:HA	1:1859:A:LYS:HG3	10	0.11
(1,2685)	1:1859:A:LYS:HA	1:1859:A:LYS:HG3	18	0.11
(1,2682)	1:1826:A:LYS:HB2	1:1871:A:ASN:HD22	4	0.11
(1,2675)	1:1865:A:ILE:HG21	1:1869:A:LEU:HD11	8	0.11
(1,2675)	1:1865:A:ILE:HG21	1:1869:A:LEU:HD12	8	0.11
(1,2675)	1:1865:A:ILE:HG21	1:1869:A:LEU:HD13	8	0.11
(1,2675)	1:1865:A:ILE:HG22	1:1869:A:LEU:HD11	8	0.11
(1,2675)	1:1865:A:ILE:HG22	1:1869:A:LEU:HD12	8	0.11
(1,2675)	1:1865:A:ILE:HG22	1:1869:A:LEU:HD13	8	0.11
(1,2675)	1:1865:A:ILE:HG23	1:1869:A:LEU:HD11	8	0.11
(1,2675)	1:1865:A:ILE:HG23	1:1869:A:LEU:HD12	8	0.11
(1,2675)	1:1865:A:ILE:HG23	1:1869:A:LEU:HD13	8	0.11
(1,2662)	1:1955:A:ASP:H	1:1956:A:ARG:H	17	0.11
(1,2651)	1:1823:A:LYS:H	1:1823:A:LYS:HB2	1	0.11
(1,2651)	1:1823:A:LYS:H	1:1823:A:LYS:HB2	19	0.11
(1,2650)	1:1904:A:SER:HB2	1:1904:A:SER:HA	19	0.11
(1,2650)	1:1904:A:SER:HB3	1:1904:A:SER:HA	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2648)	1:1853:A:LEU:HA	1:1856:A:TYR:HB3	4	0.11
(1,2648)	1:1853:A:LEU:HA	1:1856:A:TYR:HB3	10	0.11
(1,2648)	1:1853:A:LEU:HA	1:1856:A:TYR:HB3	11	0.11
(1,2648)	1:1853:A:LEU:HA	1:1856:A:TYR:HB3	13	0.11
(1,2648)	1:1853:A:LEU:HA	1:1856:A:TYR:HB3	15	0.11
(1,2648)	1:1853:A:LEU:HA	1:1856:A:TYR:HB3	19	0.11
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE1	9	0.11
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE2	9	0.11
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE1	9	0.11
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE2	9	0.11
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE1	9	0.11
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE2	9	0.11
(1,2636)	1:1909:A:VAL:HG21	1:1909:A:VAL:HA	7	0.11
(1,2636)	1:1909:A:VAL:HG22	1:1909:A:VAL:HA	7	0.11
(1,2636)	1:1909:A:VAL:HG23	1:1909:A:VAL:HA	7	0.11
(1,2613)	1:1839:A:LYS:H	1:1838:A:LYS:HG3	7	0.11
(1,2613)	1:1839:A:LYS:H	1:1838:A:LYS:HG3	10	0.11
(1,2606)	1:1840:A:ILE:HD11	1:1850:A:LEU:HA	1	0.11
(1,2606)	1:1840:A:ILE:HD12	1:1850:A:LEU:HA	1	0.11
(1,2606)	1:1840:A:ILE:HD13	1:1850:A:LEU:HA	1	0.11
(1,2606)	1:1840:A:ILE:HD11	1:1850:A:LEU:HA	9	0.11
(1,2606)	1:1840:A:ILE:HD12	1:1850:A:LEU:HA	9	0.11
(1,2606)	1:1840:A:ILE:HD13	1:1850:A:LEU:HA	9	0.11
(1,2606)	1:1840:A:ILE:HD11	1:1850:A:LEU:HA	10	0.11
(1,2606)	1:1840:A:ILE:HD12	1:1850:A:LEU:HA	10	0.11
(1,2606)	1:1840:A:ILE:HD13	1:1850:A:LEU:HA	10	0.11
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	1	0.11
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	6	0.11
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	10	0.11
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	17	0.11
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	18	0.11
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	15	0.11
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	15	0.11
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB2	20	0.11
(1,2574)	1:1855:A:GLU:HA	1:1855:A:GLU:HB3	20	0.11
(1,2564)	1:1909:A:VAL:H	1:1910:A:THR:H	11	0.11
(1,2564)	1:1909:A:VAL:H	1:1910:A:THR:H	13	0.11
(1,2564)	1:1909:A:VAL:H	1:1910:A:THR:H	15	0.11
(1,2564)	1:1909:A:VAL:H	1:1910:A:THR:H	20	0.11
(1,2559)	1:1892:A:GLU:H	1:1890:A:GLU:HA	4	0.11
(1,2559)	1:1892:A:GLU:H	1:1890:A:GLU:HA	18	0.11
(1,2559)	1:1892:A:GLU:H	1:1890:A:GLU:HA	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	14	0.11
(1,2536)	1:1848:A:GLU:H	1:1848:A:GLU:HG3	20	0.11
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	8	0.11
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	12	0.11
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	16	0.11
(1,2526)	1:1842:A:SER:HB2	1:1845:A:ASN:HD21	18	0.11
(1,2518)	1:1848:A:GLU:HB2	1:1839:A:LYS:HD2	3	0.11
(1,2518)	1:1848:A:GLU:HB2	1:1839:A:LYS:HD2	15	0.11
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	2	0.11
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	8	0.11
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	14	0.11
(1,2504)	1:1867:A:PRO:HA	1:1871:A:ASN:HD21	6	0.11
(1,2502)	1:1892:A:GLU:HG3	1:1892:A:GLU:HB3	9	0.11
(1,2502)	1:1892:A:GLU:HG3	1:1892:A:GLU:HB3	10	0.11
(1,2502)	1:1892:A:GLU:HG3	1:1892:A:GLU:HB3	16	0.11
(1,2489)	1:1893:A:GLY:H	1:1891:A:ARG:HB2	9	0.11
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	1	0.11
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	3	0.11
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	7	0.11
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	11	0.11
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	12	0.11
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	15	0.11
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	17	0.11
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	19	0.11
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	20	0.11
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE1	12	0.11
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE2	12	0.11
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE1	15	0.11
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE2	15	0.11
(1,2470)	1:1830:A:ASN:H	1:1833:A:LEU:H	8	0.11
(1,2454)	1:1818:A:SER:HB2	1:1818:A:SER:HA	9	0.11
(1,2454)	1:1818:A:SER:HB3	1:1818:A:SER:HA	9	0.11
(1,2454)	1:1818:A:SER:HB2	1:1818:A:SER:HA	15	0.11
(1,2454)	1:1818:A:SER:HB3	1:1818:A:SER:HA	15	0.11
(1,2454)	1:1818:A:SER:HB2	1:1818:A:SER:HA	16	0.11
(1,2454)	1:1818:A:SER:HB3	1:1818:A:SER:HA	16	0.11
(1,2451)	1:1861:A:SER:H	1:1860:A:TYR:HB3	1	0.11
(1,2451)	1:1861:A:SER:H	1:1860:A:TYR:HB3	4	0.11
(1,2451)	1:1861:A:SER:H	1:1860:A:TYR:HB3	6	0.11
(1,2451)	1:1861:A:SER:H	1:1860:A:TYR:HB3	10	0.11
(1,2451)	1:1861:A:SER:H	1:1860:A:TYR:HB3	15	0.11
(1,2451)	1:1861:A:SER:H	1:1860:A:TYR:HB3	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2426)	1:1907:A:MET:HA	1:1908:A:GLU:H	1	0.11
(1,2426)	1:1907:A:MET:HA	1:1908:A:GLU:H	10	0.11
(1,2426)	1:1907:A:MET:HA	1:1908:A:GLU:H	18	0.11
(1,2418)	1:1891:A:ARG:HA	1:1891:A:ARG:HG2	5	0.11
(1,2418)	1:1891:A:ARG:HA	1:1891:A:ARG:HG2	7	0.11
(1,2415)	1:1857:A:LYS:HA	1:1857:A:LYS:HG2	8	0.11
(1,2415)	1:1857:A:LYS:HA	1:1857:A:LYS:HG2	15	0.11
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	17	0.11
(1,2384)	1:1941:A:ILE:H	1:1942:A:LEU:HG	18	0.11
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	14	0.11
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	15	0.11
(1,2352)	1:1889:A:MET:HB2	1:1894:A:LYS:HB2	11	0.11
(1,2328)	1:1950:A:ASN:H	1:1951:A:THR:H	11	0.11
(1,2325)	1:1939:A:LEU:H	1:1939:A:LEU:HD21	6	0.11
(1,2325)	1:1939:A:LEU:H	1:1939:A:LEU:HD22	6	0.11
(1,2325)	1:1939:A:LEU:H	1:1939:A:LEU:HD23	6	0.11
(1,2298)	1:1891:A:ARG:H	1:1891:A:ARG:HB2	4	0.11
(1,2298)	1:1891:A:ARG:H	1:1891:A:ARG:HB2	7	0.11
(1,2287)	1:1863:A:ALA:H	1:1862:A:ASP:HA	5	0.11
(1,2287)	1:1863:A:ALA:H	1:1862:A:ASP:HA	12	0.11
(1,2287)	1:1863:A:ALA:H	1:1862:A:ASP:HA	15	0.11
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	1	0.11
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	1	0.11
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	1	0.11
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	6	0.11
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	6	0.11
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	6	0.11
(1,2284)	1:1853:A:LEU:HD21	1:1865:A:ILE:HG13	16	0.11
(1,2284)	1:1853:A:LEU:HD22	1:1865:A:ILE:HG13	16	0.11
(1,2284)	1:1853:A:LEU:HD23	1:1865:A:ILE:HG13	16	0.11
(1,2283)	1:1851:A:ALA:HA	1:1855:A:GLU:H	16	0.11
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG21	18	0.11
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG22	18	0.11
(1,2278)	1:1854:A:TYR:HB2	1:1887:A:ILE:HG23	18	0.11
(1,2268)	1:1824:A:SER:HB3	1:1825:A:SER:H	13	0.11
(1,2261)	1:1906:A:GLN:H	1:1906:A:GLN:HB2	6	0.11
(1,2261)	1:1906:A:GLN:H	1:1906:A:GLN:HB2	17	0.11
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD21	16	0.11
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD22	16	0.11
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD23	16	0.11
(1,2245)	1:1954:A:ASP:HA	1:1954:A:ASP:HB2	13	0.11
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	7	0.11
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	11	0.11
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	13	0.11
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG21	4	0.11
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG22	4	0.11
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG23	4	0.11
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG21	4	0.11
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG22	4	0.11
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG23	4	0.11
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG21	4	0.11
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG22	4	0.11
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG23	4	0.11
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG21	16	0.11
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG22	16	0.11
(1,2200)	1:1910:A:THR:HG21	1:1912:A:VAL:HG23	16	0.11
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG21	16	0.11
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG22	16	0.11
(1,2200)	1:1910:A:THR:HG22	1:1912:A:VAL:HG23	16	0.11
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG21	16	0.11
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG22	16	0.11
(1,2200)	1:1910:A:THR:HG23	1:1912:A:VAL:HG23	16	0.11
(1,2193)	1:1889:A:MET:HB2	1:1894:A:LYS:HE2	12	0.11
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG21	14	0.11
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG22	14	0.11
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG23	14	0.11
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG21	14	0.11
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG22	14	0.11
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG23	14	0.11
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG21	14	0.11
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG22	14	0.11
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG23	14	0.11
(1,2180)	1:1884:A:LEU:H	1:1850:A:LEU:HD11	20	0.11
(1,2180)	1:1884:A:LEU:H	1:1850:A:LEU:HD12	20	0.11
(1,2180)	1:1884:A:LEU:H	1:1850:A:LEU:HD13	20	0.11
(1,2179)	1:1940:A:LYS:HA	1:1943:A:ARG:HB2	14	0.11
(1,2165)	1:1841:A:GLY:H	1:1876:A:PHE:HE1	9	0.11
(1,2165)	1:1841:A:GLY:H	1:1876:A:PHE:HE2	9	0.11
(1,2162)	1:1858:A:LYS:HE3	1:1854:A:TYR:HE1	11	0.11
(1,2162)	1:1858:A:LYS:HE3	1:1854:A:TYR:HE2	11	0.11
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	5	0.11
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	8	0.11
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	1	0.11
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	1	0.11
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	1	0.11
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	4	0.11
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	4	0.11
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	4	0.11
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	5	0.11
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	5	0.11
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	5	0.11
(1,2157)	1:1851:A:ALA:HB1	1:1855:A:GLU:HB2	13	0.11
(1,2157)	1:1851:A:ALA:HB2	1:1855:A:GLU:HB2	13	0.11
(1,2157)	1:1851:A:ALA:HB3	1:1855:A:GLU:HB2	13	0.11
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	3	0.11
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	3	0.11
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	4	0.11
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	4	0.11
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	5	0.11
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	5	0.11
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	10	0.11
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	10	0.11
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	11	0.11
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	11	0.11
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	12	0.11
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	12	0.11
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	15	0.11
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	15	0.11
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG2	20	0.11
(1,2152)	1:1928:A:GLU:HB2	1:1928:A:GLU:HG3	20	0.11
(1,2134)	1:1853:A:LEU:H	1:1853:A:LEU:HB3	2	0.11
(1,2134)	1:1853:A:LEU:H	1:1853:A:LEU:HB3	10	0.11
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	2	0.11
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	2	0.11
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	2	0.11
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	12	0.11
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	12	0.11
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	12	0.11
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	20	0.11
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	20	0.11
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	20	0.11
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	2	0.11
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	3	0.11
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	16	0.11
(1,2083)	1:1854:A:TYR:H	1:1854:A:TYR:HB2	20	0.11
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	6	0.11
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	12	0.11
(1,2070)	1:1820:A:ILE:HG12	1:1821:A:ASP:H	9	0.11
(1,2070)	1:1820:A:ILE:HG12	1:1821:A:ASP:H	10	0.11
(1,2067)	1:1953:A:GLN:H	1:1953:A:GLN:HB2	4	0.11
(1,2055)	1:1922:A:ILE:HA	1:1922:A:ILE:HG12	8	0.11
(1,2055)	1:1922:A:ILE:HA	1:1922:A:ILE:HG12	10	0.11
(1,2028)	1:1824:A:SER:H	1:1823:A:LYS:HG3	10	0.11
(1,2017)	1:1838:A:LYS:HG3	1:1838:A:LYS:HE3	5	0.11
(1,1984)	1:1934:A:VAL:H	1:1934:A:VAL:HB	8	0.11
(1,1979)	1:1941:A:ILE:HG21	1:1942:A:LEU:HG	10	0.11
(1,1979)	1:1941:A:ILE:HG22	1:1942:A:LEU:HG	10	0.11
(1,1979)	1:1941:A:ILE:HG23	1:1942:A:LEU:HG	10	0.11
(1,1978)	1:1941:A:ILE:H	1:1940:A:LYS:H	1	0.11
(1,1978)	1:1941:A:ILE:H	1:1940:A:LYS:H	17	0.11
(1,1978)	1:1941:A:ILE:H	1:1940:A:LYS:H	20	0.11
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD11	2	0.11
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD12	2	0.11
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD13	2	0.11
(1,1960)	1:1828:A:LYS:HE2	1:1828:A:LYS:HD2	6	0.11
(1,1960)	1:1828:A:LYS:HE2	1:1828:A:LYS:HD3	6	0.11
(1,1960)	1:1828:A:LYS:HE3	1:1828:A:LYS:HD2	6	0.11
(1,1960)	1:1828:A:LYS:HE3	1:1828:A:LYS:HD3	6	0.11
(1,1907)	1:1858:A:LYS:HA	1:1861:A:SER:HA	6	0.11
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG21	3	0.11
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG22	3	0.11
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG23	3	0.11
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG21	8	0.11
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG22	8	0.11
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG23	8	0.11
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG21	20	0.11
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG22	20	0.11
(1,1903)	1:1906:A:GLN:H	1:1903:A:ILE:HG23	20	0.11
(1,1895)	1:1855:A:GLU:H	1:1852:A:GLU:HG2	10	0.11
(1,1895)	1:1855:A:GLU:H	1:1852:A:GLU:HG2	16	0.11
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE1	7	0.11
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE2	7	0.11
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE1	7	0.11
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE2	7	0.11
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE1	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE2	7	0.11
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE1	13	0.11
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE2	13	0.11
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE1	13	0.11
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE2	13	0.11
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE1	13	0.11
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE2	13	0.11
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE1	16	0.11
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE2	16	0.11
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE1	16	0.11
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE2	16	0.11
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE1	16	0.11
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE2	16	0.11
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE1	18	0.11
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE2	18	0.11
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE1	18	0.11
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE2	18	0.11
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE1	18	0.11
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE2	18	0.11
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE1	19	0.11
(1,1872)	1:1833:A:LEU:HD11	1:1837:A:PHE:HE2	19	0.11
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE1	19	0.11
(1,1872)	1:1833:A:LEU:HD12	1:1837:A:PHE:HE2	19	0.11
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE1	19	0.11
(1,1872)	1:1833:A:LEU:HD13	1:1837:A:PHE:HE2	19	0.11
(1,1870)	1:1956:A:ARG:H	1:1956:A:ARG:HG3	18	0.11
(1,1858)	1:1934:A:VAL:HA	1:1937:A:GLU:H	9	0.11
(1,1850)	1:1839:A:LYS:HG3	1:1839:A:LYS:HE3	20	0.11
(1,1833)	1:1941:A:ILE:H	1:1941:A:ILE:HA	6	0.11
(1,1833)	1:1941:A:ILE:H	1:1941:A:ILE:HA	8	0.11
(1,1833)	1:1941:A:ILE:H	1:1941:A:ILE:HA	9	0.11
(1,1833)	1:1941:A:ILE:H	1:1941:A:ILE:HA	20	0.11
(1,1806)	1:1840:A:ILE:HB	1:1876:A:PHE:HZ	8	0.11
(1,1806)	1:1840:A:ILE:HB	1:1876:A:PHE:HZ	17	0.11
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	1	0.11
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	2	0.11
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	4	0.11
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	5	0.11
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	9	0.11
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	11	0.11
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	13	0.11
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	20	0.11
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD21	2	0.11
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD22	2	0.11
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD23	2	0.11
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD21	10	0.11
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD22	10	0.11
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD23	10	0.11
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD21	11	0.11
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD22	11	0.11
(1,1775)	1:1883:A:GLY:HA3	1:1850:A:LEU:HD23	11	0.11
(1,1750)	1:1924:A:ASN:HB2	1:1924:A:ASN:HA	12	0.11
(1,1750)	1:1924:A:ASN:HB2	1:1924:A:ASN:HA	17	0.11
(1,1747)	1:1853:A:LEU:HD11	1:1856:A:TYR:HB2	1	0.11
(1,1747)	1:1853:A:LEU:HD12	1:1856:A:TYR:HB2	1	0.11
(1,1747)	1:1853:A:LEU:HD13	1:1856:A:TYR:HB2	1	0.11
(1,1747)	1:1853:A:LEU:HD11	1:1856:A:TYR:HB2	15	0.11
(1,1747)	1:1853:A:LEU:HD12	1:1856:A:TYR:HB2	15	0.11
(1,1747)	1:1853:A:LEU:HD13	1:1856:A:TYR:HB2	15	0.11
(1,1724)	1:1853:A:LEU:HD21	1:1869:A:LEU:HD11	1	0.11
(1,1724)	1:1853:A:LEU:HD21	1:1869:A:LEU:HD12	1	0.11
(1,1724)	1:1853:A:LEU:HD21	1:1869:A:LEU:HD13	1	0.11
(1,1724)	1:1853:A:LEU:HD22	1:1869:A:LEU:HD11	1	0.11
(1,1724)	1:1853:A:LEU:HD22	1:1869:A:LEU:HD12	1	0.11
(1,1724)	1:1853:A:LEU:HD22	1:1869:A:LEU:HD13	1	0.11
(1,1724)	1:1853:A:LEU:HD23	1:1869:A:LEU:HD11	1	0.11
(1,1724)	1:1853:A:LEU:HD23	1:1869:A:LEU:HD12	1	0.11
(1,1724)	1:1853:A:LEU:HD23	1:1869:A:LEU:HD13	1	0.11
(1,1724)	1:1853:A:LEU:HD21	1:1869:A:LEU:HD11	20	0.11
(1,1724)	1:1853:A:LEU:HD21	1:1869:A:LEU:HD12	20	0.11
(1,1724)	1:1853:A:LEU:HD21	1:1869:A:LEU:HD13	20	0.11
(1,1724)	1:1853:A:LEU:HD22	1:1869:A:LEU:HD11	20	0.11
(1,1724)	1:1853:A:LEU:HD22	1:1869:A:LEU:HD12	20	0.11
(1,1724)	1:1853:A:LEU:HD22	1:1869:A:LEU:HD13	20	0.11
(1,1724)	1:1853:A:LEU:HD23	1:1869:A:LEU:HD11	20	0.11
(1,1724)	1:1853:A:LEU:HD23	1:1869:A:LEU:HD12	20	0.11
(1,1724)	1:1853:A:LEU:HD23	1:1869:A:LEU:HD13	20	0.11
(1,1683)	1:1933:A:SER:H	1:1932:A:PRO:HB2	7	0.11
(1,1678)	1:1832:A:PHE:HD1	1:1856:A:TYR:HE1	5	0.11
(1,1678)	1:1832:A:PHE:HD1	1:1856:A:TYR:HE2	5	0.11
(1,1678)	1:1832:A:PHE:HD2	1:1856:A:TYR:HE1	5	0.11
(1,1678)	1:1832:A:PHE:HD2	1:1856:A:TYR:HE2	5	0.11
(1,1678)	1:1832:A:PHE:HD1	1:1856:A:TYR:HE1	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1678)	1:1832:A:PHE:HD1	1:1856:A:TYR:HE2	8	0.11
(1,1678)	1:1832:A:PHE:HD2	1:1856:A:TYR:HE1	8	0.11
(1,1678)	1:1832:A:PHE:HD2	1:1856:A:TYR:HE2	8	0.11
(1,1678)	1:1832:A:PHE:HD1	1:1856:A:TYR:HE1	11	0.11
(1,1678)	1:1832:A:PHE:HD1	1:1856:A:TYR:HE2	11	0.11
(1,1678)	1:1832:A:PHE:HD2	1:1856:A:TYR:HE1	11	0.11
(1,1678)	1:1832:A:PHE:HD2	1:1856:A:TYR:HE2	11	0.11
(1,1678)	1:1832:A:PHE:HD1	1:1856:A:TYR:HE1	20	0.11
(1,1678)	1:1832:A:PHE:HD1	1:1856:A:TYR:HE2	20	0.11
(1,1678)	1:1832:A:PHE:HD2	1:1856:A:TYR:HE1	20	0.11
(1,1678)	1:1832:A:PHE:HD2	1:1856:A:TYR:HE2	20	0.11
(1,1675)	1:1924:A:ASN:H	1:1924:A:ASN:HB2	1	0.11
(1,1675)	1:1924:A:ASN:H	1:1924:A:ASN:HB2	9	0.11
(1,1666)	1:1907:A:MET:HG2	1:1908:A:GLU:H	9	0.11
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	20	0.11
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	20	0.11
(1,1638)	1:1869:A:LEU:HD11	1:1876:A:PHE:HE1	5	0.11
(1,1638)	1:1869:A:LEU:HD11	1:1876:A:PHE:HE2	5	0.11
(1,1638)	1:1869:A:LEU:HD12	1:1876:A:PHE:HE1	5	0.11
(1,1638)	1:1869:A:LEU:HD12	1:1876:A:PHE:HE2	5	0.11
(1,1638)	1:1869:A:LEU:HD13	1:1876:A:PHE:HE1	5	0.11
(1,1638)	1:1869:A:LEU:HD13	1:1876:A:PHE:HE2	5	0.11
(1,1619)	1:1887:A:ILE:HG21	1:1890:A:GLU:HB2	4	0.11
(1,1619)	1:1887:A:ILE:HG22	1:1890:A:GLU:HB2	4	0.11
(1,1619)	1:1887:A:ILE:HG23	1:1890:A:GLU:HB2	4	0.11
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD11	2	0.11
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD12	2	0.11
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD13	2	0.11
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD11	2	0.11
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD12	2	0.11
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD13	2	0.11
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD11	2	0.11
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD12	2	0.11
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD13	2	0.11
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD11	10	0.11
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD12	10	0.11
(1,1618)	1:1884:A:LEU:HD11	1:1853:A:LEU:HD13	10	0.11
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD11	10	0.11
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD12	10	0.11
(1,1618)	1:1884:A:LEU:HD12	1:1853:A:LEU:HD13	10	0.11
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD11	10	0.11
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD12	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1618)	1:1884:A:LEU:HD13	1:1853:A:LEU:HD13	10	0.11
(1,1599)	1:1846:A:THR:HA	1:1842:A:SER:H	12	0.11
(1,1588)	1:1882:A:ARG:H	1:1880:A:VAL:H	10	0.11
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE2	5	0.11
(1,1587)	1:1823:A:LYS:HG3	1:1823:A:LYS:HE3	5	0.11
(1,1567)	1:1894:A:LYS:H	1:1894:A:LYS:HD2	5	0.11
(1,1567)	1:1894:A:LYS:H	1:1894:A:LYS:HD2	7	0.11
(1,1567)	1:1894:A:LYS:H	1:1894:A:LYS:HD2	14	0.11
(1,1565)	1:1838:A:LYS:HA	1:1842:A:SER:H	6	0.11
(1,1556)	1:1853:A:LEU:HD11	1:1857:A:LYS:HD2	2	0.11
(1,1556)	1:1853:A:LEU:HD12	1:1857:A:LYS:HD2	2	0.11
(1,1556)	1:1853:A:LEU:HD13	1:1857:A:LYS:HD2	2	0.11
(1,1556)	1:1853:A:LEU:HD11	1:1857:A:LYS:HD2	5	0.11
(1,1556)	1:1853:A:LEU:HD12	1:1857:A:LYS:HD2	5	0.11
(1,1556)	1:1853:A:LEU:HD13	1:1857:A:LYS:HD2	5	0.11
(1,1556)	1:1853:A:LEU:HD11	1:1857:A:LYS:HD2	15	0.11
(1,1556)	1:1853:A:LEU:HD12	1:1857:A:LYS:HD2	15	0.11
(1,1556)	1:1853:A:LEU:HD13	1:1857:A:LYS:HD2	15	0.11
(1,1504)	1:1855:A:GLU:HA	1:1858:A:LYS:HE2	3	0.11
(1,1504)	1:1855:A:GLU:HA	1:1858:A:LYS:HE2	13	0.11
(1,1504)	1:1855:A:GLU:HA	1:1858:A:LYS:HE2	20	0.11
(1,1479)	1:1867:A:PRO:HD2	1:1868:A:PHE:H	5	0.11
(1,1479)	1:1867:A:PRO:HD2	1:1868:A:PHE:H	10	0.11
(1,1458)	1:1955:A:ASP:H	1:1954:A:ASP:HA	14	0.11
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	9	0.11
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	4	0.11
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	4	0.11
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	6	0.11
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	6	0.11
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	8	0.11
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	8	0.11
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	14	0.11
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	14	0.11
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	19	0.11
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	19	0.11
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	2	0.11
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	2	0.11
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	16	0.11
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	16	0.11
(1,1416)	1:1830:A:ASN:HB2	1:1827:A:ALA:HA	17	0.11
(1,1416)	1:1830:A:ASN:HB3	1:1827:A:ALA:HA	17	0.11
(1,1415)	1:1897:A:ILE:H	1:1897:A:ILE:HG21	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1415)	1:1897:A:ILE:H	1:1897:A:ILE:HG22	16	0.11
(1,1415)	1:1897:A:ILE:H	1:1897:A:ILE:HG23	16	0.11
(1,1395)	1:1893:A:GLY:H	1:1892:A:GLU:HG3	5	0.11
(1,1395)	1:1893:A:GLY:H	1:1892:A:GLU:HG3	6	0.11
(1,1395)	1:1893:A:GLY:H	1:1892:A:GLU:HG3	12	0.11
(1,1395)	1:1893:A:GLY:H	1:1892:A:GLU:HG3	19	0.11
(1,1381)	1:1922:A:ILE:H	1:1921:A:SER:HB2	6	0.11
(1,1381)	1:1922:A:ILE:H	1:1921:A:SER:HB2	20	0.11
(1,1379)	1:1939:A:LEU:HD11	1:1839:A:LYS:HB2	13	0.11
(1,1379)	1:1939:A:LEU:HD12	1:1839:A:LYS:HB2	13	0.11
(1,1379)	1:1939:A:LEU:HD13	1:1839:A:LYS:HB2	13	0.11
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD21	3	0.11
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD22	3	0.11
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD23	3	0.11
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD21	3	0.11
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD22	3	0.11
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD23	3	0.11
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD21	3	0.11
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD22	3	0.11
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD23	3	0.11
(1,1342)	1:1859:A:LYS:H	1:1858:A:LYS:HG3	7	0.11
(1,1342)	1:1859:A:LYS:H	1:1858:A:LYS:HG3	10	0.11
(1,1342)	1:1859:A:LYS:H	1:1858:A:LYS:HG3	11	0.11
(1,1342)	1:1859:A:LYS:H	1:1858:A:LYS:HG3	18	0.11
(1,1342)	1:1859:A:LYS:H	1:1858:A:LYS:HG3	19	0.11
(1,1335)	1:1953:A:GLN:HA	1:1953:A:GLN:HG2	18	0.11
(1,1334)	1:1884:A:LEU:H	1:1882:A:ARG:HB3	7	0.11
(1,1330)	1:1893:A:GLY:H	1:1892:A:GLU:HB2	8	0.11
(1,1328)	1:1864:A:ASP:H	1:1865:A:ILE:HB	2	0.11
(1,1307)	1:1821:A:ASP:HA	1:1823:A:LYS:H	5	0.11
(1,1255)	1:1865:A:ILE:HD11	1:1857:A:LYS:HE2	6	0.11
(1,1255)	1:1865:A:ILE:HD12	1:1857:A:LYS:HE2	6	0.11
(1,1255)	1:1865:A:ILE:HD13	1:1857:A:LYS:HE2	6	0.11
(1,1253)	1:1896:A:ARG:H	1:1896:A:ARG:HG2	17	0.11
(1,1239)	1:1890:A:GLU:HA	1:1896:A:ARG:HG3	17	0.11
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	2	0.11
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	2	0.11
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	2	0.11
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	5	0.11
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	5	0.11
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	5	0.11
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	11	0.11
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	11	0.11
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	15	0.11
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	15	0.11
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	15	0.11
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD11	16	0.11
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD12	16	0.11
(1,1221)	1:1869:A:LEU:H	1:1869:A:LEU:HD13	16	0.11
(1,1200)	1:1922:A:ILE:HB	1:1922:A:ILE:H	4	0.11
(1,1200)	1:1922:A:ILE:HB	1:1922:A:ILE:H	14	0.11
(1,1195)	1:1829:A:VAL:HG21	1:1833:A:LEU:HD11	9	0.11
(1,1195)	1:1829:A:VAL:HG21	1:1833:A:LEU:HD12	9	0.11
(1,1195)	1:1829:A:VAL:HG21	1:1833:A:LEU:HD13	9	0.11
(1,1195)	1:1829:A:VAL:HG22	1:1833:A:LEU:HD11	9	0.11
(1,1195)	1:1829:A:VAL:HG22	1:1833:A:LEU:HD12	9	0.11
(1,1195)	1:1829:A:VAL:HG22	1:1833:A:LEU:HD13	9	0.11
(1,1195)	1:1829:A:VAL:HG23	1:1833:A:LEU:HD11	9	0.11
(1,1195)	1:1829:A:VAL:HG23	1:1833:A:LEU:HD12	9	0.11
(1,1195)	1:1829:A:VAL:HG23	1:1833:A:LEU:HD13	9	0.11
(1,1187)	1:1838:A:LYS:H	1:1838:A:LYS:HG3	9	0.11
(1,1187)	1:1838:A:LYS:H	1:1838:A:LYS:HG3	11	0.11
(1,1187)	1:1838:A:LYS:H	1:1838:A:LYS:HG3	13	0.11
(1,1187)	1:1838:A:LYS:H	1:1838:A:LYS:HG3	15	0.11
(1,1187)	1:1838:A:LYS:H	1:1838:A:LYS:HG3	19	0.11
(1,1173)	1:1902:A:GLY:H	1:1903:A:ILE:HD11	1	0.11
(1,1173)	1:1902:A:GLY:H	1:1903:A:ILE:HD12	1	0.11
(1,1173)	1:1902:A:GLY:H	1:1903:A:ILE:HD13	1	0.11
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG11	6	0.11
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG12	6	0.11
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG13	6	0.11
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG11	9	0.11
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG12	9	0.11
(1,1137)	1:1908:A:GLU:H	1:1909:A:VAL:HG13	9	0.11
(1,1120)	1:1941:A:ILE:HD11	1:1944:A:GLN:HE22	1	0.11
(1,1120)	1:1941:A:ILE:HD12	1:1944:A:GLN:HE22	1	0.11
(1,1120)	1:1941:A:ILE:HD13	1:1944:A:GLN:HE22	1	0.11
(1,1120)	1:1941:A:ILE:HD11	1:1944:A:GLN:HE22	10	0.11
(1,1120)	1:1941:A:ILE:HD12	1:1944:A:GLN:HE22	10	0.11
(1,1120)	1:1941:A:ILE:HD13	1:1944:A:GLN:HE22	10	0.11
(1,1090)	1:1852:A:GLU:H	1:1850:A:LEU:H	1	0.11
(1,1090)	1:1852:A:GLU:H	1:1850:A:LEU:H	6	0.11
(1,1090)	1:1852:A:GLU:H	1:1850:A:LEU:H	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1080)	1:1847:A:LYS:HA	1:1850:A:LEU:HB2	7	0.11
(1,1080)	1:1847:A:LYS:HA	1:1850:A:LEU:HB2	13	0.11
(1,1080)	1:1847:A:LYS:HA	1:1850:A:LEU:HB2	14	0.11
(1,1056)	1:1927:A:GLY:H	1:1926:A:ASN:HA	7	0.11
(1,1029)	1:1836:A:ILE:HA	1:1836:A:ILE:HG13	2	0.11
(1,1029)	1:1836:A:ILE:HA	1:1836:A:ILE:HG13	4	0.11
(1,1029)	1:1836:A:ILE:HA	1:1836:A:ILE:HG13	6	0.11
(1,1029)	1:1836:A:ILE:HA	1:1836:A:ILE:HG13	9	0.11
(1,1029)	1:1836:A:ILE:HA	1:1836:A:ILE:HG13	14	0.11
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	4	0.11
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	5	0.11
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	9	0.11
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	12	0.11
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	13	0.11
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	15	0.11
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	18	0.11
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	19	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	4	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	4	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	4	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	8	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	8	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	8	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	11	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	11	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	11	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	12	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	12	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	12	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	13	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	13	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	13	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	18	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	18	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	18	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	19	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	19	0.11
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	19	0.11
(1,1000)	1:1917:A:SER:HA	1:1918:A:THR:H	5	0.11
(1,1000)	1:1917:A:SER:HA	1:1918:A:THR:H	10	0.11
(1,1000)	1:1917:A:SER:HA	1:1918:A:THR:H	14	0.11
(1,994)	1:1889:A:MET:HE1	1:1885:A:ARG:HG2	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:1889:A:MET:HE2	1:1885:A:ARG:HG2	10	0.11
(1,994)	1:1889:A:MET:HE3	1:1885:A:ARG:HG2	10	0.11
(1,986)	1:1837:A:PHE:H	1:1840:A:ILE:H	3	0.11
(1,986)	1:1837:A:PHE:H	1:1840:A:ILE:H	5	0.11
(1,986)	1:1837:A:PHE:H	1:1840:A:ILE:H	8	0.11
(1,986)	1:1837:A:PHE:H	1:1840:A:ILE:H	9	0.11
(1,986)	1:1837:A:PHE:H	1:1840:A:ILE:H	11	0.11
(1,986)	1:1837:A:PHE:H	1:1840:A:ILE:H	12	0.11
(1,986)	1:1837:A:PHE:H	1:1840:A:ILE:H	16	0.11
(1,986)	1:1837:A:PHE:H	1:1840:A:ILE:H	20	0.11
(1,975)	1:1876:A:PHE:H	1:1876:A:PHE:HB3	10	0.11
(1,974)	1:1856:A:TYR:HD1	1:1833:A:LEU:HD11	3	0.11
(1,974)	1:1856:A:TYR:HD1	1:1833:A:LEU:HD12	3	0.11
(1,974)	1:1856:A:TYR:HD1	1:1833:A:LEU:HD13	3	0.11
(1,974)	1:1856:A:TYR:HD2	1:1833:A:LEU:HD11	3	0.11
(1,974)	1:1856:A:TYR:HD2	1:1833:A:LEU:HD12	3	0.11
(1,974)	1:1856:A:TYR:HD2	1:1833:A:LEU:HD13	3	0.11
(1,974)	1:1856:A:TYR:HD1	1:1833:A:LEU:HD11	20	0.11
(1,974)	1:1856:A:TYR:HD1	1:1833:A:LEU:HD12	20	0.11
(1,974)	1:1856:A:TYR:HD1	1:1833:A:LEU:HD13	20	0.11
(1,974)	1:1856:A:TYR:HD2	1:1833:A:LEU:HD11	20	0.11
(1,974)	1:1856:A:TYR:HD2	1:1833:A:LEU:HD12	20	0.11
(1,974)	1:1856:A:TYR:HD2	1:1833:A:LEU:HD13	20	0.11
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	2	0.11
(1,967)	1:1916:A:THR:H	1:1917:A:SER:H	19	0.11
(1,959)	1:1898:A:SER:H	1:1897:A:ILE:HG12	14	0.11
(1,952)	1:1949:A:ASP:HA	1:1949:A:ASP:HB3	7	0.11
(1,952)	1:1949:A:ASP:HA	1:1949:A:ASP:HB3	14	0.11
(1,937)	1:1894:A:LYS:H	1:1894:A:LYS:HG3	4	0.11
(1,937)	1:1894:A:LYS:H	1:1894:A:LYS:HG3	12	0.11
(1,937)	1:1894:A:LYS:H	1:1894:A:LYS:HG3	15	0.11
(1,937)	1:1894:A:LYS:H	1:1894:A:LYS:HG3	17	0.11
(1,929)	1:1922:A:ILE:HG13	1:1922:A:ILE:H	8	0.11
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB2	2	0.11
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB3	2	0.11
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB2	4	0.11
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB3	4	0.11
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB2	10	0.11
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB3	10	0.11
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB2	15	0.11
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB3	15	0.11
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB2	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,909)	1:1944:A:GLN:H	1:1944:A:GLN:HB3	18	0.11
(1,889)	1:1889:A:MET:H	1:1892:A:GLU:HG3	4	0.11
(1,889)	1:1889:A:MET:H	1:1892:A:GLU:HG3	20	0.11
(1,888)	1:1887:A:ILE:HA	1:1890:A:GLU:HG2	8	0.11
(1,888)	1:1887:A:ILE:HA	1:1890:A:GLU:HG2	17	0.11
(1,878)	1:1820:A:ILE:H	1:1820:A:ILE:HB	3	0.11
(1,878)	1:1820:A:ILE:H	1:1820:A:ILE:HB	16	0.11
(1,878)	1:1820:A:ILE:H	1:1820:A:ILE:HB	17	0.11
(1,874)	1:1823:A:LYS:H	1:1820:A:ILE:HG21	18	0.11
(1,874)	1:1823:A:LYS:H	1:1820:A:ILE:HG22	18	0.11
(1,874)	1:1823:A:LYS:H	1:1820:A:ILE:HG23	18	0.11
(1,844)	1:1890:A:GLU:HA	1:1890:A:GLU:HG2	1	0.11
(1,844)	1:1890:A:GLU:HA	1:1890:A:GLU:HG2	5	0.11
(1,844)	1:1890:A:GLU:HA	1:1890:A:GLU:HG2	10	0.11
(1,844)	1:1890:A:GLU:HA	1:1890:A:GLU:HG2	17	0.11
(1,834)	1:1886:A:VAL:H	1:1885:A:ARG:H	17	0.11
(1,828)	1:1851:A:ALA:HB1	1:1852:A:GLU:HG2	3	0.11
(1,828)	1:1851:A:ALA:HB2	1:1852:A:GLU:HG2	3	0.11
(1,828)	1:1851:A:ALA:HB3	1:1852:A:GLU:HG2	3	0.11
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	3	0.11
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	3	0.11
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	3	0.11
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB1	11	0.11
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB2	11	0.11
(1,819)	1:1848:A:GLU:H	1:1851:A:ALA:HB3	11	0.11
(1,804)	1:1845:A:ASN:H	1:1845:A:ASN:HD22	10	0.11
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG21	16	0.11
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG22	16	0.11
(1,780)	1:1919:A:VAL:HG21	1:1916:A:THR:HG23	16	0.11
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG21	16	0.11
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG22	16	0.11
(1,780)	1:1919:A:VAL:HG22	1:1916:A:THR:HG23	16	0.11
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG21	16	0.11
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG22	16	0.11
(1,780)	1:1919:A:VAL:HG23	1:1916:A:THR:HG23	16	0.11
(1,739)	1:1822:A:GLU:H	1:1822:A:GLU:HG3	4	0.11
(1,739)	1:1822:A:GLU:H	1:1822:A:GLU:HG3	17	0.11
(1,736)	1:1898:A:SER:H	1:1897:A:ILE:H	10	0.11
(1,731)	1:1952:A:LYS:H	1:1952:A:LYS:HG2	3	0.11
(1,731)	1:1952:A:LYS:H	1:1952:A:LYS:HG3	3	0.11
(1,719)	1:1877:A:GLN:H	1:1878:A:SER:HB2	20	0.11
(1,712)	1:1848:A:GLU:HG3	1:1839:A:LYS:HD2	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:1956:A:ARG:H	1:1956:A:ARG:HB3	20	0.11
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	1	0.11
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	3	0.11
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	10	0.11
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	13	0.11
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	16	0.11
(1,691)	1:1871:A:ASN:HA	1:1871:A:ASN:HD22	20	0.11
(1,679)	1:1954:A:ASP:H	1:1953:A:GLN:HB2	3	0.11
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	6	0.11
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	11	0.11
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	17	0.11
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	18	0.11
(1,669)	1:1890:A:GLU:H	1:1890:A:GLU:HG3	9	0.11
(1,669)	1:1890:A:GLU:H	1:1890:A:GLU:HG3	16	0.11
(1,666)	1:1942:A:LEU:HD21	1:1839:A:LYS:HG2	12	0.11
(1,666)	1:1942:A:LEU:HD22	1:1839:A:LYS:HG2	12	0.11
(1,666)	1:1942:A:LEU:HD23	1:1839:A:LYS:HG2	12	0.11
(1,666)	1:1942:A:LEU:HD21	1:1839:A:LYS:HG2	17	0.11
(1,666)	1:1942:A:LEU:HD22	1:1839:A:LYS:HG2	17	0.11
(1,666)	1:1942:A:LEU:HD23	1:1839:A:LYS:HG2	17	0.11
(1,632)	1:1949:A:ASP:H	1:1949:A:ASP:HB3	2	0.11
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE1	2	0.11
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE2	2	0.11
(1,631)	1:1889:A:MET:HG3	1:1889:A:MET:HE3	2	0.11
(1,630)	1:1926:A:ASN:HA	1:1926:A:ASN:HB2	17	0.11
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	2	0.11
(1,624)	1:1939:A:LEU:HB2	1:1839:A:LYS:HG3	12	0.11
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	1	0.11
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	4	0.11
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	14	0.11
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	16	0.11
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	17	0.11
(1,617)	1:1881:A:GLU:H	1:1879:A:TYR:HA	19	0.11
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	9	0.11
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	10	0.11
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	12	0.11
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	20	0.11
(1,615)	1:1880:A:VAL:H	1:1881:A:GLU:HB2	3	0.11
(1,615)	1:1880:A:VAL:H	1:1881:A:GLU:HB2	13	0.11
(1,615)	1:1880:A:VAL:H	1:1881:A:GLU:HB2	15	0.11
(1,615)	1:1880:A:VAL:H	1:1881:A:GLU:HB2	18	0.11
(1,615)	1:1880:A:VAL:H	1:1881:A:GLU:HB2	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:1880:A:VAL:H	1:1881:A:GLU:HB2	20	0.11
(1,612)	1:1900:A:SER:HB3	1:1901:A:THR:H	2	0.11
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	2	0.11
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	2	0.11
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	4	0.11
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	4	0.11
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	10	0.11
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	10	0.11
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	13	0.11
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	13	0.11
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	18	0.11
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	18	0.11
(1,602)	1:1900:A:SER:HA	1:1899:A:THR:HG21	9	0.11
(1,602)	1:1900:A:SER:HA	1:1899:A:THR:HG22	9	0.11
(1,602)	1:1900:A:SER:HA	1:1899:A:THR:HG23	9	0.11
(1,595)	1:1823:A:LYS:HA	1:1823:A:LYS:HB2	4	0.11
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	5	0.11
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	10	0.11
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	16	0.11
(1,585)	1:1923:A:GLY:H	1:1922:A:ILE:HB	7	0.11
(1,585)	1:1923:A:GLY:H	1:1922:A:ILE:HB	9	0.11
(1,585)	1:1923:A:GLY:H	1:1922:A:ILE:HB	19	0.11
(1,579)	1:1897:A:ILE:H	1:1897:A:ILE:HG12	6	0.11
(1,558)	1:1929:A:GLU:H	1:1928:A:GLU:HA	5	0.11
(1,558)	1:1929:A:GLU:H	1:1928:A:GLU:HA	15	0.11
(1,532)	1:1946:A:CYS:HB2	1:1946:A:CYS:HA	5	0.11
(1,526)	1:1885:A:ARG:HA	1:1888:A:GLU:HG2	5	0.11
(1,526)	1:1885:A:ARG:HA	1:1888:A:GLU:HG2	11	0.11
(1,526)	1:1885:A:ARG:HA	1:1888:A:GLU:HG2	20	0.11
(1,520)	1:1817:A:ALA:HB1	1:1818:A:SER:H	16	0.11
(1,520)	1:1817:A:ALA:HB2	1:1818:A:SER:H	16	0.11
(1,520)	1:1817:A:ALA:HB3	1:1818:A:SER:H	16	0.11
(1,509)	1:1865:A:ILE:HG21	1:1866:A:GLU:H	3	0.11
(1,509)	1:1865:A:ILE:HG22	1:1866:A:GLU:H	3	0.11
(1,509)	1:1865:A:ILE:HG23	1:1866:A:GLU:H	3	0.11
(1,509)	1:1865:A:ILE:HG21	1:1866:A:GLU:H	4	0.11
(1,509)	1:1865:A:ILE:HG22	1:1866:A:GLU:H	4	0.11
(1,509)	1:1865:A:ILE:HG23	1:1866:A:GLU:H	4	0.11
(1,509)	1:1865:A:ILE:HG21	1:1866:A:GLU:H	10	0.11
(1,509)	1:1865:A:ILE:HG22	1:1866:A:GLU:H	10	0.11
(1,509)	1:1865:A:ILE:HG23	1:1866:A:GLU:H	10	0.11
(1,509)	1:1865:A:ILE:HG21	1:1866:A:GLU:H	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,509)	1:1865:A:ILE:HG22	1:1866:A:GLU:H	18	0.11
(1,509)	1:1865:A:ILE:HG23	1:1866:A:GLU:H	18	0.11
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	2	0.11
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	6	0.11
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	7	0.11
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	12	0.11
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	16	0.11
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	17	0.11
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	19	0.11
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	9	0.11
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	11	0.11
(1,474)	1:1877:A:GLN:HG2	1:1874:A:GLN:HA	1	0.11
(1,474)	1:1877:A:GLN:HG2	1:1874:A:GLN:HA	2	0.11
(1,474)	1:1877:A:GLN:HG2	1:1874:A:GLN:HA	20	0.11
(1,472)	1:1894:A:LYS:H	1:1894:A:LYS:HB3	9	0.11
(1,472)	1:1894:A:LYS:H	1:1894:A:LYS:HB3	10	0.11
(1,472)	1:1894:A:LYS:H	1:1894:A:LYS:HB3	13	0.11
(1,466)	1:1917:A:SER:H	1:1917:A:SER:HB2	3	0.11
(1,466)	1:1917:A:SER:H	1:1917:A:SER:HB2	4	0.11
(1,466)	1:1917:A:SER:H	1:1917:A:SER:HB2	20	0.11
(1,461)	1:1845:A:ASN:HD21	1:1839:A:LYS:HG3	7	0.11
(1,450)	1:1896:A:ARG:HB2	1:1890:A:GLU:HG2	2	0.11
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	18	0.11
(1,444)	1:1872:A:SER:H	1:1877:A:GLN:HG3	6	0.11
(1,444)	1:1872:A:SER:H	1:1877:A:GLN:HG3	10	0.11
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	1	0.11
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	1	0.11
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	12	0.11
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	12	0.11
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	16	0.11
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	16	0.11
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	18	0.11
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	18	0.11
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	19	0.11
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	19	0.11
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	20	0.11
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	20	0.11
(1,385)	1:1952:A:LYS:H	1:1951:A:THR:HA	17	0.11
(1,383)	1:1830:A:ASN:HA	1:1833:A:LEU:HB3	5	0.11
(1,383)	1:1830:A:ASN:HA	1:1833:A:LEU:HB3	9	0.11
(1,380)	1:1838:A:LYS:HG3	1:1838:A:LYS:HE2	17	0.11
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	4	0.11
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	6	0.11
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	10	0.11
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	15	0.11
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	18	0.11
(1,377)	1:1820:A:ILE:HB	1:1823:A:LYS:HG2	8	0.11
(1,377)	1:1820:A:ILE:HB	1:1823:A:LYS:HG2	14	0.11
(1,377)	1:1820:A:ILE:HB	1:1823:A:LYS:HG2	15	0.11
(1,375)	1:1896:A:ARG:HG2	1:1896:A:ARG:HD2	7	0.11
(1,375)	1:1896:A:ARG:HG2	1:1896:A:ARG:HD3	7	0.11
(1,375)	1:1896:A:ARG:HG2	1:1896:A:ARG:HD2	14	0.11
(1,375)	1:1896:A:ARG:HG2	1:1896:A:ARG:HD3	14	0.11
(1,366)	1:1936:A:LEU:H	1:1934:A:VAL:HA	15	0.11
(1,362)	1:1854:A:TYR:HA	1:1857:A:LYS:HB2	16	0.11
(1,330)	1:1827:A:ALA:H	1:1826:A:LYS:HB3	3	0.11
(1,330)	1:1827:A:ALA:H	1:1826:A:LYS:HB3	8	0.11
(1,330)	1:1827:A:ALA:H	1:1826:A:LYS:HB3	16	0.11
(1,325)	1:1936:A:LEU:HB2	1:1933:A:SER:HA	1	0.11
(1,325)	1:1936:A:LEU:HB2	1:1933:A:SER:HA	3	0.11
(1,325)	1:1936:A:LEU:HB2	1:1933:A:SER:HA	4	0.11
(1,325)	1:1936:A:LEU:HB2	1:1933:A:SER:HA	12	0.11
(1,325)	1:1936:A:LEU:HB2	1:1933:A:SER:HA	18	0.11
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD11	11	0.11
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD12	11	0.11
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD13	11	0.11
(1,316)	1:1919:A:VAL:HG21	1:1918:A:THR:HG21	16	0.11
(1,316)	1:1919:A:VAL:HG21	1:1918:A:THR:HG22	16	0.11
(1,316)	1:1919:A:VAL:HG21	1:1918:A:THR:HG23	16	0.11
(1,316)	1:1919:A:VAL:HG22	1:1918:A:THR:HG21	16	0.11
(1,316)	1:1919:A:VAL:HG22	1:1918:A:THR:HG22	16	0.11
(1,316)	1:1919:A:VAL:HG22	1:1918:A:THR:HG23	16	0.11
(1,316)	1:1919:A:VAL:HG23	1:1918:A:THR:HG21	16	0.11
(1,316)	1:1919:A:VAL:HG23	1:1918:A:THR:HG22	16	0.11
(1,316)	1:1919:A:VAL:HG23	1:1918:A:THR:HG23	16	0.11
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	9	0.11
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	11	0.11
(1,309)	1:1938:A:ARG:HA	1:1939:A:LEU:H	20	0.11
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	3	0.11
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	3	0.11
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	13	0.11
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	13	0.11
(1,265)	1:1904:A:SER:HB2	1:1913:A:PRO:HG3	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	5	0.11
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	5	0.11
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	19	0.11
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	19	0.11
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	20	0.11
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	20	0.11
(1,247)	1:1905:A:PRO:HD3	1:1905:A:PRO:HB3	7	0.11
(1,247)	1:1905:A:PRO:HD3	1:1905:A:PRO:HB3	8	0.11
(1,247)	1:1905:A:PRO:HD3	1:1905:A:PRO:HB3	10	0.11
(1,247)	1:1905:A:PRO:HD3	1:1905:A:PRO:HB3	17	0.11
(1,246)	1:1874:A:GLN:H	1:1874:A:GLN:HG2	16	0.11
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD11	2	0.11
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD12	2	0.11
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD13	2	0.11
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD11	12	0.11
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD12	12	0.11
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD13	12	0.11
(1,239)	1:1896:A:ARG:H	1:1897:A:ILE:HB	20	0.11
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	1	0.11
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	4	0.11
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	6	0.11
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	7	0.11
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	8	0.11
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	11	0.11
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	14	0.11
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	19	0.11
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG21	14	0.11
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG22	14	0.11
(1,208)	1:1928:A:GLU:HG2	1:1930:A:VAL:HG23	14	0.11
(1,195)	1:1844:A:GLU:HA	1:1846:A:THR:HG21	9	0.11
(1,195)	1:1844:A:GLU:HA	1:1846:A:THR:HG22	9	0.11
(1,195)	1:1844:A:GLU:HA	1:1846:A:THR:HG23	9	0.11
(1,186)	1:1884:A:LEU:HD11	1:1857:A:LYS:HD3	11	0.11
(1,186)	1:1884:A:LEU:HD12	1:1857:A:LYS:HD3	11	0.11
(1,186)	1:1884:A:LEU:HD13	1:1857:A:LYS:HD3	11	0.11
(1,181)	1:1916:A:THR:H	1:1916:A:THR:HG21	7	0.11
(1,181)	1:1916:A:THR:H	1:1916:A:THR:HG22	7	0.11
(1,181)	1:1916:A:THR:H	1:1916:A:THR:HG23	7	0.11
(1,104)	1:1951:A:THR:H	1:1951:A:THR:HB	5	0.11
(1,98)	1:1879:A:TYR:H	1:1879:A:TYR:HB2	5	0.11
(1,97)	1:1927:A:GLY:H	1:1929:A:GLU:H	1	0.11
(1,96)	1:1828:A:LYS:HA	1:1831:A:ASP:HB3	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:1857:A:LYS:HA	1:1865:A:ILE:HD11	19	0.11
(1,93)	1:1857:A:LYS:HA	1:1865:A:ILE:HD12	19	0.11
(1,93)	1:1857:A:LYS:HA	1:1865:A:ILE:HD13	19	0.11
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	2	0.11
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	3	0.11
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	5	0.11
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	11	0.11
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	12	0.11
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	14	0.11
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	18	0.11
(1,69)	1:1883:A:GLY:HA2	1:1887:A:ILE:H	10	0.11
(1,69)	1:1883:A:GLY:HA2	1:1887:A:ILE:H	16	0.11
(1,55)	1:1874:A:GLN:HB2	1:1874:A:GLN:HE21	2	0.11
(1,55)	1:1874:A:GLN:HB2	1:1874:A:GLN:HE21	10	0.11
(1,55)	1:1874:A:GLN:HB2	1:1874:A:GLN:HE21	20	0.11
(1,31)	1:1827:A:ALA:H	1:1826:A:LYS:HB2	17	0.11
(3,56)	1:1945:A:ARG:N	1:1941:A:ILE:O	12	0.1
(1,3293)	1:1854:A:TYR:HD1	1:1855:A:GLU:HG2	11	0.1
(1,3293)	1:1854:A:TYR:HD2	1:1855:A:GLU:HG2	11	0.1
(1,3291)	1:1907:A:MET:HB2	1:1908:A:GLU:H	18	0.1
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	5	0.1
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	6	0.1
(1,3239)	1:1872:A:SER:HB2	1:1872:A:SER:HA	16	0.1
(1,3238)	1:1920:A:SER:H	1:1919:A:VAL:H	1	0.1
(1,3238)	1:1920:A:SER:H	1:1919:A:VAL:H	2	0.1
(1,3238)	1:1920:A:SER:H	1:1919:A:VAL:H	4	0.1
(1,3238)	1:1920:A:SER:H	1:1919:A:VAL:H	12	0.1
(1,3226)	1:1871:A:ASN:HB3	1:1871:A:ASN:HD22	4	0.1
(1,3190)	1:1923:A:GLY:H	1:1922:A:ILE:H	1	0.1
(1,3160)	1:1942:A:LEU:H	1:1944:A:GLN:H	19	0.1
(1,3159)	1:1822:A:GLU:H	1:1822:A:GLU:HG2	3	0.1
(1,3159)	1:1822:A:GLU:H	1:1822:A:GLU:HG2	4	0.1
(1,3159)	1:1822:A:GLU:H	1:1822:A:GLU:HG2	5	0.1
(1,3159)	1:1822:A:GLU:H	1:1822:A:GLU:HG2	18	0.1
(1,3144)	1:1845:A:ASN:HA	1:1845:A:ASN:HD21	7	0.1
(1,3138)	1:1926:A:ASN:H	1:1926:A:ASN:HD22	13	0.1
(1,3134)	1:1852:A:GLU:HG2	1:1852:A:GLU:HB3	3	0.1
(1,3134)	1:1852:A:GLU:HG2	1:1852:A:GLU:HB3	4	0.1
(1,3134)	1:1852:A:GLU:HG2	1:1852:A:GLU:HB3	5	0.1
(1,3134)	1:1852:A:GLU:HG2	1:1852:A:GLU:HB3	8	0.1
(1,3134)	1:1852:A:GLU:HG2	1:1852:A:GLU:HB3	16	0.1
(1,3134)	1:1852:A:GLU:HG2	1:1852:A:GLU:HB3	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3134)	1:1852:A:GLU:HG2	1:1852:A:GLU:HB3	19	0.1
(1,3102)	1:1943:A:ARG:HA	1:1946:A:CYS:HB3	10	0.1
(1,3089)	1:1859:A:LYS:HE2	1:1856:A:TYR:HB2	13	0.1
(1,3089)	1:1859:A:LYS:HE3	1:1856:A:TYR:HB2	13	0.1
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	4	0.1
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	4	0.1
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	10	0.1
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	10	0.1
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD1	16	0.1
(1,3083)	1:1884:A:LEU:HB2	1:1854:A:TYR:HD2	16	0.1
(1,3075)	1:1942:A:LEU:HB3	1:1838:A:LYS:HG3	13	0.1
(1,3032)	1:1835:A:GLU:H	1:1833:A:LEU:HB2	3	0.1
(1,3032)	1:1835:A:GLU:H	1:1833:A:LEU:HB2	4	0.1
(1,3032)	1:1835:A:GLU:H	1:1833:A:LEU:HB2	9	0.1
(1,3032)	1:1835:A:GLU:H	1:1833:A:LEU:HB2	15	0.1
(1,3032)	1:1835:A:GLU:H	1:1833:A:LEU:HB2	19	0.1
(1,3015)	1:1938:A:ARG:HB2	1:1845:A:ASN:HD21	14	0.1
(1,3014)	1:1866:A:GLU:H	1:1866:A:GLU:HA	16	0.1
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD11	4	0.1
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD12	4	0.1
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD13	4	0.1
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD11	8	0.1
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD12	8	0.1
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD13	8	0.1
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD11	9	0.1
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD12	9	0.1
(1,3002)	1:1878:A:SER:H	1:1869:A:LEU:HD13	9	0.1
(1,2955)	1:1905:A:PRO:HD2	1:1904:A:SER:HA	9	0.1
(1,2951)	1:1940:A:LYS:HD3	1:1940:A:LYS:HE2	1	0.1
(1,2951)	1:1940:A:LYS:HD3	1:1940:A:LYS:HE3	1	0.1
(1,2951)	1:1940:A:LYS:HD3	1:1940:A:LYS:HE2	3	0.1
(1,2951)	1:1940:A:LYS:HD3	1:1940:A:LYS:HE3	3	0.1
(1,2951)	1:1940:A:LYS:HD3	1:1940:A:LYS:HE2	10	0.1
(1,2951)	1:1940:A:LYS:HD3	1:1940:A:LYS:HE3	10	0.1
(1,2951)	1:1940:A:LYS:HD3	1:1940:A:LYS:HE2	16	0.1
(1,2951)	1:1940:A:LYS:HD3	1:1940:A:LYS:HE3	16	0.1
(1,2907)	1:1894:A:LYS:H	1:1894:A:LYS:HE3	18	0.1
(1,2886)	1:1905:A:PRO:HD2	1:1905:A:PRO:HB2	20	0.1
(1,2842)	1:1950:A:ASN:HB2	1:1951:A:THR:H	2	0.1
(1,2824)	1:1840:A:ILE:HD11	1:1853:A:LEU:HG	12	0.1
(1,2824)	1:1840:A:ILE:HD12	1:1853:A:LEU:HG	12	0.1
(1,2824)	1:1840:A:ILE:HD13	1:1853:A:LEU:HG	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2818)	1:1886:A:VAL:H	1:1885:A:ARG:HG3	12	0.1
(1,2818)	1:1886:A:VAL:H	1:1885:A:ARG:HG3	14	0.1
(1,2818)	1:1886:A:VAL:H	1:1885:A:ARG:HG3	15	0.1
(1,2807)	1:1889:A:MET:H	1:1888:A:GLU:HB2	5	0.1
(1,2776)	1:1916:A:THR:HB	1:1917:A:SER:H	19	0.1
(1,2760)	1:1903:A:ILE:HA	1:1903:A:ILE:HG12	17	0.1
(1,2760)	1:1903:A:ILE:HA	1:1903:A:ILE:HG12	18	0.1
(1,2745)	1:1929:A:GLU:HG2	1:1930:A:VAL:H	11	0.1
(1,2733)	1:1885:A:ARG:HA	1:1889:A:MET:H	2	0.1
(1,2668)	1:1925:A:THR:H	1:1924:A:ASN:HB2	8	0.1
(1,2648)	1:1853:A:LEU:HA	1:1856:A:TYR:HB3	9	0.1
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE1	19	0.1
(1,2637)	1:1863:A:ALA:HB1	1:1856:A:TYR:HE2	19	0.1
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE1	19	0.1
(1,2637)	1:1863:A:ALA:HB2	1:1856:A:TYR:HE2	19	0.1
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE1	19	0.1
(1,2637)	1:1863:A:ALA:HB3	1:1856:A:TYR:HE2	19	0.1
(1,2592)	1:1869:A:LEU:H	1:1869:A:LEU:HB2	13	0.1
(1,2591)	1:1927:A:GLY:H	1:1925:A:THR:HA	18	0.1
(1,2569)	1:1908:A:GLU:HG2	1:1908:A:GLU:HA	4	0.1
(1,2564)	1:1909:A:VAL:H	1:1910:A:THR:H	1	0.1
(1,2554)	1:1935:A:TYR:HA	1:1937:A:GLU:H	15	0.1
(1,2513)	1:1935:A:TYR:HA	1:1935:A:TYR:H	20	0.1
(1,2510)	1:1849:A:GLY:H	1:1840:A:ILE:HG12	20	0.1
(1,2504)	1:1867:A:PRO:HA	1:1871:A:ASN:HD21	13	0.1
(1,2502)	1:1892:A:GLU:HG3	1:1892:A:GLU:HB3	3	0.1
(1,2502)	1:1892:A:GLU:HG3	1:1892:A:GLU:HB3	6	0.1
(1,2502)	1:1892:A:GLU:HG3	1:1892:A:GLU:HB3	8	0.1
(1,2502)	1:1892:A:GLU:HG3	1:1892:A:GLU:HB3	12	0.1
(1,2502)	1:1892:A:GLU:HG3	1:1892:A:GLU:HB3	13	0.1
(1,2502)	1:1892:A:GLU:HG3	1:1892:A:GLU:HB3	14	0.1
(1,2502)	1:1892:A:GLU:HG3	1:1892:A:GLU:HB3	17	0.1
(1,2490)	1:1820:A:ILE:HD11	1:1821:A:ASP:H	5	0.1
(1,2490)	1:1820:A:ILE:HD12	1:1821:A:ASP:H	5	0.1
(1,2490)	1:1820:A:ILE:HD13	1:1821:A:ASP:H	5	0.1
(1,2490)	1:1820:A:ILE:HD11	1:1821:A:ASP:H	19	0.1
(1,2490)	1:1820:A:ILE:HD12	1:1821:A:ASP:H	19	0.1
(1,2490)	1:1820:A:ILE:HD13	1:1821:A:ASP:H	19	0.1
(1,2489)	1:1893:A:GLY:H	1:1891:A:ARG:HB2	6	0.1
(1,2489)	1:1893:A:GLY:H	1:1891:A:ARG:HB2	15	0.1
(1,2488)	1:1840:A:ILE:H	1:1839:A:LYS:HA	14	0.1
(1,2483)	1:1908:A:GLU:H	1:1908:A:GLU:HG2	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2483)	1:1908:A:GLU:H	1:1908:A:GLU:HG2	12	0.1
(1,2483)	1:1908:A:GLU:H	1:1908:A:GLU:HG2	16	0.1
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE1	3	0.1
(1,2478)	1:1831:A:ASP:H	1:1868:A:PHE:HE2	3	0.1
(1,2451)	1:1861:A:SER:H	1:1860:A:TYR:HB3	3	0.1
(1,2451)	1:1861:A:SER:H	1:1860:A:TYR:HB3	5	0.1
(1,2451)	1:1861:A:SER:H	1:1860:A:TYR:HB3	7	0.1
(1,2451)	1:1861:A:SER:H	1:1860:A:TYR:HB3	14	0.1
(1,2451)	1:1861:A:SER:H	1:1860:A:TYR:HB3	19	0.1
(1,2449)	1:1938:A:ARG:HA	1:1938:A:ARG:HB3	13	0.1
(1,2426)	1:1907:A:MET:HA	1:1908:A:GLU:H	11	0.1
(1,2424)	1:1950:A:ASN:HB2	1:1950:A:ASN:HA	12	0.1
(1,2423)	1:1931:A:GLY:H	1:1930:A:VAL:HA	13	0.1
(1,2415)	1:1857:A:LYS:HA	1:1857:A:LYS:HG2	18	0.1
(1,2415)	1:1857:A:LYS:HA	1:1857:A:LYS:HG2	19	0.1
(1,2376)	1:1890:A:GLU:H	1:1892:A:GLU:H	11	0.1
(1,2345)	1:1930:A:VAL:H	1:1930:A:VAL:HG11	6	0.1
(1,2345)	1:1930:A:VAL:H	1:1930:A:VAL:HG12	6	0.1
(1,2345)	1:1930:A:VAL:H	1:1930:A:VAL:HG13	6	0.1
(1,2339)	1:1840:A:ILE:H	1:1849:A:GLY:H	9	0.1
(1,2298)	1:1891:A:ARG:H	1:1891:A:ARG:HB2	2	0.1
(1,2298)	1:1891:A:ARG:H	1:1891:A:ARG:HB2	8	0.1
(1,2298)	1:1891:A:ARG:H	1:1891:A:ARG:HB2	9	0.1
(1,2298)	1:1891:A:ARG:H	1:1891:A:ARG:HB2	16	0.1
(1,2298)	1:1891:A:ARG:H	1:1891:A:ARG:HB2	20	0.1
(1,2287)	1:1863:A:ALA:H	1:1862:A:ASP:HA	19	0.1
(1,2281)	1:1845:A:ASN:HD22	1:1848:A:GLU:HG3	10	0.1
(1,2268)	1:1824:A:SER:HB3	1:1825:A:SER:H	8	0.1
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD21	8	0.1
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD22	8	0.1
(1,2250)	1:1940:A:LYS:HD3	1:1936:A:LEU:HD23	8	0.1
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	4	0.1
(1,2244)	1:1825:A:SER:HA	1:1826:A:LYS:H	14	0.1
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG21	7	0.1
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG22	7	0.1
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG23	7	0.1
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG21	7	0.1
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG22	7	0.1
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG23	7	0.1
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG21	7	0.1
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG22	7	0.1
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG23	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG21	13	0.1
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG22	13	0.1
(1,2184)	1:1909:A:VAL:HG21	1:1910:A:THR:HG23	13	0.1
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG21	13	0.1
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG22	13	0.1
(1,2184)	1:1909:A:VAL:HG22	1:1910:A:THR:HG23	13	0.1
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG21	13	0.1
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG22	13	0.1
(1,2184)	1:1909:A:VAL:HG23	1:1910:A:THR:HG23	13	0.1
(1,2180)	1:1884:A:LEU:H	1:1850:A:LEU:HD11	10	0.1
(1,2180)	1:1884:A:LEU:H	1:1850:A:LEU:HD12	10	0.1
(1,2180)	1:1884:A:LEU:H	1:1850:A:LEU:HD13	10	0.1
(1,2180)	1:1884:A:LEU:H	1:1850:A:LEU:HD11	11	0.1
(1,2180)	1:1884:A:LEU:H	1:1850:A:LEU:HD12	11	0.1
(1,2180)	1:1884:A:LEU:H	1:1850:A:LEU:HD13	11	0.1
(1,2165)	1:1841:A:GLY:H	1:1876:A:PHE:HE1	16	0.1
(1,2165)	1:1841:A:GLY:H	1:1876:A:PHE:HE2	16	0.1
(1,2162)	1:1858:A:LYS:HE3	1:1854:A:TYR:HE1	17	0.1
(1,2162)	1:1858:A:LYS:HE3	1:1854:A:TYR:HE2	17	0.1
(1,2160)	1:1941:A:ILE:HD11	1:1944:A:GLN:HE21	12	0.1
(1,2160)	1:1941:A:ILE:HD12	1:1944:A:GLN:HE21	12	0.1
(1,2160)	1:1941:A:ILE:HD13	1:1944:A:GLN:HE21	12	0.1
(1,2159)	1:1868:A:PHE:H	1:1867:A:PRO:HB2	14	0.1
(1,2134)	1:1853:A:LEU:H	1:1853:A:LEU:HB3	1	0.1
(1,2134)	1:1853:A:LEU:H	1:1853:A:LEU:HB3	11	0.1
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	5	0.1
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	5	0.1
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	5	0.1
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG21	8	0.1
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG22	8	0.1
(1,2130)	1:1888:A:GLU:H	1:1886:A:VAL:HG23	8	0.1
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	1	0.1
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	5	0.1
(1,2082)	1:1936:A:LEU:HA	1:1938:A:ARG:H	15	0.1
(1,2070)	1:1820:A:ILE:HG12	1:1821:A:ASP:H	11	0.1
(1,2063)	1:1887:A:ILE:HD11	1:1847:A:LYS:HE2	8	0.1
(1,2063)	1:1887:A:ILE:HD12	1:1847:A:LYS:HE2	8	0.1
(1,2063)	1:1887:A:ILE:HD13	1:1847:A:LYS:HE2	8	0.1
(1,2055)	1:1922:A:ILE:HA	1:1922:A:ILE:HG12	7	0.1
(1,2055)	1:1922:A:ILE:HA	1:1922:A:ILE:HG12	11	0.1
(1,2051)	1:1840:A:ILE:HA	1:1846:A:THR:HA	7	0.1
(1,2051)	1:1840:A:ILE:HA	1:1846:A:THR:HA	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2051)	1:1840:A:ILE:HA	1:1846:A:THR:HA	15	0.1
(1,2037)	1:1843:A:LYS:HE3	1:1844:A:GLU:HG3	7	0.1
(1,2037)	1:1843:A:LYS:HE3	1:1844:A:GLU:HG3	10	0.1
(1,2011)	1:1930:A:VAL:H	1:1929:A:GLU:HG3	17	0.1
(1,1985)	1:1886:A:VAL:HA	1:1889:A:MET:HB2	5	0.1
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD11	14	0.1
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD12	14	0.1
(1,1967)	1:1884:A:LEU:HA	1:1887:A:ILE:HD13	14	0.1
(1,1960)	1:1828:A:LYS:HE2	1:1828:A:LYS:HD2	12	0.1
(1,1960)	1:1828:A:LYS:HE2	1:1828:A:LYS:HD3	12	0.1
(1,1960)	1:1828:A:LYS:HE3	1:1828:A:LYS:HD2	12	0.1
(1,1960)	1:1828:A:LYS:HE3	1:1828:A:LYS:HD3	12	0.1
(1,1960)	1:1828:A:LYS:HE2	1:1828:A:LYS:HD2	13	0.1
(1,1960)	1:1828:A:LYS:HE2	1:1828:A:LYS:HD3	13	0.1
(1,1960)	1:1828:A:LYS:HE3	1:1828:A:LYS:HD2	13	0.1
(1,1960)	1:1828:A:LYS:HE3	1:1828:A:LYS:HD3	13	0.1
(1,1960)	1:1828:A:LYS:HE2	1:1828:A:LYS:HD2	18	0.1
(1,1960)	1:1828:A:LYS:HE2	1:1828:A:LYS:HD3	18	0.1
(1,1960)	1:1828:A:LYS:HE3	1:1828:A:LYS:HD2	18	0.1
(1,1960)	1:1828:A:LYS:HE3	1:1828:A:LYS:HD3	18	0.1
(1,1960)	1:1828:A:LYS:HE2	1:1828:A:LYS:HD2	19	0.1
(1,1960)	1:1828:A:LYS:HE2	1:1828:A:LYS:HD3	19	0.1
(1,1960)	1:1828:A:LYS:HE3	1:1828:A:LYS:HD2	19	0.1
(1,1960)	1:1828:A:LYS:HE3	1:1828:A:LYS:HD3	19	0.1
(1,1956)	1:1953:A:GLN:HA	1:1953:A:GLN:HB3	7	0.1
(1,1956)	1:1953:A:GLN:HA	1:1953:A:GLN:HB3	11	0.1
(1,1956)	1:1953:A:GLN:HA	1:1953:A:GLN:HB3	12	0.1
(1,1956)	1:1953:A:GLN:HA	1:1953:A:GLN:HB3	20	0.1
(1,1910)	1:1861:A:SER:H	1:1861:A:SER:HB2	19	0.1
(1,1907)	1:1858:A:LYS:HA	1:1861:A:SER:HA	1	0.1
(1,1870)	1:1956:A:ARG:H	1:1956:A:ARG:HG3	20	0.1
(1,1853)	1:1827:A:ALA:H	1:1826:A:LYS:HG2	4	0.1
(1,1833)	1:1941:A:ILE:H	1:1941:A:ILE:HA	3	0.1
(1,1833)	1:1941:A:ILE:H	1:1941:A:ILE:HA	4	0.1
(1,1833)	1:1941:A:ILE:H	1:1941:A:ILE:HA	12	0.1
(1,1818)	1:1919:A:VAL:HB	1:1916:A:THR:HB	3	0.1
(1,1806)	1:1840:A:ILE:HB	1:1876:A:PHE:HZ	9	0.1
(1,1806)	1:1840:A:ILE:HB	1:1876:A:PHE:HZ	18	0.1
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	3	0.1
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	7	0.1
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	8	0.1
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	14	0.1
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	18	0.1
(1,1795)	1:1859:A:LYS:HA	1:1860:A:TYR:H	19	0.1
(1,1789)	1:1840:A:ILE:HG12	1:1850:A:LEU:HD11	12	0.1
(1,1789)	1:1840:A:ILE:HG12	1:1850:A:LEU:HD12	12	0.1
(1,1789)	1:1840:A:ILE:HG12	1:1850:A:LEU:HD13	12	0.1
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD11	8	0.1
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD12	8	0.1
(1,1769)	1:1941:A:ILE:HG21	1:1941:A:ILE:HD13	8	0.1
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD11	8	0.1
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD12	8	0.1
(1,1769)	1:1941:A:ILE:HG22	1:1941:A:ILE:HD13	8	0.1
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD11	8	0.1
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD12	8	0.1
(1,1769)	1:1941:A:ILE:HG23	1:1941:A:ILE:HD13	8	0.1
(1,1747)	1:1853:A:LEU:HD11	1:1856:A:TYR:HB2	4	0.1
(1,1747)	1:1853:A:LEU:HD12	1:1856:A:TYR:HB2	4	0.1
(1,1747)	1:1853:A:LEU:HD13	1:1856:A:TYR:HB2	4	0.1
(1,1742)	1:1886:A:VAL:H	1:1886:A:VAL:HG11	17	0.1
(1,1742)	1:1886:A:VAL:H	1:1886:A:VAL:HG12	17	0.1
(1,1742)	1:1886:A:VAL:H	1:1886:A:VAL:HG13	17	0.1
(1,1724)	1:1853:A:LEU:HD21	1:1869:A:LEU:HD11	14	0.1
(1,1724)	1:1853:A:LEU:HD21	1:1869:A:LEU:HD12	14	0.1
(1,1724)	1:1853:A:LEU:HD21	1:1869:A:LEU:HD13	14	0.1
(1,1724)	1:1853:A:LEU:HD22	1:1869:A:LEU:HD11	14	0.1
(1,1724)	1:1853:A:LEU:HD22	1:1869:A:LEU:HD12	14	0.1
(1,1724)	1:1853:A:LEU:HD22	1:1869:A:LEU:HD13	14	0.1
(1,1724)	1:1853:A:LEU:HD23	1:1869:A:LEU:HD11	14	0.1
(1,1724)	1:1853:A:LEU:HD23	1:1869:A:LEU:HD12	14	0.1
(1,1724)	1:1853:A:LEU:HD23	1:1869:A:LEU:HD13	14	0.1
(1,1712)	1:1832:A:PHE:H	1:1834:A:ALA:HB1	16	0.1
(1,1712)	1:1832:A:PHE:H	1:1834:A:ALA:HB2	16	0.1
(1,1712)	1:1832:A:PHE:H	1:1834:A:ALA:HB3	16	0.1
(1,1683)	1:1933:A:SER:H	1:1932:A:PRO:HB2	5	0.1
(1,1683)	1:1933:A:SER:H	1:1932:A:PRO:HB2	13	0.1
(1,1678)	1:1832:A:PHE:HD1	1:1856:A:TYR:HE1	13	0.1
(1,1678)	1:1832:A:PHE:HD1	1:1856:A:TYR:HE2	13	0.1
(1,1678)	1:1832:A:PHE:HD2	1:1856:A:TYR:HE1	13	0.1
(1,1678)	1:1832:A:PHE:HD2	1:1856:A:TYR:HE2	13	0.1
(1,1670)	1:1895:A:GLY:H	1:1894:A:LYS:HA	1	0.1
(1,1655)	1:1835:A:GLU:HG2	1:1835:A:GLU:H	14	0.1
(1,1655)	1:1835:A:GLU:HG3	1:1835:A:GLU:H	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1638)	1:1869:A:LEU:HD11	1:1876:A:PHE:HE1	4	0.1
(1,1638)	1:1869:A:LEU:HD11	1:1876:A:PHE:HE2	4	0.1
(1,1638)	1:1869:A:LEU:HD12	1:1876:A:PHE:HE1	4	0.1
(1,1638)	1:1869:A:LEU:HD12	1:1876:A:PHE:HE2	4	0.1
(1,1638)	1:1869:A:LEU:HD13	1:1876:A:PHE:HE1	4	0.1
(1,1638)	1:1869:A:LEU:HD13	1:1876:A:PHE:HE2	4	0.1
(1,1624)	1:1941:A:ILE:HA	1:1944:A:GLN:HB2	11	0.1
(1,1624)	1:1941:A:ILE:HA	1:1944:A:GLN:HB3	11	0.1
(1,1598)	1:1955:A:ASP:H	1:1953:A:GLN:HG2	12	0.1
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD11	2	0.1
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD12	2	0.1
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD13	2	0.1
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD11	2	0.1
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD12	2	0.1
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD13	2	0.1
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD11	17	0.1
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD12	17	0.1
(1,1591)	1:1854:A:TYR:HD1	1:1887:A:ILE:HD13	17	0.1
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD11	17	0.1
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD12	17	0.1
(1,1591)	1:1854:A:TYR:HD2	1:1887:A:ILE:HD13	17	0.1
(1,1588)	1:1882:A:ARG:H	1:1880:A:VAL:H	2	0.1
(1,1588)	1:1882:A:ARG:H	1:1880:A:VAL:H	6	0.1
(1,1588)	1:1882:A:ARG:H	1:1880:A:VAL:H	14	0.1
(1,1567)	1:1894:A:LYS:H	1:1894:A:LYS:HD2	3	0.1
(1,1567)	1:1894:A:LYS:H	1:1894:A:LYS:HD2	15	0.1
(1,1504)	1:1855:A:GLU:HA	1:1858:A:LYS:HE2	5	0.1
(1,1504)	1:1855:A:GLU:HA	1:1858:A:LYS:HE2	11	0.1
(1,1504)	1:1855:A:GLU:HA	1:1858:A:LYS:HE2	12	0.1
(1,1479)	1:1867:A:PRO:HD2	1:1868:A:PHE:H	11	0.1
(1,1479)	1:1867:A:PRO:HD2	1:1868:A:PHE:H	14	0.1
(1,1470)	1:1824:A:SER:H	1:1827:A:ALA:H	17	0.1
(1,1467)	1:1862:A:ASP:H	1:1861:A:SER:HB2	2	0.1
(1,1443)	1:1904:A:SER:H	1:1903:A:ILE:HB	7	0.1
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD1	7	0.1
(1,1427)	1:1835:A:GLU:H	1:1832:A:PHE:HD2	7	0.1
(1,1415)	1:1897:A:ILE:H	1:1897:A:ILE:HG21	6	0.1
(1,1415)	1:1897:A:ILE:H	1:1897:A:ILE:HG22	6	0.1
(1,1415)	1:1897:A:ILE:H	1:1897:A:ILE:HG23	6	0.1
(1,1415)	1:1897:A:ILE:H	1:1897:A:ILE:HG21	12	0.1
(1,1415)	1:1897:A:ILE:H	1:1897:A:ILE:HG22	12	0.1
(1,1415)	1:1897:A:ILE:H	1:1897:A:ILE:HG23	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1415)	1:1897:A:ILE:H	1:1897:A:ILE:HG21	14	0.1
(1,1415)	1:1897:A:ILE:H	1:1897:A:ILE:HG22	14	0.1
(1,1415)	1:1897:A:ILE:H	1:1897:A:ILE:HG23	14	0.1
(1,1395)	1:1893:A:GLY:H	1:1892:A:GLU:HG3	20	0.1
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD21	2	0.1
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD22	2	0.1
(1,1351)	1:1880:A:VAL:HG21	1:1850:A:LEU:HD23	2	0.1
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD21	2	0.1
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD22	2	0.1
(1,1351)	1:1880:A:VAL:HG22	1:1850:A:LEU:HD23	2	0.1
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD21	2	0.1
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD22	2	0.1
(1,1351)	1:1880:A:VAL:HG23	1:1850:A:LEU:HD23	2	0.1
(1,1342)	1:1859:A:LYS:H	1:1858:A:LYS:HG3	3	0.1
(1,1342)	1:1859:A:LYS:H	1:1858:A:LYS:HG3	9	0.1
(1,1342)	1:1859:A:LYS:H	1:1858:A:LYS:HG3	12	0.1
(1,1335)	1:1953:A:GLN:HA	1:1953:A:GLN:HG2	1	0.1
(1,1335)	1:1953:A:GLN:HA	1:1953:A:GLN:HG2	2	0.1
(1,1334)	1:1884:A:LEU:H	1:1882:A:ARG:HB3	8	0.1
(1,1307)	1:1821:A:ASP:HA	1:1823:A:LYS:H	16	0.1
(1,1239)	1:1890:A:GLU:HA	1:1896:A:ARG:HG3	4	0.1
(1,1212)	1:1950:A:ASN:HB3	1:1950:A:ASN:HA	6	0.1
(1,1200)	1:1922:A:ILE:HB	1:1922:A:ILE:H	15	0.1
(1,1200)	1:1922:A:ILE:HB	1:1922:A:ILE:H	17	0.1
(1,1189)	1:1956:A:ARG:HB2	1:1956:A:ARG:HD2	15	0.1
(1,1189)	1:1956:A:ARG:HB2	1:1956:A:ARG:HD3	15	0.1
(1,1187)	1:1838:A:LYS:H	1:1838:A:LYS:HG3	2	0.1
(1,1187)	1:1838:A:LYS:H	1:1838:A:LYS:HG3	3	0.1
(1,1148)	1:1824:A:SER:H	1:1824:A:SER:HA	5	0.1
(1,1125)	1:1908:A:GLU:HB3	1:1908:A:GLU:HA	3	0.1
(1,1103)	1:1853:A:LEU:H	1:1851:A:ALA:HA	13	0.1
(1,1098)	1:1905:A:PRO:HD2	1:1904:A:SER:HB2	17	0.1
(1,1098)	1:1905:A:PRO:HD2	1:1904:A:SER:HB3	17	0.1
(1,1090)	1:1852:A:GLU:H	1:1850:A:LEU:H	12	0.1
(1,1080)	1:1847:A:LYS:HA	1:1850:A:LEU:HB2	1	0.1
(1,1080)	1:1847:A:LYS:HA	1:1850:A:LEU:HB2	9	0.1
(1,1054)	1:1830:A:ASN:HD22	1:1868:A:PHE:HE1	9	0.1
(1,1054)	1:1830:A:ASN:HD22	1:1868:A:PHE:HE2	9	0.1
(1,1029)	1:1836:A:ILE:HA	1:1836:A:ILE:HG13	1	0.1
(1,1029)	1:1836:A:ILE:HA	1:1836:A:ILE:HG13	5	0.1
(1,1029)	1:1836:A:ILE:HA	1:1836:A:ILE:HG13	8	0.1
(1,1029)	1:1836:A:ILE:HA	1:1836:A:ILE:HG13	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1029)	1:1836:A:ILE:HA	1:1836:A:ILE:HG13	12	0.1
(1,1029)	1:1836:A:ILE:HA	1:1836:A:ILE:HG13	15	0.1
(1,1029)	1:1836:A:ILE:HA	1:1836:A:ILE:HG13	16	0.1
(1,1029)	1:1836:A:ILE:HA	1:1836:A:ILE:HG13	17	0.1
(1,1029)	1:1836:A:ILE:HA	1:1836:A:ILE:HG13	20	0.1
(1,1014)	1:1846:A:THR:H	1:1845:A:ASN:H	16	0.1
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	1	0.1
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	2	0.1
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	7	0.1
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	10	0.1
(1,1013)	1:1854:A:TYR:H	1:1855:A:GLU:H	17	0.1
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	1	0.1
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	1	0.1
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	1	0.1
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	7	0.1
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	7	0.1
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	7	0.1
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	10	0.1
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	10	0.1
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	10	0.1
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	15	0.1
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	15	0.1
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	15	0.1
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB1	16	0.1
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB2	16	0.1
(1,1009)	1:1829:A:VAL:H	1:1827:A:ALA:HB3	16	0.1
(1,986)	1:1837:A:PHE:H	1:1840:A:ILE:H	1	0.1
(1,986)	1:1837:A:PHE:H	1:1840:A:ILE:H	17	0.1
(1,986)	1:1837:A:PHE:H	1:1840:A:ILE:H	18	0.1
(1,986)	1:1837:A:PHE:H	1:1840:A:ILE:H	19	0.1
(1,985)	1:1877:A:GLN:HE21	1:1869:A:LEU:HD21	7	0.1
(1,985)	1:1877:A:GLN:HE21	1:1869:A:LEU:HD22	7	0.1
(1,985)	1:1877:A:GLN:HE21	1:1869:A:LEU:HD23	7	0.1
(1,975)	1:1876:A:PHE:H	1:1876:A:PHE:HB3	13	0.1
(1,975)	1:1876:A:PHE:H	1:1876:A:PHE:HB3	20	0.1
(1,959)	1:1898:A:SER:H	1:1897:A:ILE:HG12	4	0.1
(1,959)	1:1898:A:SER:H	1:1897:A:ILE:HG12	5	0.1
(1,952)	1:1949:A:ASP:HA	1:1949:A:ASP:HB3	10	0.1
(1,952)	1:1949:A:ASP:HA	1:1949:A:ASP:HB3	11	0.1
(1,952)	1:1949:A:ASP:HA	1:1949:A:ASP:HB3	17	0.1
(1,937)	1:1894:A:LYS:H	1:1894:A:LYS:HG3	1	0.1
(1,889)	1:1889:A:MET:H	1:1892:A:GLU:HG3	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,889)	1:1889:A:MET:H	1:1892:A:GLU:HG3	19	0.1
(1,851)	1:1906:A:GLN:HB2	1:1908:A:GLU:H	18	0.1
(1,844)	1:1890:A:GLU:HA	1:1890:A:GLU:HG2	12	0.1
(1,844)	1:1890:A:GLU:HA	1:1890:A:GLU:HG2	18	0.1
(1,828)	1:1851:A:ALA:HB1	1:1852:A:GLU:HG2	20	0.1
(1,828)	1:1851:A:ALA:HB2	1:1852:A:GLU:HG2	20	0.1
(1,828)	1:1851:A:ALA:HB3	1:1852:A:GLU:HG2	20	0.1
(1,815)	1:1911:A:CYS:HA	1:1912:A:VAL:HG11	11	0.1
(1,815)	1:1911:A:CYS:HA	1:1912:A:VAL:HG12	11	0.1
(1,815)	1:1911:A:CYS:HA	1:1912:A:VAL:HG13	11	0.1
(1,808)	1:1830:A:ASN:HB2	1:1829:A:VAL:H	9	0.1
(1,749)	1:1872:A:SER:HB3	1:1877:A:GLN:HE22	16	0.1
(1,749)	1:1872:A:SER:HB3	1:1877:A:GLN:HE22	17	0.1
(1,736)	1:1898:A:SER:H	1:1897:A:ILE:H	1	0.1
(1,736)	1:1898:A:SER:H	1:1897:A:ILE:H	19	0.1
(1,719)	1:1877:A:GLN:H	1:1878:A:SER:HB2	9	0.1
(1,719)	1:1877:A:GLN:H	1:1878:A:SER:HB2	18	0.1
(1,677)	1:1952:A:LYS:H	1:1953:A:GLN:H	10	0.1
(1,675)	1:1890:A:GLU:HB3	1:1890:A:GLU:HG2	11	0.1
(1,669)	1:1890:A:GLU:H	1:1890:A:GLU:HG3	8	0.1
(1,669)	1:1890:A:GLU:H	1:1890:A:GLU:HG3	19	0.1
(1,666)	1:1942:A:LEU:HD21	1:1839:A:LYS:HG2	13	0.1
(1,666)	1:1942:A:LEU:HD22	1:1839:A:LYS:HG2	13	0.1
(1,666)	1:1942:A:LEU:HD23	1:1839:A:LYS:HG2	13	0.1
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	8	0.1
(1,616)	1:1881:A:GLU:H	1:1882:A:ARG:H	17	0.1
(1,615)	1:1880:A:VAL:H	1:1881:A:GLU:HB2	2	0.1
(1,615)	1:1880:A:VAL:H	1:1881:A:GLU:HB2	8	0.1
(1,615)	1:1880:A:VAL:H	1:1881:A:GLU:HB2	9	0.1
(1,615)	1:1880:A:VAL:H	1:1881:A:GLU:HB2	11	0.1
(1,615)	1:1880:A:VAL:H	1:1881:A:GLU:HB2	16	0.1
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	3	0.1
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	3	0.1
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG2	15	0.1
(1,603)	1:1855:A:GLU:H	1:1855:A:GLU:HG3	15	0.1
(1,593)	1:1920:A:SER:HA	1:1915:A:PRO:HB3	7	0.1
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	1	0.1
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	4	0.1
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	18	0.1
(1,590)	1:1936:A:LEU:HA	1:1939:A:LEU:H	19	0.1
(1,516)	1:1886:A:VAL:HG21	1:1882:A:ARG:HG3	9	0.1
(1,516)	1:1886:A:VAL:HG22	1:1882:A:ARG:HG3	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	1:1886:A:VAL:HG23	1:1882:A:ARG:HG3	9	0.1
(1,516)	1:1886:A:VAL:HG21	1:1882:A:ARG:HG3	13	0.1
(1,516)	1:1886:A:VAL:HG22	1:1882:A:ARG:HG3	13	0.1
(1,516)	1:1886:A:VAL:HG23	1:1882:A:ARG:HG3	13	0.1
(1,516)	1:1886:A:VAL:HG21	1:1882:A:ARG:HG3	15	0.1
(1,516)	1:1886:A:VAL:HG22	1:1882:A:ARG:HG3	15	0.1
(1,516)	1:1886:A:VAL:HG23	1:1882:A:ARG:HG3	15	0.1
(1,516)	1:1886:A:VAL:HG21	1:1882:A:ARG:HG3	18	0.1
(1,516)	1:1886:A:VAL:HG22	1:1882:A:ARG:HG3	18	0.1
(1,516)	1:1886:A:VAL:HG23	1:1882:A:ARG:HG3	18	0.1
(1,516)	1:1886:A:VAL:HG21	1:1882:A:ARG:HG3	19	0.1
(1,516)	1:1886:A:VAL:HG22	1:1882:A:ARG:HG3	19	0.1
(1,516)	1:1886:A:VAL:HG23	1:1882:A:ARG:HG3	19	0.1
(1,509)	1:1865:A:ILE:HG21	1:1866:A:GLU:H	6	0.1
(1,509)	1:1865:A:ILE:HG22	1:1866:A:GLU:H	6	0.1
(1,509)	1:1865:A:ILE:HG23	1:1866:A:GLU:H	6	0.1
(1,509)	1:1865:A:ILE:HG21	1:1866:A:GLU:H	9	0.1
(1,509)	1:1865:A:ILE:HG22	1:1866:A:GLU:H	9	0.1
(1,509)	1:1865:A:ILE:HG23	1:1866:A:GLU:H	9	0.1
(1,496)	1:1940:A:LYS:H	1:1937:A:GLU:HA	12	0.1
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	4	0.1
(1,493)	1:1952:A:LYS:HA	1:1952:A:LYS:HB3	18	0.1
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	4	0.1
(1,482)	1:1878:A:SER:H	1:1880:A:VAL:H	7	0.1
(1,466)	1:1917:A:SER:H	1:1917:A:SER:HB2	11	0.1
(1,448)	1:1826:A:LYS:H	1:1826:A:LYS:HB2	4	0.1
(1,422)	1:1862:A:ASP:H	1:1857:A:LYS:HG3	16	0.1
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD2	4	0.1
(1,393)	1:1843:A:LYS:HB3	1:1843:A:LYS:HD3	4	0.1
(1,385)	1:1952:A:LYS:H	1:1951:A:THR:HA	15	0.1
(1,378)	1:1885:A:ARG:HA	1:1885:A:ARG:HG2	16	0.1
(1,375)	1:1896:A:ARG:HG2	1:1896:A:ARG:HD2	4	0.1
(1,375)	1:1896:A:ARG:HG2	1:1896:A:ARG:HD3	4	0.1
(1,375)	1:1896:A:ARG:HG2	1:1896:A:ARG:HD2	16	0.1
(1,375)	1:1896:A:ARG:HG2	1:1896:A:ARG:HD3	16	0.1
(1,362)	1:1854:A:TYR:HA	1:1857:A:LYS:HB2	7	0.1
(1,330)	1:1827:A:ALA:H	1:1826:A:LYS:HB3	10	0.1
(1,325)	1:1936:A:LEU:HB2	1:1933:A:SER:HA	2	0.1
(1,325)	1:1936:A:LEU:HB2	1:1933:A:SER:HA	13	0.1
(1,325)	1:1936:A:LEU:HB2	1:1933:A:SER:HA	14	0.1
(1,324)	1:1889:A:MET:HE1	1:1896:A:ARG:HD2	13	0.1
(1,324)	1:1889:A:MET:HE2	1:1896:A:ARG:HD2	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,324)	1:1889:A:MET:HE3	1:1896:A:ARG:HD2	13	0.1
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD11	19	0.1
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD12	19	0.1
(1,318)	1:1886:A:VAL:HB	1:1887:A:ILE:HD13	19	0.1
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG11	3	0.1
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG12	3	0.1
(1,300)	1:1914:A:THR:HB	1:1912:A:VAL:HG13	3	0.1
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	14	0.1
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	14	0.1
(1,273)	1:1932:A:PRO:HD2	1:1932:A:PRO:HB2	18	0.1
(1,273)	1:1932:A:PRO:HD3	1:1932:A:PRO:HB2	18	0.1
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	1	0.1
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	1	0.1
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD1	18	0.1
(1,250)	1:1834:A:ALA:HA	1:1837:A:PHE:HD2	18	0.1
(1,249)	1:1865:A:ILE:HA	1:1868:A:PHE:HB3	2	0.1
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD11	4	0.1
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD12	4	0.1
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD13	4	0.1
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD11	17	0.1
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD12	17	0.1
(1,242)	1:1850:A:LEU:H	1:1887:A:ILE:HD13	17	0.1
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	3	0.1
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	9	0.1
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	12	0.1
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	15	0.1
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	16	0.1
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	17	0.1
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	18	0.1
(1,222)	1:1942:A:LEU:H	1:1942:A:LEU:HB2	20	0.1
(1,215)	1:1828:A:LYS:HA	1:1831:A:ASP:HB2	14	0.1
(1,215)	1:1828:A:LYS:HA	1:1831:A:ASP:HB2	20	0.1
(1,210)	1:1889:A:MET:H	1:1889:A:MET:HG3	18	0.1
(1,177)	1:1910:A:THR:H	1:1910:A:THR:HB	6	0.1
(1,135)	1:1939:A:LEU:HD11	1:1839:A:LYS:HD2	13	0.1
(1,135)	1:1939:A:LEU:HD12	1:1839:A:LYS:HD2	13	0.1
(1,135)	1:1939:A:LEU:HD13	1:1839:A:LYS:HD2	13	0.1
(1,135)	1:1939:A:LEU:HD11	1:1839:A:LYS:HD2	14	0.1
(1,135)	1:1939:A:LEU:HD12	1:1839:A:LYS:HD2	14	0.1
(1,135)	1:1939:A:LEU:HD13	1:1839:A:LYS:HD2	14	0.1
(1,125)	1:1822:A:GLU:HG2	1:1823:A:LYS:H	5	0.1
(1,125)	1:1822:A:GLU:HG2	1:1823:A:LYS:H	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	4	0.1
(1,71)	1:1935:A:TYR:HA	1:1936:A:LEU:H	20	0.1
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD2	14	0.1
(1,70)	1:1939:A:LEU:HD21	1:1943:A:ARG:HD3	14	0.1
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD2	14	0.1
(1,70)	1:1939:A:LEU:HD22	1:1943:A:ARG:HD3	14	0.1
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD2	14	0.1
(1,70)	1:1939:A:LEU:HD23	1:1943:A:ARG:HD3	14	0.1
(1,55)	1:1874:A:GLN:HB2	1:1874:A:GLN:HE21	3	0.1

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

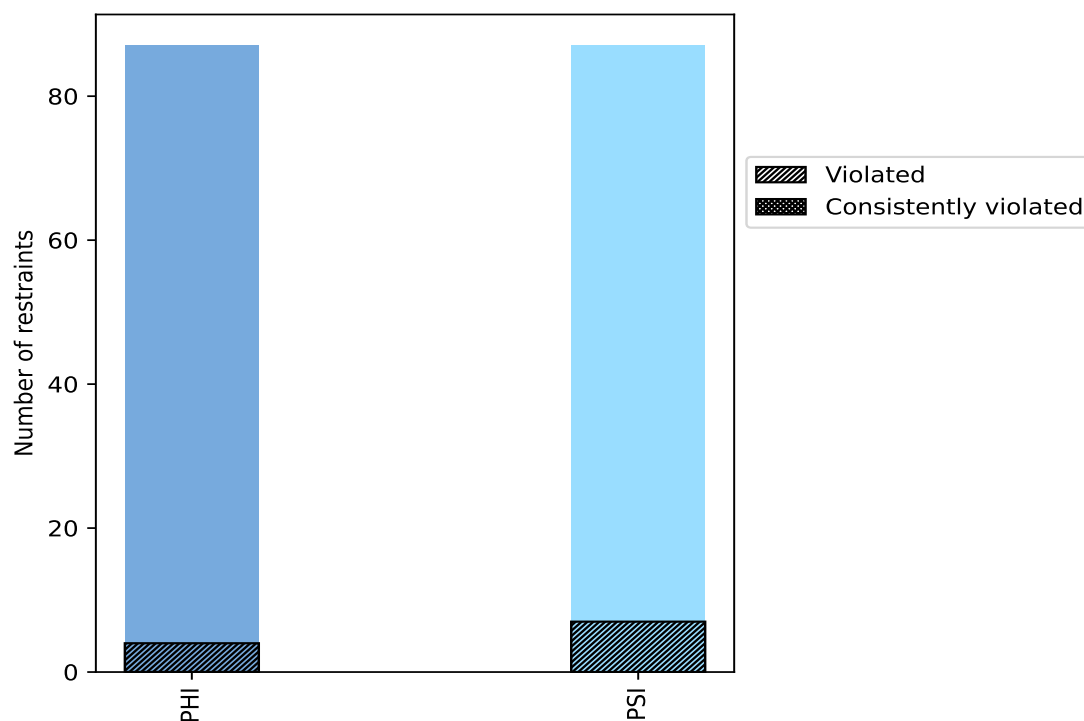
10.1 Summary of dihedral-angle violations [i](#)

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	87	50.0	4	4.6	2.3	0	0.0	0.0
PSI	87	50.0	7	8.0	4.0	0	0.0	0.0
Total	174	100.0	11	6.3	6.3	0	0.0	0.0

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

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



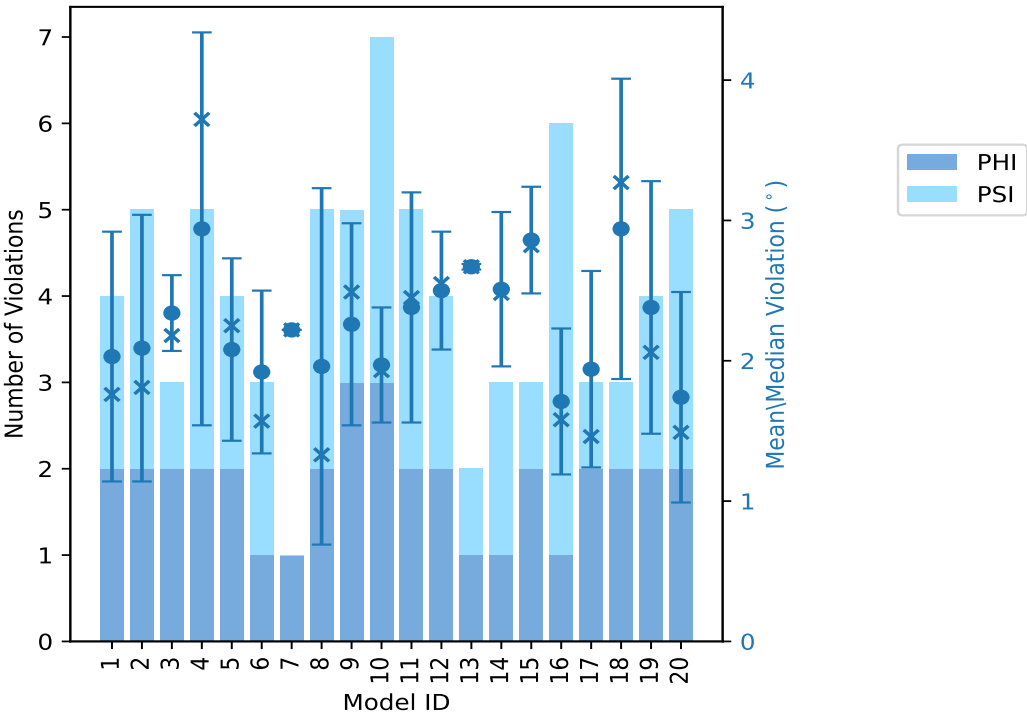
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	2	2	4	2.03	3.46	0.89	1.76
2	2	3	5	2.09	3.86	0.95	1.81
3	2	1	3	2.34	2.73	0.27	2.18
4	2	3	5	2.94	4.66	1.4	3.72
5	2	2	4	2.08	2.76	0.65	2.25
6	1	2	3	1.92	2.74	0.58	1.57
7	1	0	1	2.22	2.22	0.0	2.22
8	2	3	5	1.96	4.5	1.27	1.33
9	3	2	5	2.26	3.31	0.72	2.49
10	3	4	7	1.97	2.7	0.41	1.93
11	2	3	5	2.38	3.48	0.82	2.45
12	2	2	4	2.5	3.03	0.42	2.55
13	1	1	2	2.67	2.69	0.02	2.67
14	1	2	3	2.51	3.2	0.55	2.48
15	2	1	3	2.86	3.34	0.38	2.82
16	1	5	6	1.71	2.5	0.52	1.58
17	2	1	3	1.94	2.93	0.7	1.46
18	2	1	3	2.94	4.05	1.07	3.27
19	2	2	4	2.38	3.89	0.9	2.06
20	2	3	5	1.74	3.2	0.75	1.49

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



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

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

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

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

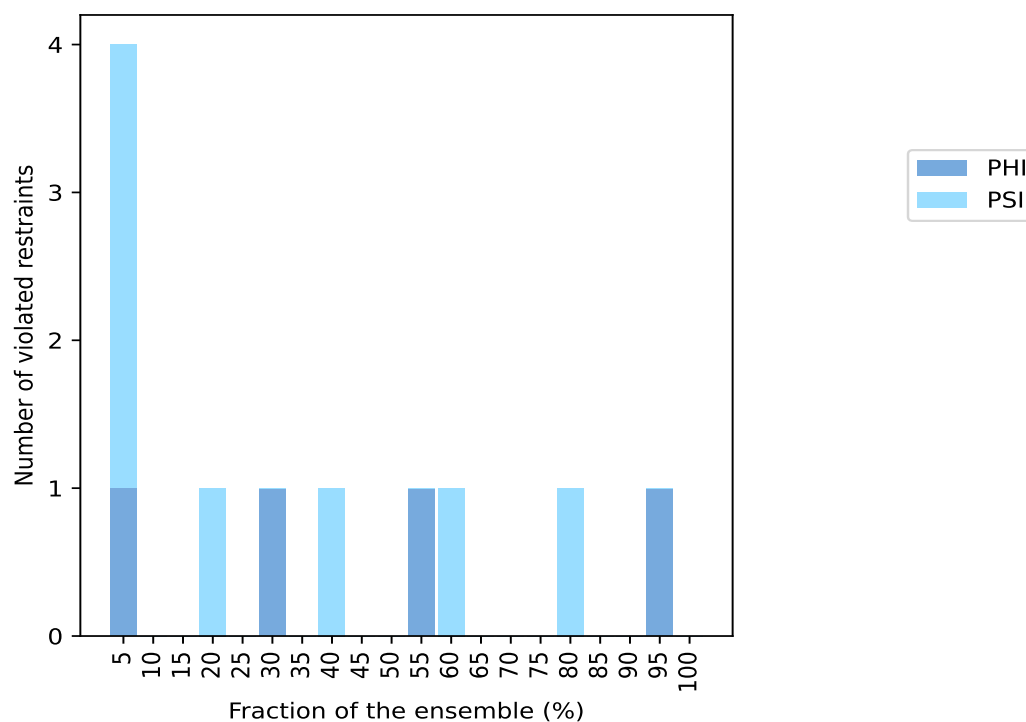
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	1	1	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	1	1	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
1	0	1	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

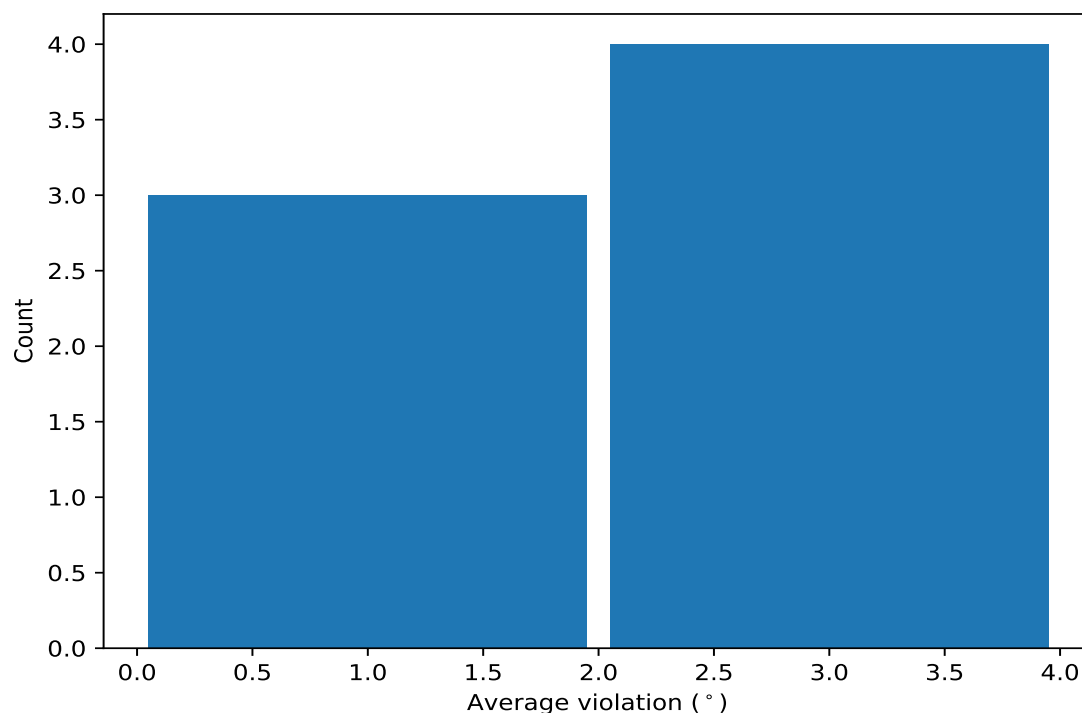


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

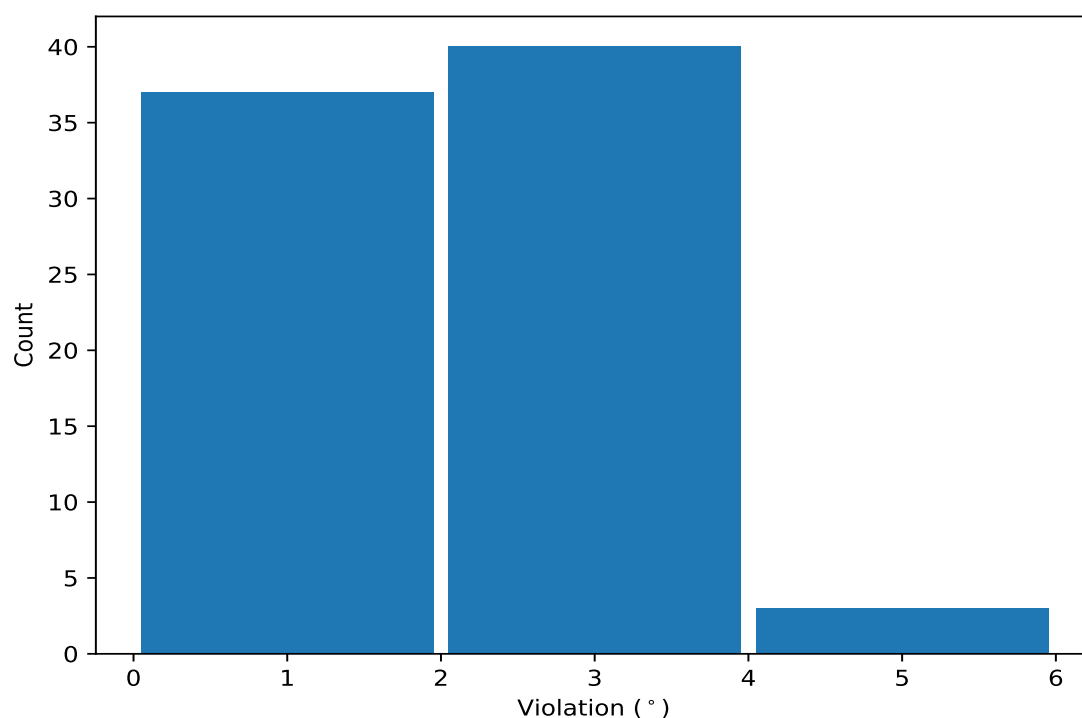
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Medi
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	19	2.79	0.83	2.76
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	16	1.77	0.38	1.83
(1,128)	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	1:1909:A:VAL:N	12	2.45	0.71	2.47
(1,123)	1:1905:A:PRO:C	1:1906:A:GLN:N	1:1906:A:GLN:CA	1:1906:A:GLN:C	11	2.37	0.89	2.22
(1,28)	1:1841:A:GLY:N	1:1841:A:GLY:CA	1:1841:A:GLY:C	1:1842:A:SER:N	8	1.35	0.24	1.33
(1,127)	1:1907:A:MET:C	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	6	2.66	1.11	2.35
(1,82)	1:1876:A:PHE:N	1:1876:A:PHE:CA	1:1876:A:PHE:C	1:1877:A:GLN:N	4	1.4	0.49	1.12

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

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

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

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,127)	1:1907:A:MET:C	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	4	4.66
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	8	4.5
(1,123)	1:1905:A:PRO:C	1:1906:A:GLN:N	1:1906:A:GLN:CA	1:1906:A:GLN:C	18	4.05
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	19	3.89
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	2	3.86
(1,128)	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	1:1909:A:VAL:N	4	3.76
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	4	3.72
(1,127)	1:1907:A:MET:C	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	11	3.48
(1,123)	1:1905:A:PRO:C	1:1906:A:GLN:N	1:1906:A:GLN:CA	1:1906:A:GLN:C	1	3.46
(1,123)	1:1905:A:PRO:C	1:1906:A:GLN:N	1:1906:A:GLN:CA	1:1906:A:GLN:C	15	3.34
(1,128)	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	1:1909:A:VAL:N	9	3.31
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	18	3.27
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	14	3.2
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	20	3.2
(1,128)	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	1:1909:A:VAL:N	12	3.03
(1,128)	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	1:1909:A:VAL:N	11	2.94
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	17	2.93
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	15	2.82
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	5	2.76
(1,128)	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	1:1909:A:VAL:N	6	2.74
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	3	2.73

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,34)	1:1845:A:ASN:N	1:1845:A:ASN:CA	1:1845:A:ASN:C	1:1846:A:THR:N	10	2.7
(1,128)	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	1:1909:A:VAL:N	13	2.69
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	13	2.65
(1,137)	1:1913:A:PRO:C	1:1914:A:THR:N	1:1914:A:THR:CA	1:1914:A:THR:C	9	2.59
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	12	2.56
(1,123)	1:1905:A:PRO:C	1:1906:A:GLN:N	1:1906:A:GLN:CA	1:1906:A:GLN:C	12	2.55
(1,144)	1:1931:A:GLY:N	1:1931:A:GLY:CA	1:1931:A:GLY:C	1:1932:A:PRO:N	16	2.5
(1,127)	1:1907:A:MET:C	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	9	2.49
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	14	2.48
(1,123)	1:1905:A:PRO:C	1:1906:A:GLN:N	1:1906:A:GLN:CA	1:1906:A:GLN:C	5	2.47
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	11	2.45
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	15	2.41
(1,128)	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	1:1909:A:VAL:N	19	2.25
(1,82)	1:1876:A:PHE:N	1:1876:A:PHE:CA	1:1876:A:PHE:C	1:1877:A:GLN:N	16	2.24
(1,123)	1:1905:A:PRO:C	1:1906:A:GLN:N	1:1906:A:GLN:CA	1:1906:A:GLN:C	7	2.22
(1,127)	1:1907:A:MET:C	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	10	2.21
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	3	2.18
(1,128)	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	1:1909:A:VAL:N	2	2.13
(1,123)	1:1905:A:PRO:C	1:1906:A:GLN:N	1:1906:A:GLN:CA	1:1906:A:GLN:C	3	2.12
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1	2.08
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	10	2.04
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	5	2.03
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	11	1.95
(1,123)	1:1905:A:PRO:C	1:1906:A:GLN:N	1:1906:A:GLN:CA	1:1906:A:GLN:C	10	1.93
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	10	1.89
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	19	1.86
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	12	1.85
(1,28)	1:1841:A:GLY:N	1:1841:A:GLY:CA	1:1841:A:GLY:C	1:1842:A:SER:N	14	1.85
(1,128)	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	1:1909:A:VAL:N	10	1.83
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	2	1.81
(1,128)	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	1:1909:A:VAL:N	16	1.75
(1,128)	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	1:1909:A:VAL:N	20	1.63
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	6	1.57
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	9	1.57
(1,127)	1:1907:A:MET:C	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	2	1.55
(1,127)	1:1907:A:MET:C	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	19	1.54
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	18	1.5
(1,28)	1:1841:A:GLY:N	1:1841:A:GLY:CA	1:1841:A:GLY:C	1:1842:A:SER:N	20	1.49
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	4	1.48
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	17	1.46
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	1	1.44
(1,28)	1:1841:A:GLY:N	1:1841:A:GLY:CA	1:1841:A:GLY:C	1:1842:A:SER:N	6	1.44
(1,123)	1:1905:A:PRO:C	1:1906:A:GLN:N	1:1906:A:GLN:CA	1:1906:A:GLN:C	17	1.43
(1,173)	1:1945:A:ARG:C	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	16	1.42
(1,128)	1:1908:A:GLU:N	1:1908:A:GLU:CA	1:1908:A:GLU:C	1:1909:A:VAL:N	8	1.39
(1,28)	1:1841:A:GLY:N	1:1841:A:GLY:CA	1:1841:A:GLY:C	1:1842:A:SER:N	8	1.33
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	8	1.32
(1,28)	1:1841:A:GLY:N	1:1841:A:GLY:CA	1:1841:A:GLY:C	1:1842:A:SER:N	9	1.32
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	16	1.29
(1,123)	1:1905:A:PRO:C	1:1906:A:GLN:N	1:1906:A:GLN:CA	1:1906:A:GLN:C	8	1.28
(1,174)	1:1946:A:CYS:N	1:1946:A:CYS:CA	1:1946:A:CYS:C	1:1947:A:GLY:N	20	1.22

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,28)	1:1841:A:GLY:N	1:1841:A:GLY:CA	1:1841:A:GLY:C	1:1842:A:SER:N	10	1.22
(1,123)	1:1905:A:PRO:C	1:1906:A:GLN:N	1:1906:A:GLN:CA	1:1906:A:GLN:C	20	1.18
(1,82)	1:1876:A:PHE:N	1:1876:A:PHE:CA	1:1876:A:PHE:C	1:1877:A:GLN:N	1	1.15
(1,82)	1:1876:A:PHE:N	1:1876:A:PHE:CA	1:1876:A:PHE:C	1:1877:A:GLN:N	2	1.1
(1,82)	1:1876:A:PHE:N	1:1876:A:PHE:CA	1:1876:A:PHE:C	1:1877:A:GLN:N	4	1.1
(1,28)	1:1841:A:GLY:N	1:1841:A:GLY:CA	1:1841:A:GLY:C	1:1842:A:SER:N	11	1.09
(1,120)	1:1904:A:SER:N	1:1904:A:SER:CA	1:1904:A:SER:C	1:1905:A:PRO:N	16	1.05
(1,28)	1:1841:A:GLY:N	1:1841:A:GLY:CA	1:1841:A:GLY:C	1:1842:A:SER:N	5	1.05