

wwPDB NMR Structure Validation Summary Report (i)

Apr 2, 2020 – 11:19 AM CDT

PDB ID : 2KO1

Title: Solution NMR structure of the ACT domain from GTP pyrophosphokinase

of Chlorobium tepidum. Northeast Structural Genomics Consortium Target

CtR148A

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Deposited on : 2009-09-08

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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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)

NmrClust : Kelley et al. (1996)

MolProbity: 4.02b-467

Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)

RCI : v 1n 11 5 13 A (Berjanski et al., 2005)

PANAV : Wang et al. (2010)

 $ShiftChecker \quad : \quad 2.6. dev1$

BMRB Restraints Analalysis : v1.2

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

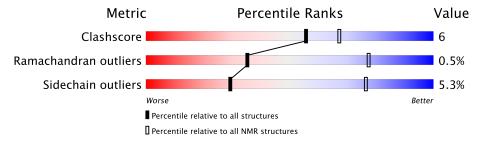
Validation Pipeline (wwPDB-VP) : 2.6.dev1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $SOLUTION\ NMR$

The overall completeness of chemical shifts assignment is 64%.

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 $(\# \mathrm{Entries})$	$ m NMR~archive \ (\#Entries)$		
Clashscore	136327	12091		
Ramachandran outliers	132723	10835		
Sidechain outliers	132532	10811		

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 <=5%

Mol	Chain	Length	Quality of chain		
1	A	88	76%	13%	11%
1	В	88	76%	14%	10%



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:4-A:81, B:3-B:81 (157)		0.32	1				

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 4 clusters and 3 single-model clusters were found.

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



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2858 atoms, of which 1452 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called GTP pyrophosphokinase.

Mol	Chain	Residues		Atoms					Trace
1	Λ	88	Total	С	Н	N	О	S	0
1	A	00	1429	442	726	128	128	5	0
1	D	88	Total	С	Н	N	О	S	0
1	Б	00	1429	442	726	128	128	5	U

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP Q8KC80
A	16	ASN	ILE	ENGINEERED	UNP Q8KC80
A	81	LEU	-	EXPRESSION TAG	UNP Q8KC80
A	82	GLU	-	EXPRESSION TAG	UNP Q8KC80
A	83	HIS	-	EXPRESSION TAG	UNP Q8KC80
A	84	HIS	-	EXPRESSION TAG	UNP Q8KC80
A	85	HIS	-	EXPRESSION TAG	UNP Q8KC80
A	86	HIS	-	EXPRESSION TAG	UNP Q8KC80
A	87	HIS	-	EXPRESSION TAG	UNP Q8KC80
A	88	HIS	-	EXPRESSION TAG	UNP Q8KC80
В	1	MET	-	INITIATING METHIONINE	UNP Q8KC80
В	16	ASN	ILE	ENGINEERED	UNP Q8KC80
В	81	LEU	-	EXPRESSION TAG	UNP Q8KC80
В	82	GLU	-	EXPRESSION TAG	UNP Q8KC80
В	83	HIS	-	EXPRESSION TAG	UNP Q8KC80
В	84	HIS	-	EXPRESSION TAG	UNP Q8KC80
В	85	HIS	-	EXPRESSION TAG	UNP Q8KC80
В	86	HIS	-	EXPRESSION TAG	UNP Q8KC80
В	87	HIS	-	EXPRESSION TAG	UNP Q8KC80
В	88	HIS	-	EXPRESSION TAG	UNP Q8KC80

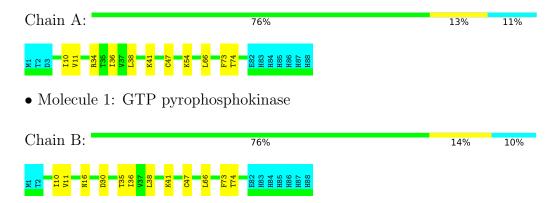


4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

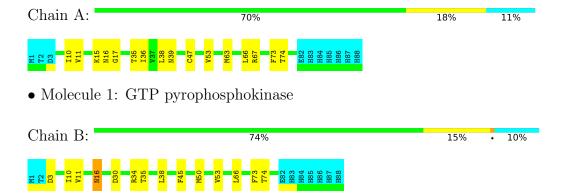
• Molecule 1: GTP pyrophosphokinase



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

• Molecule 1: GTP pyrophosphokinase





Refinement protocol and experimental data overview (i) 5



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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: target function.

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

Software name	Classification	Version
CYANA	structure solution	3.0
CNS	refinement	1.2.1

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)	2ko1_nmr.cif
Number of chemical shift lists	1
Total number of shifts	2170
Number of shifts mapped to atoms	1348
Number of unparsed shifts	312
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	510
Assignment completeness (well-defined parts)	64%

No validations of the models with respect to experimental NMR restraints is performed at this time.



6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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	610	650	650	8±2
1	В	618	654	654	9±3
All	All	24560	26080	26080	288

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 6.

5 of 104 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	$Distance(\mathring{A})$	${f Models}$	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:B:10:ILE:HD11	1:B:66:LEU:HD13	0.71	1.62	3	11
1:B:36:ILE:HD11	1:B:47:CYS:SG	0.66	2.29	14	10
1:A:10:ILE:HD11	1:A:66:LEU:HD13	0.66	1.65	18	14
1:A:36:ILE:HD11	1:A:47:CYS:SG	0.65	2.31	5	9
1:A:15:LYS:O	1:A:17:GLY:N	0.59	2.35	20	3

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 she	ws the	number	of resid	lues for	which	the	backbone	conforma	ation
was ana	alysed and the	total numb	er of re	esidues.							

Mol	Chain	Analysed Favoured Allowed		Outliers	Percentiles		
1	A	78/88 (89%)	75±2 (96±3%)	3±2 (4±3%)	0±0 (0±1%)	40	79
1	В	79/88 (90%)	75±2 (95±2%)	4±2 (4±2%)	0±1 (1±1%)	31	76
All	All	3140/3520 (89%)	2996 (95%)	129 (4%)	15 (0%)	35	77

5 of 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	В	16	ASN	5
1	A	16	ASN	4
1	A	42	ASP	2
1	В	17	GLY	2
1	В	43	GLY	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	A	70/80 (88%)	66±2 (95±2%)	$4\pm 2 \ (5\pm 2\%)$	29	76	
1	В	71/80 (89%)	67±1 (95±2%)	4±1 (5±2%)	30	77	
All	All	2820/3200 (88%)	2670 (95%)	150 (5%)	29	76	

5 of 41 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	В	73	PHE	19
1	A	41	LYS	17
1	В	41	LYS	13
1	A	73	PHE	13
1	В	30	ASP	11



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 carbohydrates 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 (i)

The completeness of assignment taking into account all chemical shift lists is 64% for the well-defined parts and 59% for the entire structure.

7.1 Chemical shift list 1

File name: 2ko1_nmr.cif

Chemical shift list name: nef_chemical_shift_list_aco.tbl

7.1.1 Bookkeeping (i)

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

Total number of shifts	2170
Number of shifts mapped to atoms	1348
Number of unparsed shifts	312
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	510
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

• Chemical shift has been reported more than once. First 5 (of 312) occurrences are reported below.

Shift ID	Chain	Res	Tuno	Type Atom		Shift Dat	a
	Chain	nes	Type	Atom	Value	Uncertainty	Ambiguity
4	A	2	THR	HG2%	1.335	0.020	1
5	A	2	THR	HG2%	1.335	0.020	1
21	A	4	PHE	HB%	3.080	0.020	1
23	A	4	PHE	HD%	7.184	0.020	1
38	A	5	LEU	HD1%	0.475	0.020	1

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

• No matching atoms found in structure. First 5 (of 510) occurrences are reported below.

Chain	Pog	Type	Atom		Shift Dat	a
Chain	nes	Type	Atom	Value	Shift Dat Uncertainty	Ambiguity
A	21	GLN	HBx	2.243	0.02	2
В	44	ILE	HG1x	1.482	0.02	2



Continued from previous page...

Chain	Pag	Ттто	rno Atom		Shift Dat	a
Chain	nes	Туре	Atom	Value	Shift Dat Uncertainty	Ambiguity
A	62	LEU	HBx	1.26	0.02	2
В	41	LYS	HB%	1.815	0.02	1
A	33	ILE	HG1x	1.751	0.02	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\mathrm{C}_{\alpha}$	164	-0.11 ± 0.13	None needed ($< 0.5 \text{ ppm}$)
$^{13}C_{\beta}$	152	-0.03 ± 0.11	None needed ($< 0.5 \text{ ppm}$)
¹³ C′	162	0.07 ± 0.13	None needed ($< 0.5 \text{ ppm}$)
^{15}N	162	-0.06 ± 0.17	None needed (< 0.5 ppm)

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 64%, i.e. 1256 atoms were assigned a chemical shift out of a possible 1959. 30 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Backbone	771/785 (98%)	302/314 (96%)	312/314 (99%)	157/157 (100%)
Sidechain	445/1084 (41%)	72/622 (12%)	347/406 (85%)	26/56~(46%)
Aromatic	40/90 (44%)	20/50 (40%)	20/40 (50%)	0/0 (%)
Overall	1256/1959~(64%)	394/986 (40%)	679/760 (89%)	183/213 (86%)

7.1.4 Statistically unusual chemical shifts (i)

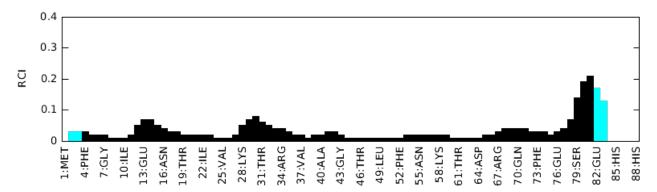
There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

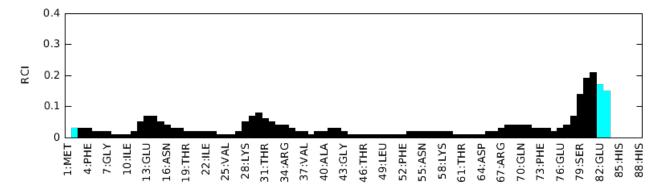
The images below report random coil index values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted 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.



Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:





8 Distance restraints analysis

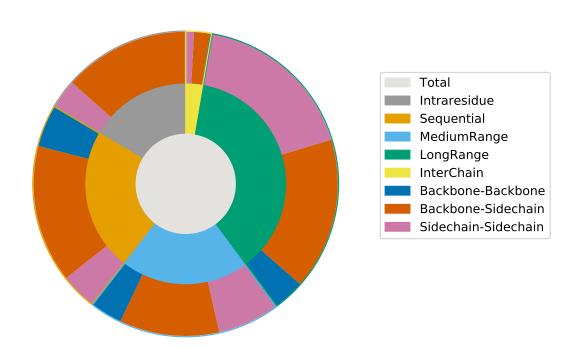
8.1 Distance restraints summary

Restraints are counted in different categories based on the atoms involved in each restraint.

Dogtroints type	$\mathbf{B} ext{-}\mathbf{B}^1(\mathbf{H}^4)$	$\mathbf{B} ext{-}\mathbf{S}^2(\mathbf{H}^4)$	S-S ³ (H ⁴)	Total			
Restraints type	D-D ² (H ²)	D-S -(I 1-)	S-S°(H-)	$Total(H^4)$	RR^5	$\%^6$	
Intraresidue (i-j =0)	0(0)	673(0)	154(0)	827(0)	0.6	16.5	
Sequential (i-j =1)	226(0)	733(0)	195(0)	1154(0)	0.8	23.0	
Medium range ($ i-j >1$ and $ i-j <5$)	172(0)	532(0)	331(0)	1035(0)	0.7	20.6	
Long range (i-j ≥5)	170(0)	810(0)	882(0)	1862(0)	1.3	37.1	
Inter chain	8(0)	84(0)	44(0)	136(0)	0.1	2.7	
Total	576(0)	2832(0)	1606(0)	5014(0)	3.4	100.0	

¹number of backbone to backbone restraints, ²number of backbone to sidechain restraints, ³number of sidechain to sidechain restraints, ⁴number of hydrogen bonds in that category, ⁵number of restraints per residue, ⁶percentage of restraints in that category. There are 0 unmapped restraints

8.1.1 Pie chart: Distance restraints summary





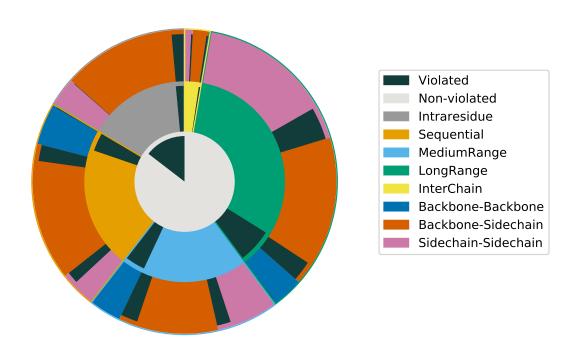
8.2 Distance violations summary

The following table provides the summary of violated restraints. Restraints that are violated at least in one model are counted as violated.

Dogtrojeta temo	$B-B^{1}(\%^{4})$	$B-S^2(\%^4)$	$S-S^3(\%^4)$	Total		
Restraints type	D-D (%)	D-3 (%)	S-S'(%)	$Total(\%^4)$	RR^5	$\%^6$
Intraresidue (i-j =0)	0(0.0)	71(10.5)	3(1.9)	74(8.9)	0.1	10.1
Sequential (i-j =1)	11(4.9)	88(12.0)	64(32.8)	163(14.1)	0.1	22.3
Medium range ($ i-j >1$ and $ i-j <5$)	8(4.7)	93(17.5)	76(23.0)	177(17.1)	0.1	24.2
Long range (i-j ≥5)	10(5.9)	111(13.7)	178(20.2)	299(16.1)	0.2	40.9
Inter chain	0(0.0)	9(10.7)	9(20.5)	18(13.2)	0.0	2.5
Total	29(5.0)	372(13.1)	330(20.5)	731(14.6)	0.5	100.0

¹number of backbone to backbone restraints, ²number of backbone to sidechain restraints, ³number of sidechain to sidechain restraints, ⁴percentage of violations with respect to total restrains in that category, ⁵number of restraints per residue, ⁶percentage of violation with respect to total violations.

8.2.1 Pie-chart: Distance violations summary





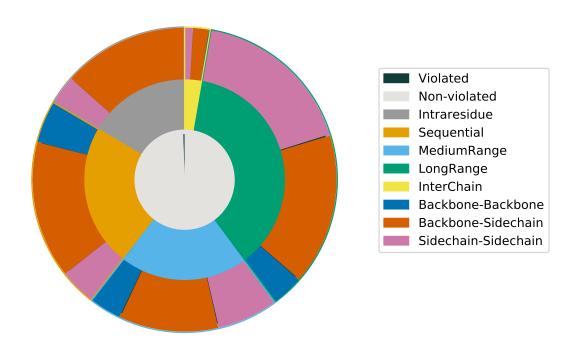
8.3 Consistent distance violations summary

The following table provides the summary of consistently violated restraints. Restraints that are violated in all models are counted as consistently violated.

Dogtroints type	$B-B^{1}(\%^{4})$	$B-S^2(\%^4)$	$S-S^3(\%^4)$	Total		
Restraints type	D-D (%)	D-5 (%)	S-S'(%)	$Total(\%^4)$	RR^5	$\%^6$
Intraresidue ($ i-j =0$)	0(0.0)	0(0.0)	0(0.0)	0(0.0)	0.0	0.0
Sequential (i-j =1)	0(0.0)	2(0.3)	1(0.5)	3(0.3)	0.0	12.5
Medium range ($ i-j >1$ and $ i-j <5$)	1(0.6)	5(0.9)	4(1.2)	10(1.0)	0.0	41.7
Long range (i-j ≥5)	0(0.0)	4(0.5)	7(0.8)	11(0.6)	0.0	45.8
Inter chain	0(0.0)	0(0.0)	0(0.0)	0(0.0)	0.0	0.0
Total	1(0.2)	11(0.4)	12(0.7)	24(0.5)	0.0	100.0

¹number of backbone to backbone restraints, ²number of backbone to sidechain restraints, ³number of sidechain to sidechain restraints, ⁴percentage of violations with respect to total restrains in that category, ⁵number of restraints per residue, ⁶percentage of violation with respect to total violations

8.3.1 Pie-chart: Consistent distance violations





8.4 Residual distance violations

Violation are counted in different bin sizes and listed below

Range (Å)	Avg. No. of violated restraints per model	Max violation (Å)
0-0.2	182.1	0.2
0.2-0.5	2.3	0.39
0.5-1.0	None	None
1.0-2.0	None	None
2.0-5.0	None	None
5.0<	None	None

8.5 Distance violations in ensemble

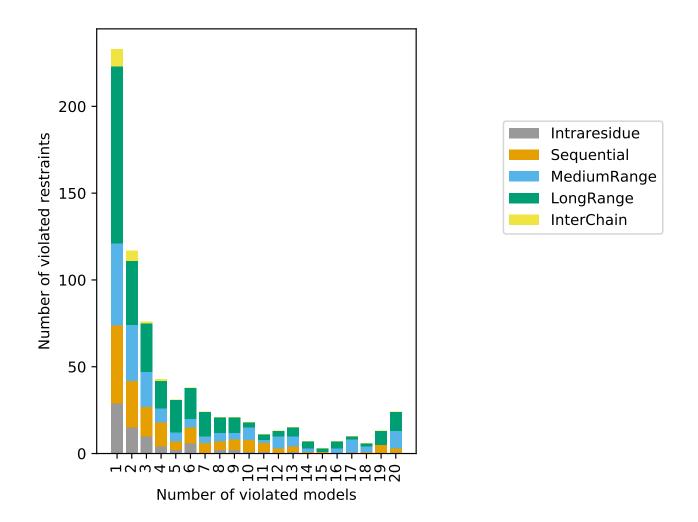
The restraints are grouped based on the number of violated models and listed here.

I		f violat		strair	nts	No. of violated models
IR^1	SQ^2	MR^3	$ LR^4 $	$ IC^5 $	Total	10. of violated models
29	45	47	102	10	233	1
15	27	32	37	6	117	2
10	17	20	28	1	76	3
4	14	8	16	1	43	4
2	5	5	19	0	31	5
6	9	5	18	0	38	6
0	6	4	14	0	24	7
2	5	5	9	0	21	8
2	6	4	9	0	21	9
1	7	7	3	0	18	10
1	5	2	3	0	11	11
0	3	7	3	0	13	12
1	3	6	5	0	15	13
0	1	2	4	0	7	14
0	1	0	2	0	3	15
0	0	3	4	0	7	16
1	0	7	2	0	10	17
0	1	3	2	0	6	18
0	5	0	8	0	13	19
0	3	10	11	0	24	20

 $^{^1 \}rm intraresidue$ restraints, $^2 \rm sequential$ restraints, $^3 \rm medium$ range restraints, $^4 \rm long$ range restraints, $^5 \rm inter$ chain restraints



8.5.1 Bar graph: No. of models vs No. of violations



753 intraresidue restraints, 991 sequential restraints, 858 medium range restraints,1563 long range restraints and 118 inter chain restraints are not violated. In total, 4283 restraints are not violated in any of the models

8.6 Violations in each model

The following table lists the violation count in each model in the ensemble

Model ID		N	o. of v	riolati	Mean (Å)	Max (Å)		
Model ID	IR^1	SQ^2	$ m MR^3$	LR^4	IC^5	Total	Mean (A)	Max (A)
1	7	45	50	79	0	181	0.06	0.39
2	13	38	52	74	3	180	0.05	0.36
3	14	42	59	68	3	186	0.05	0.32
4	13	38	58	77	2	188	0.05	0.21
5	14	46	59	67	1	187	0.05	0.36



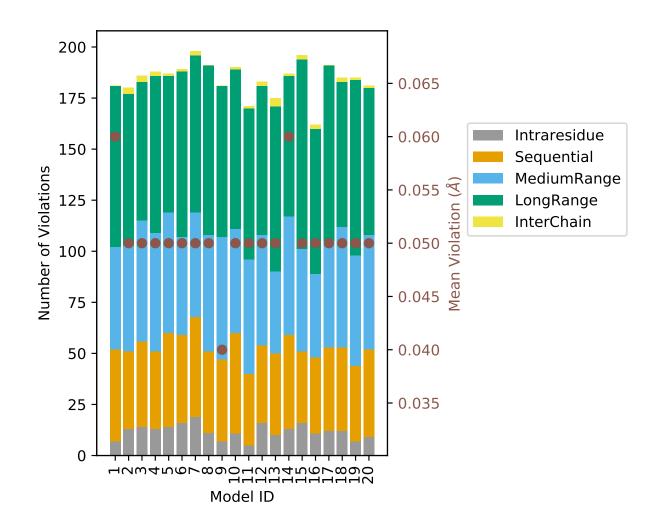
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Model ID		N	o. of v	iolati	ons		Mean (Å)	Max (Å)	
Model 1D	IR^1	SQ^2	MR^3	LR^4	IC^5	Total	Mean (A)	Max (A)	
6	16	43	48	81	1	189	0.05	0.21	
7	19	49	51	77	2	198	0.05	0.25	
8	11	40	57	83	0	191	0.05	0.29	
9	7	40	60	74	0	181	0.04	0.16	
10	11	49	51	78	1	190	0.05	0.3	
11	5	35	56	74	1	171	0.05	0.24	
12	16	38	54	73	2	183	0.05	0.24	
13	10	40	40	81	4	175	0.05	0.37	
14	13	46	58	69	1	187	0.06	0.28	
15	16	35	50	93	2	196	0.05	0.33	
16	11	37	41	71	2	162	0.05	0.27	
17	12	41	52	86	0	191	0.05	0.18	
18	12	41	59	71	2	185	0.05	0.34	
19	7	37	54	86	1	185	0.05	0.33	
20	9	43	56	72	1	181	0.05	0.29	

 $^{^1}$ intraresidue restraints, 2 iequential restraints, 3 iedium range restraints, 4 long range restraints, 5 inter chain restraints



8.6.1 Bar graph: Violations in each model

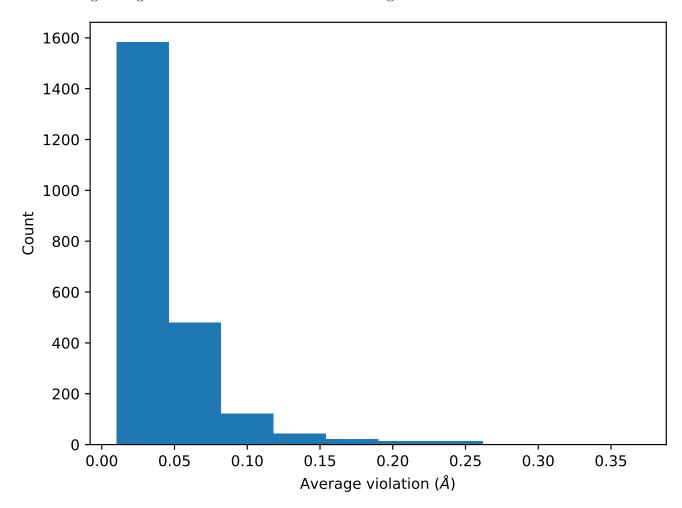




8.7 Most violated distance restraints

8.7.1 Histogram : Distribution of mean distance violations

The following histogram shows the distribution of average violations of each restraint.



8.7.2 Table: Most violated distance restraints

The following tale lists the average violation of each restraint sorted by number of violated models

Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	20	0.05	0.09
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	20	0.06	0.1
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	20	0.14	0.32
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	20	0.14	0.32
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	20	0.14	0.32
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	20	0.14	0.32



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	20	0.07	0.13
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	20	0.07	0.13
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	20	0.07	0.13
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	20	0.06	0.08
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	20	0.06	0.08
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	20	0.06	0.08
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	20	0.06	0.08
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	20	0.06	0.08
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	20	0.06	0.08
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	20	0.06	0.11
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	20	0.06	0.11
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	20	0.06	0.11
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	20	0.06	0.11
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	20	0.06	0.11
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	20	0.06	0.11
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE1	20	0.06	0.11
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE2	20	0.06	0.11
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE1	20	0.06	0.11
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE2	20	0.06	0.11
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE1	20	0.05	0.09
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE2	20	0.05	0.09
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE1	20	0.05	0.09
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE2	20	0.05	0.09
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	20	0.09	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	20	0.09	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	20	0.09	0.11
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	20	0.08	0.13
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	20	0.08	0.13
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	20	0.08	0.13
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	20	0.07	0.1
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	20	0.07	0.1
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	20	0.07	0.1
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	20	0.1	0.14
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	20	0.1	0.14
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	20	0.1	0.14
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	20	0.09	0.17
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	20	0.09	0.17
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	20	0.09	0.17
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	20	0.12	0.17
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	20	0.11	0.16
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	20	0.06	0.14
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	20	0.06	0.14



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	20	0.06	0.14
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	20	0.06	0.11
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	20	0.06	0.11
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	20	0.06	0.11
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	20	0.1	0.21
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	20	0.1	0.21
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	20	0.1	0.21
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	20	0.06	0.15
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	20	0.06	0.15
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	20	0.06	0.15
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	20	0.07	0.08
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	20	0.07	0.08
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	20	0.07	0.08
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	20	0.07	0.13
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	20	0.07	0.13
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	20	0.07	0.13
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	20	0.06	0.09
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	20	0.06	0.09
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	20	0.06	0.09
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	20	0.1	0.14
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	20	0.08	0.13
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	20	0.08	0.13
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	20	0.08	0.13
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	19	0.03	0.07
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	19	0.07	0.12
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	19	0.07	0.12
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	19	0.07	0.12
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	19	0.06	0.09
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	19	0.06	0.09
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	19	0.06	0.09
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	19	0.06	0.09
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	19	0.06	0.09
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	19	0.06	0.09
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	19	0.06	0.11
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	19	0.06	0.11
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	19	0.06	0.11
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	19	0.06	0.11
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	19	0.06	0.11
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	19	0.06	0.11
(1,2816)	1:B:50:MET:HE1	1:B:51:ILE:HG13	19	0.04	0.07
(1,2816)	1:B:50:MET:HE2	1:B:51:ILE:HG13	19	0.04	0.07
(1,2816)	1:B:50:MET:HE3	1:B:51:ILE:HG13	19	0.04	0.07



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	19	0.04	0.08
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	19	0.04	0.08
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	19	0.04	0.08
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	19	0.05	0.12
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	19	0.04	0.07
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	19	0.09	0.16
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	19	0.09	0.16
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	19	0.09	0.16
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	19	0.08	0.13
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	19	0.08	0.13
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	19	0.08	0.13
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	19	0.08	0.12
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	19	0.08	0.12
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	19	0.08	0.12
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	19	0.08	0.16
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	19	0.08	0.16
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	19	0.08	0.16
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	19	0.08	0.16
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	19	0.08	0.16
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	19	0.08	0.16
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	19	0.08	0.16
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	19	0.08	0.16
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	19	0.08	0.16
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	19	0.04	0.13
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	19	0.04	0.13
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	19	0.04	0.13
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	19	0.04	0.13
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	19	0.04	0.13
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	19	0.04	0.13
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	18	0.08	0.13
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	18	0.08	0.13
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	18	0.08	0.13
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	18	0.02	0.05
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	18	0.13	0.21
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	18	0.13	0.21
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	18	0.13	0.21
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	18	0.09	0.14
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	18	0.07	0.12
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	18	0.07	0.12
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	18	0.07	0.12
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	18	0.07	0.12
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	18	0.07	0.12



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	18	0.07	0.12
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	18	0.07	0.12
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	18	0.07	0.12
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	18	0.07	0.12
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	18	0.05	0.16
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	18	0.05	0.16
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	18	0.05	0.16
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG2	17	0.06	0.11
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	17	0.06	0.11
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	17	0.06	0.11
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG3	17	0.06	0.11
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	17	0.06	0.11
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	17	0.06	0.11
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE1	17	0.05	0.11
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE2	17	0.05	0.11
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE3	17	0.05	0.11
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE1	17	0.05	0.11
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE2	17	0.05	0.11
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE3	17	0.05	0.11
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	17	0.06	0.13
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	17	0.06	0.13
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	17	0.06	0.13
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	17	0.06	0.13
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	17	0.06	0.13
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	17	0.06	0.13
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	17	0.04	0.07
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	17	0.04	0.07
(1,3591)	1:A:20:ASN:HA	1:A:22:ILE:HB	17	0.04	0.07
(1,3413)	1:B:63:MET:HE1	1:B:76:GLU:HA	17	0.05	0.08
(1,3413)	1:B:63:MET:HE2	1:B:76:GLU:HA	17	0.05	0.08
(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	17	0.05	0.08
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	17	0.05	0.09
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	17	0.05	0.09
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	17	0.05	0.09
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	17	0.06	0.1
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	17	0.06	0.1
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	17	0.06	0.1
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	17	0.04	0.1
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	17	0.04	0.1
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	17	0.04	0.1
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	17	0.05	0.09
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	16	0.1	0.26



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,3592)	1:B:20:ASN:HA	1:B:22:ILE:HB	16	0.05	0.09
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	16	0.09	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	16	0.09	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	16	0.09	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	16	0.09	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	16	0.09	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	16	0.09	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	16	0.09	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	16	0.09	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	16	0.09	0.14
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	16	0.04	0.1
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	16	0.04	0.1
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	16	0.04	0.1
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	16	0.04	0.1
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	16	0.04	0.1
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG23	16	0.04	0.1
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	16	0.04	0.1
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	16	0.04	0.1
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	16	0.04	0.1
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	16	0.04	0.08
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	16	0.04	0.08
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	16	0.04	0.08
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	16	0.04	0.08
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	16	0.04	0.08
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	16	0.04	0.08
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	16	0.05	0.08
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	16	0.05	0.08
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	16	0.05	0.08
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	16	0.05	0.1
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD11	15	0.03	0.05
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD12	15	0.03	0.05
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD13	15	0.03	0.05
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	15	0.09	0.36
(1,3412)	1:A:63:MET:HE1	1:A:76:GLU:HA	15	0.05	0.07
(1,3412)	1:A:63:MET:HE2	1:A:76:GLU:HA	15	0.05	0.07
(1,3412)	1:A:63:MET:HE3	1:A:76:GLU:HA	15	0.05	0.07
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB2	14	0.02	0.04
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB3	14	0.02	0.04
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	14	0.16	0.28
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	14	0.16	0.28
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	14	0.16	0.28
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	14	0.16	0.28



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,4205)	1:B:29:PHE:HD1	1:B:65:LYS:HD2	14	0.05	0.1
(1,4205)	1:B:29:PHE:HD2	1:B:65:LYS:HD2	14	0.05	0.1
(1,4186)	1:A:4:PHE:HZ	1:A:6:ALA:HA	14	0.02	0.04
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	14	0.09	0.14
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	14	0.09	0.14
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	14	0.09	0.14
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	14	0.09	0.17
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	14	0.09	0.17
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	14	0.09	0.17
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	14	0.09	0.17
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	14	0.09	0.17
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	14	0.09	0.17
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	14	0.09	0.17
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	14	0.09	0.17
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	14	0.09	0.17
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	14	0.07	0.12
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	14	0.07	0.12
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	14	0.07	0.12
(1,899)	1:B:51:ILE:HG12	1:B:52:PHE:H	13	0.03	0.05
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD1	13	0.05	0.1
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD2	13	0.05	0.1
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE1	13	0.05	0.12
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE2	13	0.05	0.12
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE3	13	0.05	0.12
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE1	13	0.05	0.12
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE2	13	0.05	0.12
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE3	13	0.05	0.12
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB2	13	0.03	0.06
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB3	13	0.03	0.06
(1,4323)	1:B:52:PHE:HD1	1:B:53:VAL:H	13	0.04	0.07
(1,4323)	1:B:52:PHE:HD2	1:B:53:VAL:H	13	0.04	0.07
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG2	13	0.03	0.05
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG3	13	0.03	0.05
(1,3421)	1:B:63:MET:HE1	1:B:77:ARG:H	13	0.03	0.06
(1,3421)	1:B:63:MET:HE2	1:B:77:ARG:H	13	0.03	0.06
(1,3421)	1:B:63:MET:HE3	1:B:77:ARG:H	13	0.03	0.06
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD21	13	0.03	0.06
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD22	13	0.03	0.06
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD23	13	0.03	0.06
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	13	0.08	0.11
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	13	0.08	0.11
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	13	0.08	0.11



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2182)	1:B:29:PHE:HD1	1:B:31:THR:HB	13	0.04	0.08
(1,2182)	1:B:29:PHE:HD2	1:B:31:THR:HB	13	0.04	0.08
(1,2181)	1:A:29:PHE:HD1	1:A:31:THR:HB	13	0.05	0.09
(1,2181)	1:A:29:PHE:HD2	1:A:31:THR:HB	13	0.05	0.09
(1,2088)	1:B:25:VAL:HG11	1:B:27:SER:H	13	0.02	0.04
(1,2088)	1:B:25:VAL:HG12	1:B:27:SER:H	13	0.02	0.04
(1,2088)	1:B:25:VAL:HG13	1:B:27:SER:H	13	0.02	0.04
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG11	13	0.06	0.14
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG12	13	0.06	0.14
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG13	13	0.06	0.14
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG11	13	0.06	0.14
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG12	13	0.06	0.14
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG13	13	0.06	0.14
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG21	13	0.04	0.1
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG22	13	0.04	0.1
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG23	13	0.04	0.1
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG21	13	0.04	0.1
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG22	13	0.04	0.1
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG23	13	0.04	0.1
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG21	13	0.04	0.1
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG22	13	0.04	0.1
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG23	13	0.04	0.1
(1,1103)	1:A:62:LEU:HD11	1:A:65:LYS:H	13	0.02	0.03
(1,1103)	1:A:62:LEU:HD12	1:A:65:LYS:H	13	0.02	0.03
(1,1103)	1:A:62:LEU:HD13	1:A:65:LYS:H	13	0.02	0.03
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD1	12	0.04	0.06
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD2	12	0.04	0.06
(1,545)	1:A:29:PHE:HD1	1:A:31:THR:H	12	0.07	0.18
(1,545)	1:A:29:PHE:HD2	1:A:31:THR:H	12	0.07	0.18
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB2	12	0.07	0.16
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB3	12	0.07	0.16
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB2	12	0.07	0.16
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB3	12	0.07	0.16
(1,4187)	1:B:4:PHE:HZ	1:B:6:ALA:HA	12	0.02	0.05
(1,4144)	1:A:4:PHE:HD1	1:A:5:LEU:H	12	0.02	0.04
(1,4144)	1:A:4:PHE:HD2	1:A:5:LEU:H	12	0.02	0.04
(1,3994)	1:A:82:GLU:H	1:A:83:HIS:HB3	12	0.08	0.15
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD11	12	0.03	0.07
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD12	12	0.03	0.07
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD13	12	0.03	0.07
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD11	12	0.04	0.1
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD12	12	0.04	0.1



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD13	12	0.04	0.1
(1,381)	1:B:22:ILE:H	1:B:23:THR:HG1	12	0.02	0.04
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG11	12	0.03	0.07
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG12	12	0.03	0.07
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG13	12	0.03	0.07
(1,2667)	1:A:23:THR:HG1	1:A:47:CYS:HB3	12	0.03	0.06
(1,1106)	1:B:62:LEU:HD11	1:B:66:LEU:H	12	0.02	0.05
(1,1106)	1:B:62:LEU:HD12	1:B:66:LEU:H	12	0.02	0.05
(1,1106)	1:B:62:LEU:HD13	1:B:66:LEU:H	12	0.02	0.05
(1,1104)	1:B:62:LEU:HD11	1:B:65:LYS:H	12	0.03	0.07
(1,1104)	1:B:62:LEU:HD12	1:B:65:LYS:H	12	0.03	0.07
(1,1104)	1:B:62:LEU:HD13	1:B:65:LYS:H	12	0.03	0.07
(1,4322)	1:A:52:PHE:HD1	1:A:53:VAL:H	11	0.03	0.06
(1,4322)	1:A:52:PHE:HD2	1:A:53:VAL:H	11	0.03	0.06
(1,4204)	1:A:29:PHE:HD1	1:A:65:LYS:HD2	11	0.03	0.06
(1,4204)	1:A:29:PHE:HD2	1:A:65:LYS:HD2	11	0.03	0.06
(1,4145)	1:B:4:PHE:HD1	1:B:5:LEU:H	11	0.02	0.04
(1,4145)	1:B:4:PHE:HD2	1:B:5:LEU:H	11	0.02	0.04
(1,4053)	1:B:41:LYS:HG2	1:B:42:ASP:HA	11	0.07	0.13
(1,4053)	1:B:41:LYS:HG3	1:B:42:ASP:HA	11	0.07	0.13
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD11	11	0.04	0.08
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD12	11	0.04	0.08
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD13	11	0.04	0.08
(1,3889)	1:A:82:GLU:HA	1:A:83:HIS:HB2	11	0.04	0.1
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	11	0.19	0.33
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	11	0.19	0.33
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE1	11	0.08	0.14
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE2	11	0.08	0.14
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE3	11	0.08	0.14
(1,2485)	1:A:40:ALA:HA	1:A:45:PHE:HA	11	0.03	0.08
(1,2387)	1:A:37:VAL:HG21	1:A:38:LEU:H	11	0.02	0.04
(1,2387)	1:A:37:VAL:HG22	1:A:38:LEU:H	11	0.02	0.04
(1,2387)	1:A:37:VAL:HG23	1:A:38:LEU:H	11	0.02	0.04
(1,1105)	1:A:62:LEU:HD11	1:A:66:LEU:H	11	0.04	0.07
(1,1105)	1:A:62:LEU:HD12	1:A:66:LEU:H	11	0.04	0.07
(1,1105)	1:A:62:LEU:HD13	1:A:66:LEU:H	11	0.04	0.07
(1,563)	1:A:32:ASN:HD21	1:A:33:ILE:HB	10	0.05	0.12
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG2	10	0.02	0.04
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG3	10	0.02	0.04
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB2	10	0.08	0.11
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB3	10	0.08	0.11
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB2	10	0.08	0.11



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB3	10	0.08	0.11
(1,4388)	1:A:81:LEU:HB2	1:A:83:HIS:HD2	10	0.04	0.08
(1,4388)	1:A:81:LEU:HB3	1:A:83:HIS:HD2	10	0.04	0.08
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG21	10	0.04	0.08
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG22	10	0.04	0.08
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG23	10	0.04	0.08
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG21	10	0.03	0.06
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG22	10	0.03	0.06
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG23	10	0.03	0.06
(1,4119)	1:B:80:ASN:HA	1:B:81:LEU:HG	10	0.04	0.07
(1,3593)	1:A:66:LEU:HA	1:A:69:VAL:HB	10	0.03	0.07
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG21	10	0.03	0.05
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG22	10	0.03	0.05
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG23	10	0.03	0.05
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG21	10	0.03	0.06
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG22	10	0.03	0.06
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG23	10	0.03	0.06
(1,2583)	1:A:44:ILE:HD11	1:A:46:THR:HB	10	0.03	0.06
(1,2583)	1:A:44:ILE:HD12	1:A:46:THR:HB	10	0.03	0.06
(1,2583)	1:A:44:ILE:HD13	1:A:46:THR:HB	10	0.03	0.06
(1,2424)	1:B:38:LEU:HD11	1:B:39:ASN:H	10	0.03	0.07
(1,2424)	1:B:38:LEU:HD12	1:B:39:ASN:H	10	0.03	0.07
(1,2424)	1:B:38:LEU:HD13	1:B:39:ASN:H	10	0.03	0.07
(1,2087)	1:A:25:VAL:HG11	1:A:27:SER:H	10	0.02	0.04
(1,2087)	1:A:25:VAL:HG12	1:A:27:SER:H	10	0.02	0.04
(1,2087)	1:A:25:VAL:HG13	1:A:27:SER:H	10	0.02	0.04
(1,208)	1:B:16:ASN:HA	1:B:17:GLY:H	10	0.05	0.07
(1,207)	1:A:16:ASN:HA	1:A:17:GLY:H	10	0.05	0.07
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG11	10	0.04	0.09
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG12	10	0.04	0.09
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG13	10	0.04	0.09
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG11	10	0.04	0.09
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG12	10	0.04	0.09
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG13	10	0.04	0.09
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD11	10	0.02	0.04
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD12	10	0.02	0.04
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD13	10	0.02	0.04
(1,1020)	1:A:58:LYS:HZ1	1:A:61:THR:H	10	0.07	0.13
(1,1020)	1:A:58:LYS:HZ2	1:A:61:THR:H	10	0.07	0.13
(1,1020)	1:A:58:LYS:HZ3	1:A:61:THR:H	10	0.07	0.13
(1,898)	1:A:51:ILE:HG12	1:A:52:PHE:H	9	0.03	0.05
(1,719)	1:B:41:LYS:H	1:B:46:THR:H	9	0.05	0.08



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD11	9	0.04	0.07
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD12	9	0.04	0.07
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD13	9	0.04	0.07
(1,546)	1:B:29:PHE:HD1	1:B:31:THR:H	9	0.03	0.1
(1,546)	1:B:29:PHE:HD2	1:B:31:THR:H	9	0.03	0.1
(1,5005)	1:B:77:ARG:H	1:B:77:ARG:HG2	9	0.02	0.04
(1,5005)	1:B:77:ARG:H	1:B:77:ARG:HG3	9	0.02	0.04
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD21	9	0.04	0.06
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD22	9	0.04	0.06
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD21	9	0.04	0.06
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD22	9	0.04	0.06
(1,4386)	1:A:5:LEU:HG	1:A:83:HIS:HD2	9	0.02	0.06
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE1	9	0.02	0.05
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE2	9	0.02	0.05
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE1	9	0.02	0.05
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE2	9	0.02	0.05
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE1	9	0.02	0.05
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE2	9	0.02	0.05
(1,4036)	1:A:15:LYS:HA	1:A:17:GLY:H	9	0.13	0.33
(1,380)	1:A:22:ILE:H	1:A:23:THR:HG1	9	0.02	0.03
(1,3420)	1:A:63:MET:HE1	1:A:77:ARG:H	9	0.03	0.05
(1,3420)	1:A:63:MET:HE2	1:A:77:ARG:H	9	0.03	0.05
(1,3420)	1:A:63:MET:HE3	1:A:77:ARG:H	9	0.03	0.05
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD2	9	0.04	0.07
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD3	9	0.04	0.07
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG21	9	0.02	0.03
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG22	9	0.02	0.03
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG23	9	0.02	0.03
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD21	9	0.03	0.07
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD22	9	0.03	0.07
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD23	9	0.03	0.07
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD21	9	0.03	0.07
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD22	9	0.03	0.07
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD23	9	0.03	0.07
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD21	9	0.03	0.07
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD22	9	0.03	0.07
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD23	9	0.03	0.07
(1,2639)	1:A:46:THR:HG21	1:A:47:CYS:H	9	0.02	0.04
(1,2639)	1:A:46:THR:HG22	1:A:47:CYS:H	9	0.02	0.04
(1,2639)	1:A:46:THR:HG23	1:A:47:CYS:H	9	0.02	0.04
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG21	9	0.02	0.04
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG22	9	0.02	0.04



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG23	9	0.02	0.04
(1,2379)	1:A:37:VAL:HG21	1:A:48:ASN:HD22	9	0.02	0.03
(1,2379)	1:A:37:VAL:HG22	1:A:48:ASN:HD22	9	0.02	0.03
(1,2379)	1:A:37:VAL:HG23	1:A:48:ASN:HD22	9	0.02	0.03
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	9	0.15	0.18
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	9	0.15	0.18
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	9	0.15	0.18
(1,2257)	1:A:35:THR:HB	1:A:50:MET:HB2	9	0.02	0.04
(1,1932)	1:A:21:GLN:HE21	1:A:22:ILE:HA	9	0.02	0.04
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD11	9	0.04	0.06
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD12	9	0.04	0.06
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD13	9	0.04	0.06
(1,832)	1:A:47:CYS:HG	1:A:48:ASN:H	8	0.02	0.03
(1,4613)	1:A:42:ASP:HB2	1:A:44:ILE:HG12	8	0.04	0.07
(1,4613)	1:A:42:ASP:HB3	1:A:44:ILE:HG12	8	0.04	0.07
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD11	8	0.03	0.06
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD12	8	0.03	0.06
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD13	8	0.03	0.06
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD11	8	0.03	0.06
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD12	8	0.03	0.06
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD13	8	0.03	0.06
(1,4310)	1:A:5:LEU:HA	1:A:52:PHE:HD1	8	0.02	0.05
(1,4310)	1:A:5:LEU:HA	1:A:52:PHE:HD2	8	0.02	0.05
(1,4118)	1:A:80:ASN:HA	1:A:81:LEU:HG	8	0.04	0.1
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD11	8	0.03	0.05
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD12	8	0.03	0.05
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD13	8	0.03	0.05
(1,3562)	1:B:15:LYS:HE2	1:B:18:MET:H	8	0.03	0.06
(1,3562)	1:B:15:LYS:HE3	1:B:18:MET:H	8	0.03	0.06
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	8	0.21	0.29
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	8	0.21	0.29
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD11	8	0.02	0.04
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD12	8	0.02	0.04
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD13	8	0.02	0.04
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD11	8	0.02	0.04
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD12	8	0.02	0.04
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD13	8	0.02	0.04
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD11	8	0.02	0.04
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD12	8	0.02	0.04
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD13	8	0.02	0.04
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD11	8	0.03	0.05
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD12	8	0.03	0.05



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD13	8	0.03	0.05
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD11	8	0.03	0.05
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD12	8	0.03	0.05
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD13	8	0.03	0.05
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD11	8	0.03	0.05
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD12	8	0.03	0.05
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD13	8	0.03	0.05
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD11	8	0.03	0.05
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD12	8	0.03	0.05
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD13	8	0.03	0.05
(1,278)	1:B:20:ASN:H	1:B:20:ASN:HD22	8	0.13	0.18
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD11	8	0.01	0.02
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD12	8	0.01	0.02
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD13	8	0.01	0.02
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD11	8	0.01	0.02
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD12	8	0.01	0.02
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD13	8	0.01	0.02
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD11	8	0.01	0.02
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD12	8	0.01	0.02
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD13	8	0.01	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD21	8	0.02	0.04
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD22	8	0.02	0.04
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD23	8	0.02	0.04
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD21	8	0.02	0.04
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD22	8	0.02	0.04
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD23	8	0.02	0.04
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD21	8	0.02	0.04
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD22	8	0.02	0.04
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD23	8	0.02	0.04
(1,2668)	1:B:23:THR:HG1	1:B:47:CYS:HB3	8	0.04	0.06
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG21	8	0.03	0.05
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG22	8	0.03	0.05
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG23	8	0.03	0.05
(1,2486)	1:B:40:ALA:HA	1:B:45:PHE:HA	8	0.03	0.04
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD21	8	0.03	0.04
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD22	8	0.03	0.04
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD23	8	0.03	0.04
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	8	0.16	0.19
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	8	0.16	0.19
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	8	0.16	0.19
(1,1860)	1:A:18:MET:HE1	1:A:71:GLY:HA2	8	0.02	0.03
(1,1860)	1:A:18:MET:HE2	1:A:71:GLY:HA2	8	0.02	0.03



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1860)	1:A:18:MET:HE3	1:A:71:GLY:HA2	8	0.02	0.03
(1,1212)	1:B:69:VAL:HG11	1:B:71:GLY:H	8	0.03	0.08
(1,1212)	1:B:69:VAL:HG12	1:B:71:GLY:H	8	0.03	0.08
(1,1212)	1:B:69:VAL:HG13	1:B:71:GLY:H	8	0.03	0.08
(1,4976)	1:B:63:MET:HE1	1:B:77:ARG:HB2	7	0.04	0.1
(1,4976)	1:B:63:MET:HE1	1:B:77:ARG:HB3	7	0.04	0.1
(1,4976)	1:B:63:MET:HE2	1:B:77:ARG:HB2	7	0.04	0.1
(1,4976)	1:B:63:MET:HE2	1:B:77:ARG:HB3	7	0.04	0.1
(1,4976)	1:B:63:MET:HE3	1:B:77:ARG:HB2	7	0.04	0.1
(1,4976)	1:B:63:MET:HE3	1:B:77:ARG:HB3	7	0.04	0.1
(1,4899)	1:B:39:ASN:HD21	1:B:46:THR:HB	7	0.04	0.09
(1,4899)	1:B:39:ASN:HD22	1:B:46:THR:HB	7	0.04	0.09
(1,4898)	1:B:39:ASN:HD21	1:B:41:LYS:HE2	7	0.03	0.06
(1,4898)	1:B:39:ASN:HD21	1:B:41:LYS:HE3	7	0.03	0.06
(1,4898)	1:B:39:ASN:HD22	1:B:41:LYS:HE2	7	0.03	0.06
(1,4898)	1:B:39:ASN:HD22	1:B:41:LYS:HE3	7	0.03	0.06
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD21	7	0.09	0.11
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD22	7	0.09	0.11
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD21	7	0.09	0.11
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD22	7	0.09	0.11
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD21	7	0.09	0.11
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD22	7	0.09	0.11
(1,4387)	1:B:5:LEU:HG	1:B:83:HIS:HD2	7	0.03	0.05
(1,4329)	1:B:5:LEU:HD21	1:B:52:PHE:HE1	7	0.02	0.03
(1,4329)	1:B:5:LEU:HD21	1:B:52:PHE:HE2	7	0.02	0.03
(1,4329)	1:B:5:LEU:HD22	1:B:52:PHE:HE1	7	0.02	0.03
(1,4329)	1:B:5:LEU:HD22	1:B:52:PHE:HE2	7	0.02	0.03
(1,4329)	1:B:5:LEU:HD23	1:B:52:PHE:HE1	7	0.02	0.03
(1,4329)	1:B:5:LEU:HD23	1:B:52:PHE:HE2	7	0.02	0.03
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD21	7	0.02	0.02
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD22	7	0.02	0.02
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD23	7	0.02	0.02
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD21	7	0.02	0.02
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD22	7	0.02	0.02
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD23	7	0.02	0.02
(1,3890)	1:B:82:GLU:HA	1:B:83:HIS:HB2	7	0.04	0.09
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD21	7	0.02	0.03
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD22	7	0.02	0.03
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD23	7	0.02	0.03
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD21	7	0.02	0.03
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD22	7	0.02	0.03
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD23	7	0.02	0.03



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,3758)	1:B:6:ALA:HB1	1:B:77:ARG:HD2	7	0.04	0.07
(1,3758)	1:B:6:ALA:HB1	1:B:77:ARG:HD3	7	0.04	0.07
(1,3758)	1:B:6:ALA:HB2	1:B:77:ARG:HD2	7	0.04	0.07
(1,3758)	1:B:6:ALA:HB2	1:B:77:ARG:HD3	7	0.04	0.07
(1,3758)	1:B:6:ALA:HB3	1:B:77:ARG:HD2	7	0.04	0.07
(1,3758)	1:B:6:ALA:HB3	1:B:77:ARG:HD3	7	0.04	0.07
(1,3734)	1:B:74:THR:HA	1:B:76:GLU:HG2	7	0.04	0.09
(1,3734)	1:B:74:THR:HA	1:B:76:GLU:HG3	7	0.04	0.09
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG11	7	0.03	0.05
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG12	7	0.03	0.05
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG13	7	0.03	0.05
(1,3614)	1:B:69:VAL:H	1:B:70:GLN:HB2	7	0.03	0.07
(1,3614)	1:B:69:VAL:H	1:B:70:GLN:HB3	7	0.03	0.07
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB2	7	0.06	0.14
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB3	7	0.06	0.14
(1,3561)	1:A:15:LYS:HE2	1:A:18:MET:H	7	0.04	0.08
(1,3561)	1:A:15:LYS:HE3	1:A:18:MET:H	7	0.04	0.08
(1,3422)	1:A:9:ARG:H	1:A:63:MET:HE1	7	0.03	0.07
(1,3422)	1:A:9:ARG:H	1:A:63:MET:HE2	7	0.03	0.07
(1,3422)	1:A:9:ARG:H	1:A:63:MET:HE3	7	0.03	0.07
(1,3410)	1:A:63:MET:HE1	1:A:77:ARG:HA	7	0.05	0.12
(1,3410)	1:A:63:MET:HE2	1:A:77:ARG:HA	7	0.05	0.12
(1,3410)	1:A:63:MET:HE3	1:A:77:ARG:HA	7	0.05	0.12
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD21	7	0.02	0.03
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD22	7	0.02	0.03
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD23	7	0.02	0.03
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD21	7	0.02	0.03
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD22	7	0.02	0.03
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD23	7	0.02	0.03
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD21	7	0.02	0.03
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD22	7	0.02	0.03
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD23	7	0.02	0.03
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD21	7	0.02	0.04
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD22	7	0.02	0.04
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD23	7	0.02	0.04
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD21	7	0.02	0.04
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD22	7	0.02	0.04
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD23	7	0.02	0.04
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD21	7	0.02	0.04
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD22	7	0.02	0.04
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD23	7	0.02	0.04
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG21	7	0.02	0.02



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG22	7	0.02	0.02
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG23	7	0.02	0.02
(1,2552)	1:B:44:ILE:HG13	1:B:45:PHE:H	7	0.03	0.05
(1,2282)	1:B:36:ILE:HG21	1:B:37:VAL:HB	7	0.02	0.04
(1,2282)	1:B:36:ILE:HG22	1:B:37:VAL:HB	7	0.02	0.04
(1,2282)	1:B:36:ILE:HG23	1:B:37:VAL:HB	7	0.02	0.04
(1,2258)	1:B:35:THR:HB	1:B:50:MET:HB2	7	0.03	0.05
(1,1933)	1:B:21:GLN:HE21	1:B:22:ILE:HA	7	0.01	0.02
(1,4906)	1:B:42:ASP:HB2	1:B:44:ILE:HG12	6	0.05	0.07
(1,4906)	1:B:42:ASP:HB3	1:B:44:ILE:HG12	6	0.05	0.07
(1,4887)	1:B:37:VAL:HG11	1:B:48:ASN:HD21	6	0.03	0.07
(1,4887)	1:B:37:VAL:HG11	1:B:48:ASN:HD22	6	0.03	0.07
(1,4887)	1:B:37:VAL:HG12	1:B:48:ASN:HD21	6	0.03	0.07
(1,4887)	1:B:37:VAL:HG12	1:B:48:ASN:HD22	6	0.03	0.07
(1,4887)	1:B:37:VAL:HG13	1:B:48:ASN:HD21	6	0.03	0.07
(1,4887)	1:B:37:VAL:HG13	1:B:48:ASN:HD22	6	0.03	0.07
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD11	6	0.03	0.06
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD12	6	0.03	0.06
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD13	6	0.03	0.06
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD11	6	0.03	0.06
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD12	6	0.03	0.06
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD13	6	0.03	0.06
(1,4690)	1:A:67:ARG:H	1:A:67:ARG:HG2	6	0.01	0.02
(1,4690)	1:A:67:ARG:H	1:A:67:ARG:HG3	6	0.01	0.02
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD21	6	0.11	0.15
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD22	6	0.11	0.15
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD21	6	0.11	0.15
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD22	6	0.11	0.15
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD21	6	0.11	0.15
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD22	6	0.11	0.15
(1,4560)	1:A:31:THR:HG21	1:A:58:LYS:HE2	6	0.08	0.12
(1,4560)	1:A:31:THR:HG21	1:A:58:LYS:HE3	6	0.08	0.12
(1,4560)	1:A:31:THR:HG22	1:A:58:LYS:HE2	6	0.08	0.12
(1,4560)	1:A:31:THR:HG22	1:A:58:LYS:HE3	6	0.08	0.12
(1,4560)	1:A:31:THR:HG23	1:A:58:LYS:HE2	6	0.08	0.12
(1,4560)	1:A:31:THR:HG23	1:A:58:LYS:HE3	6	0.08	0.12
(1,4389)	1:B:81:LEU:HB2	1:B:83:HIS:HD2	6	0.03	0.06
(1,4389)	1:B:81:LEU:HB3	1:B:83:HIS:HD2	6	0.03	0.06
(1,4353)	1:B:44:ILE:HG13	1:B:73:PHE:HE1	6	0.05	0.1
(1,4353)	1:B:44:ILE:HG13	1:B:73:PHE:HE2	6	0.05	0.1
(1,4138)	1:A:4:PHE:HD1	1:A:54:LYS:HA	6	0.02	0.04
(1,4138)	1:A:4:PHE:HD2	1:A:54:LYS:HA	6	0.02	0.04



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,4129)	1:B:83:HIS:HA	1:B:83:HIS:HD2	6	0.03	0.05
(1,4112)	1:A:77:ARG:HG3	1:A:79:SER:HA	6	0.02	0.04
(1,4090)	1:A:73:PHE:HA	1:A:73:PHE:HD1	6	0.02	0.02
(1,4090)	1:A:73:PHE:HA	1:A:73:PHE:HD2	6	0.02	0.02
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD11	6	0.03	0.04
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD12	6	0.03	0.04
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD13	6	0.03	0.04
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD11	6	0.03	0.04
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD12	6	0.03	0.04
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD13	6	0.03	0.04
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD11	6	0.03	0.04
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD12	6	0.03	0.04
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD13	6	0.03	0.04
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD21	6	0.02	0.04
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD22	6	0.02	0.04
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD23	6	0.02	0.04
(1,3753)	1:A:59:LEU:HD11	1:A:77:ARG:HD2	6	0.02	0.03
(1,3753)	1:A:59:LEU:HD11	1:A:77:ARG:HD3	6	0.02	0.03
(1,3753)	1:A:59:LEU:HD12	1:A:77:ARG:HD2	6	0.02	0.03
(1,3753)	1:A:59:LEU:HD12	1:A:77:ARG:HD3	6	0.02	0.03
(1,3753)	1:A:59:LEU:HD13	1:A:77:ARG:HD2	6	0.02	0.03
(1,3753)	1:A:59:LEU:HD13	1:A:77:ARG:HD3	6	0.02	0.03
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG21	6	0.02	0.03
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG22	6	0.02	0.03
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG23	6	0.02	0.03
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG21	6	0.02	0.03
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG22	6	0.02	0.03
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG23	6	0.02	0.03
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG21	6	0.02	0.05
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG22	6	0.02	0.05
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG23	6	0.02	0.05
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG21	6	0.02	0.05
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG22	6	0.02	0.05
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG23	6	0.02	0.05
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG21	6	0.02	0.05
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG22	6	0.02	0.05
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG23	6	0.02	0.05
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG11	6	0.11	0.26
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG12	6	0.11	0.26
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG13	6	0.11	0.26
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG11	6	0.11	0.26
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG12	6	0.11	0.26



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG13	6	0.11	0.26
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE1	6	0.05	0.07
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE2	6	0.05	0.07
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE3	6	0.05	0.07
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE1	6	0.05	0.07
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE2	6	0.05	0.07
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE3	6	0.05	0.07
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE1	6	0.05	0.07
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE2	6	0.05	0.07
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE3	6	0.05	0.07
(1,3130)	1:B:4:PHE:HD1	1:B:56:THR:HG21	6	0.04	0.06
(1,3130)	1:B:4:PHE:HD1	1:B:56:THR:HG22	6	0.04	0.06
(1,3130)	1:B:4:PHE:HD1	1:B:56:THR:HG23	6	0.04	0.06
(1,3130)	1:B:4:PHE:HD2	1:B:56:THR:HG21	6	0.04	0.06
(1,3130)	1:B:4:PHE:HD2	1:B:56:THR:HG22	6	0.04	0.06
(1,3130)	1:B:4:PHE:HD2	1:B:56:THR:HG23	6	0.04	0.06
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE2	6	0.23	0.34
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE3	6	0.23	0.34
(1,3091)	1:A:54:LYS:HA	1:A:54:LYS:HD2	6	0.03	0.07
(1,3091)	1:A:54:LYS:HA	1:A:54:LYS:HD3	6	0.03	0.07
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG11	6	0.03	0.04
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG12	6	0.03	0.04
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG13	6	0.03	0.04
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD11	6	0.05	0.07
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD12	6	0.05	0.07
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD13	6	0.05	0.07
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD11	6	0.05	0.07
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD12	6	0.05	0.07
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD13	6	0.05	0.07
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD11	6	0.02	0.03
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD12	6	0.02	0.03
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD13	6	0.02	0.03
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD11	6	0.02	0.03
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD12	6	0.02	0.03
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD13	6	0.02	0.03
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD11	6	0.02	0.02
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD12	6	0.02	0.02
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD13	6	0.02	0.02
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD11	6	0.02	0.02
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD12	6	0.02	0.02
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD13	6	0.02	0.02
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD11	6	0.02	0.02



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD12	6	0.02	0.02
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD13	6	0.02	0.02
(1,2640)	1:B:46:THR:HG21	1:B:47:CYS:H	6	0.02	0.03
(1,2640)	1:B:46:THR:HG22	1:B:47:CYS:H	6	0.02	0.03
(1,2640)	1:B:46:THR:HG23	1:B:47:CYS:H	6	0.02	0.03
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD11	6	0.02	0.04
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD12	6	0.02	0.04
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD13	6	0.02	0.04
(1,2388)	1:B:37:VAL:HG21	1:B:38:LEU:H	6	0.02	0.03
(1,2388)	1:B:37:VAL:HG22	1:B:38:LEU:H	6	0.02	0.03
(1,2388)	1:B:37:VAL:HG23	1:B:38:LEU:H	6	0.02	0.03
(1,217)	1:B:18:MET:H	1:B:18:MET:HG3	6	0.02	0.03
(1,1832)	1:B:16:ASN:HB3	1:B:17:GLY:H	6	0.07	0.09
(1,1809)	1:B:11:VAL:HG21	1:B:41:LYS:HE2	6	0.06	0.14
(1,1809)	1:B:11:VAL:HG21	1:B:41:LYS:HE3	6	0.06	0.14
(1,1809)	1:B:11:VAL:HG22	1:B:41:LYS:HE2	6	0.06	0.14
(1,1809)	1:B:11:VAL:HG22	1:B:41:LYS:HE3	6	0.06	0.14
(1,1809)	1:B:11:VAL:HG23	1:B:41:LYS:HE2	6	0.06	0.14
(1,1809)	1:B:11:VAL:HG23	1:B:41:LYS:HE3	6	0.06	0.14
(1,1576)	1:A:9:ARG:HD2	1:A:11:VAL:HB	6	0.02	0.03
(1,1576)	1:A:9:ARG:HD3	1:A:11:VAL:HB	6	0.02	0.03
(1,1552)	1:B:8:ILE:HD11	1:B:77:ARG:HA	6	0.03	0.04
(1,1552)	1:B:8:ILE:HD12	1:B:77:ARG:HA	6	0.03	0.04
(1,1552)	1:B:8:ILE:HD13	1:B:77:ARG:HA	6	0.03	0.04
(1,1378)	1:B:40:ALA:H	1:B:41:LYS:HD2	6	0.05	0.15
(1,1378)	1:B:40:ALA:H	1:B:41:LYS:HD3	6	0.05	0.15
(1,1196)	1:B:69:VAL:H	1:B:70:GLN:H	6	0.02	0.05
(1,1150)	1:B:67:ARG:HE	1:B:75:VAL:HB	6	0.04	0.07
(1,833)	1:B:47:CYS:HG	1:B:48:ASN:H	5	0.02	0.04
(1,615)	1:B:35:THR:H	1:B:83:HIS:HE1	5	0.03	0.05
(1,4851)	1:B:31:THR:HG21	1:B:58:LYS:HE2	5	0.08	0.12
(1,4851)	1:B:31:THR:HG21	1:B:58:LYS:HE3	5	0.08	0.12
(1,4851)	1:B:31:THR:HG22	1:B:58:LYS:HE2	5	0.08	0.12
(1,4851)	1:B:31:THR:HG22	1:B:58:LYS:HE3	5	0.08	0.12
(1,4851)	1:B:31:THR:HG23	1:B:58:LYS:HE2	5	0.08	0.12
(1,4851)	1:B:31:THR:HG23	1:B:58:LYS:HE3	5	0.08	0.12
(1,4640)	1:A:54:LYS:HG2	1:A:55:ASN:HD21	5	0.03	0.08
(1,4640)	1:A:54:LYS:HG2	1:A:55:ASN:HD22	5	0.03	0.08
(1,4640)	1:A:54:LYS:HG3	1:A:55:ASN:HD21	5	0.03	0.08
(1,4640)	1:A:54:LYS:HG3	1:A:55:ASN:HD22	5	0.03	0.08
(1,4538)	1:A:27:SER:HG	1:A:28:LYS:HD2	5	0.07	0.12
(1,4538)	1:A:27:SER:HG	1:A:28:LYS:HD3	5	0.07	0.12



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(1,4352) 1:	:A:44:ILE:HG13 :A:44:ILE:HG13	1:A:73:PHE:HE1	5	0.04	
(' /	· A·44·ILE·HG13		J	0.04	0.09
(1,4328) 1	.11.11.11111111111111111111111111111111	1:A:73:PHE:HE2	5	0.04	0.09
	:A:5:LEU:HD21	1:A:52:PHE:HE1	5	0.02	0.02
(1,4328) 1	:A:5:LEU:HD21	1:A:52:PHE:HE2	5	0.02	0.02
(1,4328) 1	:A:5:LEU:HD22	1:A:52:PHE:HE1	5	0.02	0.02
(1,4328) 1	:A:5:LEU:HD22	1:A:52:PHE:HE2	5	0.02	0.02
(1,4328) 1	:A:5:LEU:HD23	1:A:52:PHE:HE1	5	0.02	0.02
(1,4328) 1	:A:5:LEU:HD23	1:A:52:PHE:HE2	5	0.02	0.02
(1,4132) 1	:A:4:PHE:HD1	1:A:59:LEU:HD21	5	0.02	0.02
(1,4132) 1	:A:4:PHE:HD1	1:A:59:LEU:HD22	5	0.02	0.02
(1,4132) 1	:A:4:PHE:HD1	1:A:59:LEU:HD23	5	0.02	0.02
(1,4132) 1	:A:4:PHE:HD2	1:A:59:LEU:HD21	5	0.02	0.02
(1,4132) 1	:A:4:PHE:HD2	1:A:59:LEU:HD22	5	0.02	0.02
(1,4132) 1	:A:4:PHE:HD2	1:A:59:LEU:HD23	5	0.02	0.02
(1,4052) 1	:A:41:LYS:HG2	1:A:42:ASP:HA	5	0.05	0.1
(1,4052) 1	:A:41:LYS:HG3	1:A:42:ASP:HA	5	0.05	0.1
(1,4049)	1:B:41:LYS:HA	1:B:41:LYS:HD2	5	0.02	0.03
(1,4049)	1:B:41:LYS:HA	1:B:41:LYS:HD3	5	0.02	0.03
(1,3984) 1	:A:5:LEU:HD11	1:A:81:LEU:HD11	5	0.05	0.07
(1,3984) 1	:A:5:LEU:HD11	1:A:81:LEU:HD12	5	0.05	0.07
(1,3984) 1	:A:5:LEU:HD11	1:A:81:LEU:HD13	5	0.05	0.07
(1,3984) 1	:A:5:LEU:HD12	1:A:81:LEU:HD11	5	0.05	0.07
(1,3984) 1	:A:5:LEU:HD12	1:A:81:LEU:HD12	5	0.05	0.07
(1,3984) 1	:A:5:LEU:HD12	1:A:81:LEU:HD13	5	0.05	0.07
(1,3984) 1	:A:5:LEU:HD13	1:A:81:LEU:HD11	5	0.05	0.07
(1,3984) 1	:A:5:LEU:HD13	1:A:81:LEU:HD12	5	0.05	0.07
(1,3984) 1	:A:5:LEU:HD13	1:A:81:LEU:HD13	5	0.05	0.07
(1,3824) 1	:B:9:ARG:HD2	1:B:78:LEU:HD21	5	0.03	0.05
(1,3824) 1	:B:9:ARG:HD2	1:B:78:LEU:HD22	5	0.03	0.05
(1,3824) 1	:B:9:ARG:HD2	1:B:78:LEU:HD23	5	0.03	0.05
(1,3824) 1	:B:9:ARG:HD3	1:B:78:LEU:HD21	5	0.03	0.05
(1,3824) 1	:B:9:ARG:HD3	1:B:78:LEU:HD22	5	0.03	0.05
(1,3824) 1	:B:9:ARG:HD3	1:B:78:LEU:HD23	5	0.03	0.05
(1,3821) 1	:A:9:ARG:HB2	1:A:78:LEU:HD21	5	0.02	0.03
(1,3821) 1	:A:9:ARG:HB2	1:A:78:LEU:HD22	5	0.02	0.03
(1,3821) 1	:A:9:ARG:HB2	1:A:78:LEU:HD23	5	0.02	0.03
(1,3821) 1	:A:9:ARG:HB3	1:A:78:LEU:HD21	5	0.02	0.03
(1,3821) 1	:A:9:ARG:HB3	1:A:78:LEU:HD22	5	0.02	0.03
(1,3821) 1	:A:9:ARG:HB3	1:A:78:LEU:HD23	5	0.02	0.03
(1,3798) 1	:B:9:ARG:HD2	1:B:78:LEU:HD11	5	0.05	0.09
(1,3798) 1	:B:9:ARG:HD2	1:B:78:LEU:HD12	5	0.05	0.09
(1,3798) 1	:B:9:ARG:HD2	1:B:78:LEU:HD13	5	0.05	0.09



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD11	5	0.05	0.09
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD12	5	0.05	0.09
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD13	5	0.05	0.09
(1,3754)	1:B:59:LEU:HD11	1:B:77:ARG:HD2	5	0.04	0.06
(1,3754)	1:B:59:LEU:HD11	1:B:77:ARG:HD3	5	0.04	0.06
(1,3754)	1:B:59:LEU:HD12	1:B:77:ARG:HD2	5	0.04	0.06
(1,3754)	1:B:59:LEU:HD12	1:B:77:ARG:HD3	5	0.04	0.06
(1,3754)	1:B:59:LEU:HD13	1:B:77:ARG:HD2	5	0.04	0.06
(1,3754)	1:B:59:LEU:HD13	1:B:77:ARG:HD3	5	0.04	0.06
(1,3733)	1:A:74:THR:HA	1:A:76:GLU:HG2	5	0.05	0.07
(1,3733)	1:A:74:THR:HA	1:A:76:GLU:HG3	5	0.05	0.07
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG11	5	0.13	0.18
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG12	5	0.13	0.18
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG13	5	0.13	0.18
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG11	5	0.13	0.18
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG12	5	0.13	0.18
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG13	5	0.13	0.18
(1,3559)	1:A:15:LYS:HE2	1:A:16:ASN:HD21	5	0.07	0.12
(1,3559)	1:A:15:LYS:HE3	1:A:16:ASN:HD21	5	0.07	0.12
(1,3287)	1:A:61:THR:HG21	1:A:65:LYS:HE2	5	0.03	0.06
(1,3287)	1:A:61:THR:HG21	1:A:65:LYS:HE3	5	0.03	0.06
(1,3287)	1:A:61:THR:HG22	1:A:65:LYS:HE2	5	0.03	0.06
(1,3287)	1:A:61:THR:HG22	1:A:65:LYS:HE3	5	0.03	0.06
(1,3287)	1:A:61:THR:HG23	1:A:65:LYS:HE2	5	0.03	0.06
(1,3287)	1:A:61:THR:HG23	1:A:65:LYS:HE3	5	0.03	0.06
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG11	5	0.02	0.05
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG12	5	0.02	0.05
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG13	5	0.02	0.05
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD11	5	0.04	0.07
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD12	5	0.04	0.07
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD13	5	0.04	0.07
(1,2792)	1:B:8:ILE:H	1:B:50:MET:HG3	5	0.03	0.06
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD11	5	0.02	0.03
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD12	5	0.02	0.03
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD13	5	0.02	0.03
(1,2584)	1:B:44:ILE:HD11	1:B:46:THR:HB	5	0.03	0.04
(1,2584)	1:B:44:ILE:HD12	1:B:46:THR:HB	5	0.03	0.04
(1,2584)	1:B:44:ILE:HD13	1:B:46:THR:HB	5	0.03	0.04
(1,2380)	1:B:37:VAL:HG21	1:B:48:ASN:HD22	5	0.02	0.04
(1,2380)	1:B:37:VAL:HG22	1:B:48:ASN:HD22	5	0.02	0.04
(1,2380)	1:B:37:VAL:HG23	1:B:48:ASN:HD22	5	0.02	0.04
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD11	5	0.02	0.03



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD12	5	0.02	0.03
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD13	5	0.02	0.03
(1,1861)	1:B:18:MET:HE1	1:B:71:GLY:HA2	5	0.01	0.02
(1,1861)	1:B:18:MET:HE2	1:B:71:GLY:HA2	5	0.01	0.02
(1,1861)	1:B:18:MET:HE3	1:B:71:GLY:HA2	5	0.01	0.02
(1,175)	1:A:15:LYS:H	1:A:18:MET:HG2	5	0.07	0.14
(1,1577)	1:B:9:ARG:HD2	1:B:11:VAL:HB	5	0.02	0.04
(1,1577)	1:B:9:ARG:HD3	1:B:11:VAL:HB	5	0.02	0.04
(1,1414)	1:B:3:ASP:HB2	1:B:53:VAL:H	5	0.05	0.08
(1,1413)	1:A:3:ASP:HB2	1:A:53:VAL:H	5	0.07	0.11
(1,908)	1:A:3:ASP:HB3	1:A:53:VAL:H	4	0.04	0.06
(1,761)	1:B:43:GLY:H	1:B:44:ILE:H	4	0.04	0.06
(1,718)	1:A:41:LYS:H	1:A:46:THR:H	4	0.06	0.11
(1,5002)	1:B:69:VAL:HG11	1:B:70:GLN:HE21	4	0.06	0.12
(1,5002)	1:B:69:VAL:HG11	1:B:70:GLN:HE22	4	0.06	0.12
(1,5002)	1:B:69:VAL:HG12	1:B:70:GLN:HE21	4	0.06	0.12
(1,5002)	1:B:69:VAL:HG12	1:B:70:GLN:HE22	4	0.06	0.12
(1,5002)	1:B:69:VAL:HG13	1:B:70:GLN:HE21	4	0.06	0.12
(1,5002)	1:B:69:VAL:HG13	1:B:70:GLN:HE22	4	0.06	0.12
(1,4936)	1:B:54:LYS:HE2	1:B:55:ASN:HD21	4	0.04	0.07
(1,4936)	1:B:54:LYS:HE2	1:B:55:ASN:HD22	4	0.04	0.07
(1,4936)	1:B:54:LYS:HE3	1:B:55:ASN:HD21	4	0.04	0.07
(1,4936)	1:B:54:LYS:HE3	1:B:55:ASN:HD22	4	0.04	0.07
(1,4606)	1:A:39:ASN:HD21	1:A:46:THR:HG21	4	0.04	0.05
(1,4606)	1:A:39:ASN:HD21	1:A:46:THR:HG22	4	0.04	0.05
(1,4606)	1:A:39:ASN:HD21	1:A:46:THR:HG23	4	0.04	0.05
(1,4606)	1:A:39:ASN:HD22	1:A:46:THR:HG21	4	0.04	0.05
(1,4606)	1:A:39:ASN:HD22	1:A:46:THR:HG22	4	0.04	0.05
(1,4606)	1:A:39:ASN:HD22	1:A:46:THR:HG23	4	0.04	0.05
(1,4593)	1:A:37:VAL:HG11	1:A:48:ASN:HD21	4	0.04	0.07
(1,4593)	1:A:37:VAL:HG11	1:A:48:ASN:HD22	4	0.04	0.07
(1,4593)	1:A:37:VAL:HG12	1:A:48:ASN:HD21	4	0.04	0.07
(1,4593)	1:A:37:VAL:HG12	1:A:48:ASN:HD22	4	0.04	0.07
(1,4593)	1:A:37:VAL:HG13	1:A:48:ASN:HD21	4	0.04	0.07
(1,4593)	1:A:37:VAL:HG13	1:A:48:ASN:HD22	4	0.04	0.07
(1,4496)	1:A:20:ASN:HB2	1:A:21:GLN:HE21	4	0.02	0.03
(1,4496)	1:A:20:ASN:HB3	1:A:21:GLN:HE21	4	0.02	0.03
(1,4397)	1:B:82:GLU:HA	1:B:83:HIS:HD2	4	0.07	0.15
(1,4264)	1:A:22:ILE:HD11	1:A:45:PHE:HE1	4	0.02	0.04
(1,4264)	1:A:22:ILE:HD11	1:A:45:PHE:HE2	4	0.02	0.04
(1,4264)	1:A:22:ILE:HD12	1:A:45:PHE:HE1	4	0.02	0.04
(1,4264)	1:A:22:ILE:HD12	1:A:45:PHE:HE2	4	0.02	0.04



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,4264)	1:A:22:ILE:HD13	1:A:45:PHE:HE1	4	0.02	0.04
(1,4264)	1:A:22:ILE:HD13	1:A:45:PHE:HE2	4	0.02	0.04
(1,416)	1:A:24:GLY:H	1:A:27:SER:HG	4	0.01	0.02
(1,4150)	1:A:4:PHE:HE1	1:A:59:LEU:HD21	4	0.01	0.01
(1,4150)	1:A:4:PHE:HE1	1:A:59:LEU:HD22	4	0.01	0.01
(1,4150)	1:A:4:PHE:HE1	1:A:59:LEU:HD23	4	0.01	0.01
(1,4150)	1:A:4:PHE:HE2	1:A:59:LEU:HD21	4	0.01	0.01
(1,4150)	1:A:4:PHE:HE2	1:A:59:LEU:HD22	4	0.01	0.01
(1,4150)	1:A:4:PHE:HE2	1:A:59:LEU:HD23	4	0.01	0.01
(1,4128)	1:A:83:HIS:HA	1:A:83:HIS:HD2	4	0.02	0.06
(1,3888)	1:B:8:ILE:H	1:B:81:LEU:HD21	4	0.02	0.03
(1,3888)	1:B:8:ILE:H	1:B:81:LEU:HD22	4	0.02	0.03
(1,3888)	1:B:8:ILE:H	1:B:81:LEU:HD23	4	0.02	0.03
(1,3594)	1:B:66:LEU:HA	1:B:69:VAL:HB	4	0.03	0.04
(1,3560)	1:B:15:LYS:HE2	1:B:16:ASN:HD21	4	0.07	0.12
(1,3560)	1:B:15:LYS:HE3	1:B:16:ASN:HD21	4	0.07	0.12
(1,3483)	1:A:41:LYS:HE2	1:A:44:ILE:H	4	0.05	0.11
(1,3483)	1:A:41:LYS:HE3	1:A:44:ILE:H	4	0.05	0.11
(1,3335)	1:B:58:LYS:HE2	1:B:62:LEU:HD11	4	0.03	0.05
(1,3335)	1:B:58:LYS:HE2	1:B:62:LEU:HD12	4	0.03	0.05
(1,3335)	1:B:58:LYS:HE2	1:B:62:LEU:HD13	4	0.03	0.05
(1,3331)	1:B:62:LEU:HD11	1:B:66:LEU:HG	4	0.01	0.02
(1,3331)	1:B:62:LEU:HD12	1:B:66:LEU:HG	4	0.01	0.02
(1,3331)	1:B:62:LEU:HD13	1:B:66:LEU:HG	4	0.01	0.02
(1,3212)	1:B:6:ALA:HB1	1:B:59:LEU:HD11	4	0.02	0.04
(1,3212)	1:B:6:ALA:HB1	1:B:59:LEU:HD12	4	0.02	0.04
(1,3212)	1:B:6:ALA:HB1	1:B:59:LEU:HD13	4	0.02	0.04
(1,3212)	1:B:6:ALA:HB2	1:B:59:LEU:HD11	4	0.02	0.04
(1,3212)	1:B:6:ALA:HB2	1:B:59:LEU:HD12	4	0.02	0.04
(1,3212)	1:B:6:ALA:HB2	1:B:59:LEU:HD13	4	0.02	0.04
(1,3212)	1:B:6:ALA:HB3	1:B:59:LEU:HD11	4	0.02	0.04
(1,3212)	1:B:6:ALA:HB3	1:B:59:LEU:HD12	4	0.02	0.04
(1,3212)	1:B:6:ALA:HB3	1:B:59:LEU:HD13	4	0.02	0.04
(1,3176)	1:B:30:ASP:HB2	1:B:58:LYS:HD2	4	0.06	0.09
(1,3176)	1:B:30:ASP:HB2	1:B:58:LYS:HD3	4	0.06	0.09
(1,3176)	1:B:30:ASP:HB3	1:B:58:LYS:HD2	4	0.06	0.09
(1,3176)	1:B:30:ASP:HB3	1:B:58:LYS:HD3	4	0.06	0.09
(1,3175)	1:A:30:ASP:HB2	1:A:58:LYS:HD2	4	0.05	0.08
(1,3175)	1:A:30:ASP:HB2	1:A:58:LYS:HD3	4	0.05	0.08
(1,3175)	1:A:30:ASP:HB3	1:A:58:LYS:HD2	4	0.05	0.08
(1,3175)	1:A:30:ASP:HB3	1:A:58:LYS:HD3	4	0.05	0.08
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG21	4	0.04	0.12



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG22	4	0.04	0.12
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG23	4	0.04	0.12
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG21	4	0.04	0.12
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG22	4	0.04	0.12
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG23	4	0.04	0.12
(1,3099)	1:A:54:LYS:H	1:A:54:LYS:HD2	4	0.08	0.15
(1,3099)	1:A:54:LYS:H	1:A:54:LYS:HD3	4	0.08	0.15
(1,3093)	1:A:15:LYS:HD2	1:A:16:ASN:HD22	4	0.05	0.09
(1,3093)	1:A:15:LYS:HD3	1:A:16:ASN:HD22	4	0.05	0.09
(1,2924)	1:B:51:ILE:HD11	1:B:62:LEU:HD21	4	0.04	0.05
(1,2924)	1:B:51:ILE:HD11	1:B:62:LEU:HD22	4	0.04	0.05
(1,2924)	1:B:51:ILE:HD11	1:B:62:LEU:HD23	4	0.04	0.05
(1,2924)	1:B:51:ILE:HD12	1:B:62:LEU:HD21	4	0.04	0.05
(1,2924)	1:B:51:ILE:HD12	1:B:62:LEU:HD22	4	0.04	0.05
(1,2924)	1:B:51:ILE:HD12	1:B:62:LEU:HD23	4	0.04	0.05
(1,2924)	1:B:51:ILE:HD13	1:B:62:LEU:HD21	4	0.04	0.05
(1,2924)	1:B:51:ILE:HD13	1:B:62:LEU:HD22	4	0.04	0.05
(1,2924)	1:B:51:ILE:HD13	1:B:62:LEU:HD23	4	0.04	0.05
(1,277)	1:A:20:ASN:H	1:A:20:ASN:HD22	4	0.16	0.19
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG21	4	0.13	0.18
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG22	4	0.13	0.18
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG23	4	0.13	0.18
(1,2618)	1:B:9:ARG:HD2	1:B:46:THR:HG21	4	0.04	0.07
(1,2618)	1:B:9:ARG:HD2	1:B:46:THR:HG22	4	0.04	0.07
(1,2618)	1:B:9:ARG:HD2	1:B:46:THR:HG23	4	0.04	0.07
(1,2618)	1:B:9:ARG:HD3	1:B:46:THR:HG21	4	0.04	0.07
(1,2618)	1:B:9:ARG:HD3	1:B:46:THR:HG22	4	0.04	0.07
(1,2618)	1:B:9:ARG:HD3	1:B:46:THR:HG23	4	0.04	0.07
(1,2551)	1:A:44:ILE:HG13	1:A:45:PHE:H	4	0.02	0.06
(1,2432)	1:A:38:LEU:HD21	1:B:35:THR:HG21	4	0.02	0.03
(1,2432)	1:A:38:LEU:HD21	1:B:35:THR:HG22	4	0.02	0.03
(1,2432)	1:A:38:LEU:HD21	1:B:35:THR:HG23	4	0.02	0.03
(1,2432)	1:A:38:LEU:HD22	1:B:35:THR:HG21	4	0.02	0.03
(1,2432)	1:A:38:LEU:HD22	1:B:35:THR:HG22	4	0.02	0.03
(1,2432)	1:A:38:LEU:HD22	1:B:35:THR:HG23	4	0.02	0.03
(1,2432)	1:A:38:LEU:HD23	1:B:35:THR:HG21	4	0.02	0.03
(1,2432)	1:A:38:LEU:HD23	1:B:35:THR:HG22	4	0.02	0.03
(1,2432)	1:A:38:LEU:HD23	1:B:35:THR:HG23	4	0.02	0.03
(1,2423)	1:A:38:LEU:HD11	1:A:39:ASN:H	4	0.04	0.06
(1,2423)	1:A:38:LEU:HD12	1:A:39:ASN:H	4	0.04	0.06
(1,2423)	1:A:38:LEU:HD13	1:A:39:ASN:H	4	0.04	0.06
(1,235)	1:B:15:LYS:HG2	1:B:19:THR:H	4	0.02	0.03



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(1,235) 1:B:15:LYS:HG3 1:B:19:THR:F (1,234) 1:A:15:LYS:HG2 1:A:19:THR:F (1,234) 1:A:15:LYS:HG3 1:A:19:THR:F (1,2173) 1:A:68:LYS:HA 1:A:68:LYS:HE (1,200) 1:B:15:LYS:HE2 1:B:16:ASN:HD	1 4 1 4 1 2 4 2 4 4 2 2 4	0.02 0.04 0.04 0.09	0.03 0.09 0.09
(1,234) 1:A:15:LYS:HG3 1:A:19:THR:H (1,2173) 1:A:68:LYS:HA 1:A:68:LYS:HD	1 4 02 4 22 4	0.04	
(1,2173) 1:A:68:LYS:HA 1:A:68:LYS:HE	22 4 22 4		0.09
	22 4	0.09	
(1,200) 1:B:15:LYS:HE2 1:B:16:ASN:HD			0.13
() = = = = = = = = = = = = = = = = =		0.04	0.06
(1,200) 1:B:15:LYS:HE3 1:B:16:ASN:HD	$22 \mid 4$	0.04	0.06
(1,1941) 1:B:22:ILE:HB 1:B:47:CYS:He	G 4	0.01	0.02
(1,1831) 1:A:16:ASN:HB3 1:A:17:GLY:H	[4	0.06	0.08
(1,1815) 1:B:68:LYS:HE2 1:B:69:VAL:HG	21 4	0.11	0.17
(1,1815) 1:B:68:LYS:HE2 1:B:69:VAL:HG	22 4	0.11	0.17
(1,1815) 1:B:68:LYS:HE2 1:B:69:VAL:HG	23 4	0.11	0.17
(1,1815) 1:B:68:LYS:HE3 1:B:69:VAL:HG	21 4	0.11	0.17
(1,1815) 1:B:68:LYS:HE3 1:B:69:VAL:HG	22 4	0.11	0.17
(1,1815) 1:B:68:LYS:HE3 1:B:69:VAL:HG	23 4	0.11	0.17
(1,1814) 1:A:68:LYS:HE2 1:A:69:VAL:HG	21 4	0.06	0.16
(1,1814) 1:A:68:LYS:HE2 1:A:69:VAL:HG	22 4	0.06	0.16
(1,1814) 1:A:68:LYS:HE2 1:A:69:VAL:HG	23 4	0.06	0.16
(1,1814) 1:A:68:LYS:HE3 1:A:69:VAL:HG	21 4	0.06	0.16
(1,1814) 1:A:68:LYS:HE3 1:A:69:VAL:HG	22 4	0.06	0.16
(1,1814) 1:A:68:LYS:HE3 1:A:69:VAL:HG	23 4	0.06	0.16
(1,181) 1:A:15:LYS:H 1:A:44:ILE:HA	A 4	0.02	0.03
(1,1558) 1:B:24:GLY:H 1:B:26:ILE:HD	11 4	0.03	0.06
(1,1558) 1:B:24:GLY:H 1:B:26:ILE:HD	12 4	0.03	0.06
(1,1558) 1:B:24:GLY:H 1:B:26:ILE:HD	13 4	0.03	0.06
(1,1195) 1:A:69:VAL:H 1:A:70:GLN:H	[4	0.03	0.06
(1,939) 1:B:54:LYS:HE2 1:B:55:ASN:HD	22 3	0.03	0.04
(1,939) 1:B:54:LYS:HE3 1:B:55:ASN:HD		0.03	0.04
(1,909) 1:B:3:ASP:HB3 1:B:53:VAL:H		0.04	0.06
(1,83) 1:B:9:ARG:HE 1:B:11:VAL:HG	21 3	0.04	0.08
(1,83) 1:B:9:ARG:HE 1:B:11:VAL:HG	22 3	0.04	0.08
(1,83) 1:B:9:ARG:HE 1:B:11:VAL:HG		0.04	0.08
(1,565) 1:B:32:ASN:HA 1:B:32:ASN:HD		0.01	0.02
(1,541) 1:A:30:ASP:HA 1:A:31:THR:F	I 3	0.02	0.04
(1,4883) 1:B:37:VAL:HB 1:B:48:ASN:HF	_	0.01	0.02
(1,4883) 1:B:37:VAL:HB 1:B:48:ASN:HF	3	0.01	0.02
(1,4872) 1:B:34:ARG:HG2 1:B:52:PHE:HI		0.05	0.06
(1,4872) 1:B:34:ARG:HG2 1:B:52:PHE:HI)2 3	0.05	0.06
(1,4872) 1:B:34:ARG:HG3 1:B:52:PHE:HI	_	0.05	0.06
(1,4872) 1:B:34:ARG:HG3 1:B:52:PHE:HI)2 3	0.05	0.06
(1,4861) 1:B:32:ASN:HD21 1:B:33:ILE:HI		0.06	0.1
(1,4861) 1:B:32:ASN:HD22 1:B:33:ILE:HH	3	0.06	0.1
(1,4854) 1:B:32:ASN:HA 1:B:32:ASN:HD	21 3	0.02	0.02



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,4854)	1:B:32:ASN:HA	1:B:32:ASN:HD22	3	0.02	0.02
(1,4775)	1:B:16:ASN:HB2	1:B:17:GLY:H	3	0.04	0.05
(1,4775)	1:B:16:ASN:HB3	1:B:17:GLY:H	3	0.04	0.05
(1,4768)	1:B:15:LYS:HG2	1:B:16:ASN:HD21	3	0.08	0.1
(1,4768)	1:B:15:LYS:HG2	1:B:16:ASN:HD22	3	0.08	0.1
(1,4768)	1:B:15:LYS:HG3	1:B:16:ASN:HD21	3	0.08	0.1
(1,4768)	1:B:15:LYS:HG3	1:B:16:ASN:HD22	3	0.08	0.1
(1,4715)	1:A:81:LEU:H	1:A:82:GLU:HG2	3	0.32	0.36
(1,4715)	1:A:81:LEU:H	1:A:82:GLU:HG3	3	0.32	0.36
(1,4643)	1:A:54:LYS:HE2	1:A:55:ASN:HD21	3	0.06	0.15
(1,4643)	1:A:54:LYS:HE2	1:A:55:ASN:HD22	3	0.06	0.15
(1,4643)	1:A:54:LYS:HE3	1:A:55:ASN:HD21	3	0.06	0.15
(1,4643)	1:A:54:LYS:HE3	1:A:55:ASN:HD22	3	0.06	0.15
(1,4605)	1:A:39:ASN:HD21	1:A:46:THR:HB	3	0.03	0.04
(1,4605)	1:A:39:ASN:HD22	1:A:46:THR:HB	3	0.03	0.04
(1,4514)	1:A:24:GLY:HA2	1:A:28:LYS:HE2	3	0.04	0.06
(1,4514)	1:A:24:GLY:HA2	1:A:28:LYS:HE3	3	0.04	0.06
(1,4514)	1:A:24:GLY:HA3	1:A:28:LYS:HE2	3	0.04	0.06
(1,4514)	1:A:24:GLY:HA3	1:A:28:LYS:HE3	3	0.04	0.06
(1,4457)	1:A:15:LYS:HB2	1:A:18:MET:HB2	3	0.05	0.09
(1,4457)	1:A:15:LYS:HB2	1:A:18:MET:HB3	3	0.05	0.09
(1,4457)	1:A:15:LYS:HB3	1:A:18:MET:HB2	3	0.05	0.09
(1,4457)	1:A:15:LYS:HB3	1:A:18:MET:HB3	3	0.05	0.09
(1,4343)	1:B:29:PHE:HE1	1:B:65:LYS:HE2	3	0.05	0.1
(1,4343)	1:B:29:PHE:HE1	1:B:65:LYS:HE3	3	0.05	0.1
(1,4343)	1:B:29:PHE:HE2	1:B:65:LYS:HE2	3	0.05	0.1
(1,4343)	1:B:29:PHE:HE2	1:B:65:LYS:HE3	3	0.05	0.1
(1,4311)	1:B:5:LEU:HA	1:B:52:PHE:HD1	3	0.02	0.03
(1,4311)	1:B:5:LEU:HA	1:B:52:PHE:HD2	3	0.02	0.03
(1,4234)	1:A:45:PHE:HD1	1:A:47:CYS:HG	3	0.04	0.06
(1,4234)	1:A:45:PHE:HD2	1:A:47:CYS:HG	3	0.04	0.06
(1,4211)	1:B:29:PHE:H	1:B:29:PHE:HD1	3	0.03	0.06
(1,4211)	1:B:29:PHE:H	1:B:29:PHE:HD2	3	0.03	0.06
(1,4209)	1:B:29:PHE:HA	1:B:29:PHE:HD1	3	0.07	0.11
(1,4209)	1:B:29:PHE:HA	1:B:29:PHE:HD2	3	0.07	0.11
(1,4208)	1:A:29:PHE:HA	1:A:29:PHE:HD1	3	0.03	0.05
(1,4208)	1:A:29:PHE:HA	1:A:29:PHE:HD2	3	0.03	0.05
(1,4133)	1:B:4:PHE:HD1	1:B:59:LEU:HD21	3	0.02	0.03
(1,4133)	1:B:4:PHE:HD1	1:B:59:LEU:HD22	3	0.02	0.03
(1,4133)	1:B:4:PHE:HD1	1:B:59:LEU:HD23	3	0.02	0.03
(1,4133)	1:B:4:PHE:HD2	1:B:59:LEU:HD21	3	0.02	0.03
(1,4133)	1:B:4:PHE:HD2	1:B:59:LEU:HD22	3	0.02	0.03



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,4133)	1:B:4:PHE:HD2	1:B:59:LEU:HD23	3	0.02	0.03
(1,4113)	1:B:77:ARG:HG3	1:B:79:SER:HA	3	0.02	0.03
(1,4111)	1:B:79:SER:HA	1:B:81:LEU:HG	3	0.02	0.03
(1,3987)	1:B:81:LEU:HD11	1:B:83:HIS:HB3	3	0.07	0.08
(1,3987)	1:B:81:LEU:HD12	1:B:83:HIS:HB3	3	0.07	0.08
(1,3987)	1:B:81:LEU:HD13	1:B:83:HIS:HB3	3	0.07	0.08
(1,3916)	1:B:18:MET:HE1	1:B:72:VAL:HG21	3	0.02	0.03
(1,3916)	1:B:18:MET:HE1	1:B:72:VAL:HG22	3	0.02	0.03
(1,3916)	1:B:18:MET:HE1	1:B:72:VAL:HG23	3	0.02	0.03
(1,3916)	1:B:18:MET:HE2	1:B:72:VAL:HG21	3	0.02	0.03
(1,3916)	1:B:18:MET:HE2	1:B:72:VAL:HG22	3	0.02	0.03
(1,3916)	1:B:18:MET:HE2	1:B:72:VAL:HG23	3	0.02	0.03
(1,3916)	1:B:18:MET:HE3	1:B:72:VAL:HG21	3	0.02	0.03
(1,3916)	1:B:18:MET:HE3	1:B:72:VAL:HG22	3	0.02	0.03
(1,3916)	1:B:18:MET:HE3	1:B:72:VAL:HG23	3	0.02	0.03
(1,3842)	1:B:80:ASN:HB2	1:B:81:LEU:HD21	3	0.02	0.03
(1,3842)	1:B:80:ASN:HB2	1:B:81:LEU:HD22	3	0.02	0.03
(1,3842)	1:B:80:ASN:HB2	1:B:81:LEU:HD23	3	0.02	0.03
(1,3764)	1:B:4:PHE:HZ	1:B:77:ARG:HD2	3	0.03	0.04
(1,3764)	1:B:4:PHE:HZ	1:B:77:ARG:HD3	3	0.03	0.04
(1,3686)	1:B:10:ILE:HA	1:B:74:THR:HB	3	0.02	0.02
(1,3622)	1:B:69:VAL:HA	1:B:70:GLN:HG2	3	0.16	0.25
(1,3622)	1:B:69:VAL:HA	1:B:70:GLN:HG3	3	0.16	0.25
(1,3484)	1:B:41:LYS:HE2	1:B:44:ILE:H	3	0.11	0.19
(1,3484)	1:B:41:LYS:HE3	1:B:44:ILE:H	3	0.11	0.19
(1,3423)	1:B:9:ARG:H	1:B:63:MET:HE1	3	0.05	0.08
(1,3423)	1:B:9:ARG:H	1:B:63:MET:HE2	3	0.05	0.08
(1,3423)	1:B:9:ARG:H	1:B:63:MET:HE3	3	0.05	0.08
(1,3411)	1:B:63:MET:HE1	1:B:77:ARG:HA	3	0.05	0.06
(1,3411)	1:B:63:MET:HE2	1:B:77:ARG:HA	3	0.05	0.06
(1,3411)	1:B:63:MET:HE3	1:B:77:ARG:HA	3	0.05	0.06
(1,3330)	1:A:62:LEU:HD11	1:A:66:LEU:HG	3	0.01	0.02
(1,3330)	1:A:62:LEU:HD12	1:A:66:LEU:HG	3	0.01	0.02
(1,3330)	1:A:62:LEU:HD13	1:A:66:LEU:HG	3	0.01	0.02
(1,3288)	1:B:61:THR:HG21	1:B:65:LYS:HE2	3	0.02	0.02
(1,3288)	1:B:61:THR:HG21	1:B:65:LYS:HE3	3	0.02	0.02
(1,3288)	1:B:61:THR:HG22	1:B:65:LYS:HE2	3	0.02	0.02
(1,3288)	1:B:61:THR:HG22	1:B:65:LYS:HE3	3	0.02	0.02
(1,3288)	1:B:61:THR:HG23	1:B:65:LYS:HE2	3	0.02	0.02
(1,3288)	1:B:61:THR:HG23	1:B:65:LYS:HE3	3	0.02	0.02
(1,3224)	1:B:6:ALA:HB1	1:B:59:LEU:HD21	3	0.03	0.04
(1,3224)	1:B:6:ALA:HB1	1:B:59:LEU:HD22	3	0.03	0.04



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,3224)	1:B:6:ALA:HB1	1:B:59:LEU:HD23	3	0.03	0.04
(1,3224)	1:B:6:ALA:HB2	1:B:59:LEU:HD21	3	0.03	0.04
(1,3224)	1:B:6:ALA:HB2	1:B:59:LEU:HD22	3	0.03	0.04
(1,3224)	1:B:6:ALA:HB2	1:B:59:LEU:HD23	3	0.03	0.04
(1,3224)	1:B:6:ALA:HB3	1:B:59:LEU:HD21	3	0.03	0.04
(1,3224)	1:B:6:ALA:HB3	1:B:59:LEU:HD22	3	0.03	0.04
(1,3224)	1:B:6:ALA:HB3	1:B:59:LEU:HD23	3	0.03	0.04
(1,3186)	1:B:58:LYS:H	1:B:58:LYS:HD2	3	0.05	0.06
(1,3186)	1:B:58:LYS:H	1:B:58:LYS:HD3	3	0.05	0.06
(1,3185)	1:A:58:LYS:H	1:A:58:LYS:HD2	3	0.03	0.04
(1,3185)	1:A:58:LYS:H	1:A:58:LYS:HD3	3	0.03	0.04
(1,3104)	1:B:54:LYS:HE2	1:B:55:ASN:HD21	3	0.08	0.09
(1,3104)	1:B:54:LYS:HE3	1:B:55:ASN:HD21	3	0.08	0.09
(1,3103)	1:A:54:LYS:HE2	1:A:55:ASN:HD21	3	0.16	0.21
(1,3103)	1:A:54:LYS:HE3	1:A:55:ASN:HD21	3	0.16	0.21
(1,3098)	1:B:15:LYS:HD2	1:B:16:ASN:HD21	3	0.08	0.12
(1,3098)	1:B:15:LYS:HD3	1:B:16:ASN:HD21	3	0.08	0.12
(1,2902)	1:A:51:ILE:HG21	1:B:20:ASN:HD22	3	0.04	0.06
(1,2902)	1:A:51:ILE:HG22	1:B:20:ASN:HD22	3	0.04	0.06
(1,2902)	1:A:51:ILE:HG23	1:B:20:ASN:HD22	3	0.04	0.06
(1,2882)	1:B:8:ILE:HG21	1:B:62:LEU:HD11	3	0.04	0.06
(1,2882)	1:B:8:ILE:HG21	1:B:62:LEU:HD12	3	0.04	0.06
(1,2882)	1:B:8:ILE:HG21	1:B:62:LEU:HD13	3	0.04	0.06
(1,2882)	1:B:8:ILE:HG22	1:B:62:LEU:HD11	3	0.04	0.06
(1,2882)	1:B:8:ILE:HG22	1:B:62:LEU:HD12	3	0.04	0.06
(1,2882)	1:B:8:ILE:HG22	1:B:62:LEU:HD13	3	0.04	0.06
(1,2882)	1:B:8:ILE:HG23	1:B:62:LEU:HD11	3	0.04	0.06
(1,2882)	1:B:8:ILE:HG23	1:B:62:LEU:HD12	3	0.04	0.06
(1,2882)	1:B:8:ILE:HG23	1:B:62:LEU:HD13	3	0.04	0.06
(1,2791)	1:A:8:ILE:H	1:A:50:MET:HG3	3	0.04	0.07
(1,2617)	1:A:9:ARG:HD2	1:A:46:THR:HG21	3	0.02	0.02
(1,2617)	1:A:9:ARG:HD2	1:A:46:THR:HG22	3	0.02	0.02
(1,2617)	1:A:9:ARG:HD2	1:A:46:THR:HG23	3	0.02	0.02
(1,2617)	1:A:9:ARG:HD3	1:A:46:THR:HG21	3	0.02	0.02
(1,2617)	1:A:9:ARG:HD3	1:A:46:THR:HG22	3	0.02	0.02
(1,2617)	1:A:9:ARG:HD3	1:A:46:THR:HG23	3	0.02	0.02
(1,2595)	1:A:44:ILE:H	1:A:44:ILE:HD11	3	0.02	0.04
(1,2595)	1:A:44:ILE:H	1:A:44:ILE:HD12	3	0.02	0.04
(1,2595)	1:A:44:ILE:H	1:A:44:ILE:HD13	3	0.02	0.04
(1,2590)	1:B:44:ILE:HD11	1:B:73:PHE:HD1	3	0.02	0.04
(1,2590)	1:B:44:ILE:HD11	1:B:73:PHE:HD2	3	0.02	0.04
(1,2590)	1:B:44:ILE:HD12	1:B:73:PHE:HD1	3	0.02	0.04



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2590)	1:B:44:ILE:HD12	1:B:73:PHE:HD2	3	0.02	0.04
(1,2590)	1:B:44:ILE:HD13	1:B:73:PHE:HD1	3	0.02	0.04
(1,2590)	1:B:44:ILE:HD13	1:B:73:PHE:HD2	3	0.02	0.04
(1,2589)	1:A:44:ILE:HD11	1:A:73:PHE:HD1	3	0.01	0.02
(1,2589)	1:A:44:ILE:HD11	1:A:73:PHE:HD2	3	0.01	0.02
(1,2589)	1:A:44:ILE:HD12	1:A:73:PHE:HD1	3	0.01	0.02
(1,2589)	1:A:44:ILE:HD12	1:A:73:PHE:HD2	3	0.01	0.02
(1,2589)	1:A:44:ILE:HD13	1:A:73:PHE:HD1	3	0.01	0.02
(1,2589)	1:A:44:ILE:HD13	1:A:73:PHE:HD2	3	0.01	0.02
(1,2586)	1:B:13:GLU:HA	1:B:44:ILE:HD11	3	0.03	0.04
(1,2586)	1:B:13:GLU:HA	1:B:44:ILE:HD12	3	0.03	0.04
(1,2586)	1:B:13:GLU:HA	1:B:44:ILE:HD13	3	0.03	0.04
(1,2576)	1:B:44:ILE:HG21	1:B:45:PHE:H	3	0.03	0.05
(1,2576)	1:B:44:ILE:HG22	1:B:45:PHE:H	3	0.03	0.05
(1,2576)	1:B:44:ILE:HG23	1:B:45:PHE:H	3	0.03	0.05
(1,2575)	1:A:44:ILE:HG21	1:A:45:PHE:H	3	0.04	0.06
(1,2575)	1:A:44:ILE:HG22	1:A:45:PHE:H	3	0.04	0.06
(1,2575)	1:A:44:ILE:HG23	1:A:45:PHE:H	3	0.04	0.06
(1,2526)	1:B:13:GLU:HA	1:B:44:ILE:HB	3	0.01	0.02
(1,2525)	1:A:13:GLU:HA	1:A:44:ILE:HB	3	0.02	0.03
(1,2501)	1:A:15:LYS:H	1:A:40:ALA:HB1	3	0.03	0.04
(1,2501)	1:A:15:LYS:H	1:A:40:ALA:HB2	3	0.03	0.04
(1,2501)	1:A:15:LYS:H	1:A:40:ALA:HB3	3	0.03	0.04
(1,2448)	1:B:23:THR:HG1	1:B:38:LEU:HD21	3	0.03	0.05
(1,2448)	1:B:23:THR:HG1	1:B:38:LEU:HD22	3	0.03	0.05
(1,2448)	1:B:23:THR:HG1	1:B:38:LEU:HD23	3	0.03	0.05
(1,2417)	1:A:38:LEU:HD11	1:A:45:PHE:HZ	3	0.01	0.02
(1,2417)	1:A:38:LEU:HD12	1:A:45:PHE:HZ	3	0.01	0.02
(1,2417)	1:A:38:LEU:HD13	1:A:45:PHE:HZ	3	0.01	0.02
(1,2281)	1:A:36:ILE:HG21	1:A:37:VAL:HB	3	0.02	0.03
(1,2281)	1:A:36:ILE:HG22	1:A:37:VAL:HB	3	0.02	0.03
(1,2281)	1:A:36:ILE:HG23	1:A:37:VAL:HB	3	0.02	0.03
(1,2248)	1:B:33:ILE:HD11	1:B:34:ARG:H	3	0.03	0.05
(1,2248)	1:B:33:ILE:HD12	1:B:34:ARG:H	3	0.03	0.05
(1,2248)	1:B:33:ILE:HD13	1:B:34:ARG:H	3	0.03	0.05
(1,2175)	1:A:25:VAL:HA	1:A:28:LYS:HE2	3	0.02	0.03
(1,2175)	1:A:25:VAL:HA	1:A:28:LYS:HE3	3	0.02	0.03
(1,2020)	1:B:22:ILE:HA	1:B:22:ILE:HD11	3	0.01	0.01
(1,2020)	1:B:22:ILE:HA	1:B:22:ILE:HD12	3	0.01	0.01
(1,2020)	1:B:22:ILE:HA	1:B:22:ILE:HD13	3	0.01	0.01
(1,1971)	1:B:20:ASN:H	1:B:22:ILE:HG13	3	0.01	0.01
(1,1970)	1:A:20:ASN:H	1:A:22:ILE:HG13	3	0.02	0.03



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(1,1837) 1:A:18:MET:HA 1:A:21:GLN:HG2 3 0.02 (1,1837) 1:A:18:MET:HA 1:A:21:GLN:HG3 3 0.02 (1,1813) 1:B:25:VAL:HG21 1:B:65:LYS:HE2 3 0.08 (1,1813) 1:B:25:VAL:HG21 1:B:65:LYS:HE3 3 0.08 (1,1813) 1:B:25:VAL:HG22 1:B:65:LYS:HE2 3 0.08 (1,1813) 1:B:25:VAL:HG22 1:B:65:LYS:HE3 3 0.08 (1,1813) 1:B:25:VAL:HG23 1:B:65:LYS:HE2 3 0.08 (1,1813) 1:B:25:VAL:HG23 1:B:65:LYS:HE3 3 0.08 (1,1812) 1:A:25:VAL:HG21 1:A:65:LYS:HE2 3 0.04	0.04 0.04 0.12 0.12 0.12 0.12 0.12 0.12 0.07 0.07
(1,1813) 1:B:25:VAL:HG21 1:B:65:LYS:HE2 3 0.08 (1,1813) 1:B:25:VAL:HG21 1:B:65:LYS:HE3 3 0.08 (1,1813) 1:B:25:VAL:HG22 1:B:65:LYS:HE2 3 0.08 (1,1813) 1:B:25:VAL:HG22 1:B:65:LYS:HE3 3 0.08 (1,1813) 1:B:25:VAL:HG23 1:B:65:LYS:HE2 3 0.08 (1,1813) 1:B:25:VAL:HG23 1:B:65:LYS:HE2 3 0.08	0.12 0.12 0.12 0.12 0.12 0.12 0.12 0.07 0.07
(1,1813) 1:B:25:VAL:HG21 1:B:65:LYS:HE3 3 0.08 (1,1813) 1:B:25:VAL:HG22 1:B:65:LYS:HE2 3 0.08 (1,1813) 1:B:25:VAL:HG22 1:B:65:LYS:HE3 3 0.08 (1,1813) 1:B:25:VAL:HG23 1:B:65:LYS:HE2 3 0.08 (1,1813) 1:B:25:VAL:HG23 1:B:65:LYS:HE3 3 0.08	0.12 0.12 0.12 0.12 0.12 0.07 0.07
(1,1813) 1:B:25:VAL:HG22 1:B:65:LYS:HE2 3 0.08 (1,1813) 1:B:25:VAL:HG22 1:B:65:LYS:HE3 3 0.08 (1,1813) 1:B:25:VAL:HG23 1:B:65:LYS:HE2 3 0.08 (1,1813) 1:B:25:VAL:HG23 1:B:65:LYS:HE3 3 0.08 (1,1813) 1:B:25:VAL:HG23 1:B:65:LYS:HE3 3 0.08	0.12 0.12 0.12 0.12 0.07 0.07
(1,1813) 1:B:25:VAL:HG22 1:B:65:LYS:HE3 3 0.08 (1,1813) 1:B:25:VAL:HG23 1:B:65:LYS:HE2 3 0.08 (1,1813) 1:B:25:VAL:HG23 1:B:65:LYS:HE3 3 0.08	0.12 0.12 0.12 0.07 0.07
(1,1813) 1:B:25:VAL:HG23 1:B:65:LYS:HE2 3 0.08 (1,1813) 1:B:25:VAL:HG23 1:B:65:LYS:HE3 3 0.08	0.12 0.12 0.07 0.07
(1,1813) 1:B:25:VAL:HG23 1:B:65:LYS:HE3 3 0.08	0.12 0.07 0.07
	0.07 0.07
(1.1812) $1 \cdot \Delta \cdot 25 \cdot V\Delta I \cdot HC21$ $1 \cdot \Delta \cdot 65 \cdot IVS \cdot HF2$ 3 0.04	0.07
(1,1812) 1:A:25:VAL:HG21 1:A:65:LYS:HE3 3 0.04	0.07
(1,1812) 1:A:25:VAL:HG22 1:A:65:LYS:HE2 3 0.04	0.07
(1,1812) 1:A:25:VAL:HG22 1:A:65:LYS:HE3 3 0.04	0.07
(1,1812) 1:A:25:VAL:HG23 1:A:65:LYS:HE2 3 0.04	0.07
(1,1812) 1:A:25:VAL:HG23 1:A:65:LYS:HE3 3 0.04	0.07
(1,1797) 1:B:15:LYS:HG2 1:B:18:MET:HE1 3 0.03	0.04
(1,1797) 1:B:15:LYS:HG2 1:B:18:MET:HE2 3 0.03	0.04
(1,1797) 1:B:15:LYS:HG2 1:B:18:MET:HE3 3 0.03	0.04
(1,1797) 1:B:15:LYS:HG3 1:B:18:MET:HE1 3 0.03	0.04
(1,1797) 1:B:15:LYS:HG3 1:B:18:MET:HE2 3 0.03	0.04
(1,1797) 1:B:15:LYS:HG3 1:B:18:MET:HE3 3 0.03	0.04
(1,172) 1:B:13:GLU:HG2 1:B:15:LYS:H 3 0.02	0.04
(1,172) 1:B:13:GLU:HG3 1:B:15:LYS:H 3 0.02	0.04
(1,171) 1:A:13:GLU:HG2 1:A:15:LYS:H 3 0.02	0.03
(1,171) 1:A:13:GLU:HG3 1:A:15:LYS:H 3 0.02	0.03
(1,1699) 1:B:11:VAL:HG21 1:B:45:PHE:HE1 3 0.02	0.02
(1,1699) 1:B:11:VAL:HG21 1:B:45:PHE:HE2 3 0.02	0.02
(1,1699) 1:B:11:VAL:HG22 1:B:45:PHE:HE1 3 0.02	0.02
(1,1699) 1:B:11:VAL:HG22 1:B:45:PHE:HE2 3 0.02	0.02
(1,1699) 1:B:11:VAL:HG23 1:B:45:PHE:HE1 3 0.02	0.02
(1,1699) 1:B:11:VAL:HG23 1:B:45:PHE:HE2 3 0.02	0.02
(1,167) 1:A:15:LYS:H 1:A:18:MET:HE1 3 0.02	0.03
(1,167) 1:A:15:LYS:H 1:A:18:MET:HE2 3 0.02	0.03
(1,167) 1:A:15:LYS:H 1:A:18:MET:HE3 3 0.02	0.03
(1,1356) 1:B:82:GLU:H 1:B:82:GLU:HG2 3 0.03	0.04
(1,1356) 1:B:82:GLU:H 1:B:82:GLU:HG3 3 0.03	0.04
(1,1330) 1:B:78:LEU:HD21 1:B:79:SER:H 3 0.06	0.1
(1,1330) 1:B:78:LEU:HD22 1:B:79:SER:H 3 0.06	0.1
(1,1330) 1:B:78:LEU:HD23 1:B:79:SER:H 3 0.06	0.1
(1,1211) 1:A:69:VAL:HG11 1:A:71:GLY:H 3 0.02	0.03
(1,1211) 1:A:69:VAL:HG12 1:A:71:GLY:H 3 0.02	0.03
(1,1211) 1:A:69:VAL:HG13 1:A:71:GLY:H 3 0.02	0.03
(1,1124) 1:B:67:ARG:H 1:B:69:VAL:HG21 3 0.02	0.02



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1124)	1:B:67:ARG:H	1:B:69:VAL:HG22	3	0.02	0.02
(1,1124)	1:B:67:ARG:H	1:B:69:VAL:HG23	3	0.02	0.02
(1,1067)	1:B:64:ASP:H	1:B:75:VAL:HG11	3	0.03	0.06
(1,1067)	1:B:64:ASP:H	1:B:75:VAL:HG12	3	0.03	0.06
(1,1067)	1:B:64:ASP:H	1:B:75:VAL:HG13	3	0.03	0.06
(1,839)	1:B:48:ASN:HD21	1:B:78:LEU:HD21	2	0.03	0.03
(1,839)	1:B:48:ASN:HD21	1:B:78:LEU:HD22	2	0.03	0.03
(1,839)	1:B:48:ASN:HD21	1:B:78:LEU:HD23	2	0.03	0.03
(1,838)	1:A:48:ASN:HD21	1:A:78:LEU:HD21	2	0.03	0.03
(1,838)	1:A:48:ASN:HD21	1:A:78:LEU:HD22	2	0.03	0.03
(1,838)	1:A:48:ASN:HD21	1:A:78:LEU:HD23	2	0.03	0.03
(1,829)	1:B:36:ILE:HD11	1:B:48:ASN:H	2	0.01	0.01
(1,829)	1:B:36:ILE:HD12	1:B:48:ASN:H	2	0.01	0.01
(1,829)	1:B:36:ILE:HD13	1:B:48:ASN:H	2	0.01	0.01
(1,82)	1:A:9:ARG:HE	1:A:11:VAL:HG21	2	0.08	0.12
(1,82)	1:A:9:ARG:HE	1:A:11:VAL:HG22	2	0.08	0.12
(1,82)	1:A:9:ARG:HE	1:A:11:VAL:HG23	2	0.08	0.12
(1,744)	1:A:44:ILE:H	1:A:44:ILE:HG21	2	0.01	0.02
(1,744)	1:A:44:ILE:H	1:A:44:ILE:HG22	2	0.01	0.02
(1,744)	1:A:44:ILE:H	1:A:44:ILE:HG23	2	0.01	0.02
(1,726)	1:A:41:LYS:HB2	1:A:42:ASP:H	2	0.04	0.06
(1,726)	1:A:41:LYS:HB3	1:A:42:ASP:H	2	0.04	0.06
(1,668)	1:A:39:ASN:H	1:A:48:ASN:H	2	0.05	0.07
(1,614)	1:A:35:THR:H	1:A:83:HIS:HE1	2	0.04	0.06
(1,568)	1:A:20:ASN:H	1:B:32:ASN:HD21	2	0.07	0.07
(1,542)	1:B:30:ASP:HA	1:B:31:THR:H	2	0.02	0.03
(1,5014)	1:B:81:LEU:H	1:B:82:GLU:HG2	2	0.14	0.25
(1,5014)	1:B:81:LEU:H	1:B:82:GLU:HG3	2	0.14	0.25
(1,4959)	1:B:59:LEU:HD11	1:B:77:ARG:HG2	2	0.06	0.08
(1,4959)	1:B:59:LEU:HD11	1:B:77:ARG:HG3	2	0.06	0.08
(1,4959)	1:B:59:LEU:HD12	1:B:77:ARG:HG2	2	0.06	0.08
(1,4959)	1:B:59:LEU:HD12	1:B:77:ARG:HG3	2	0.06	0.08
(1,4959)	1:B:59:LEU:HD13	1:B:77:ARG:HG2	2	0.06	0.08
(1,4959)	1:B:59:LEU:HD13	1:B:77:ARG:HG3	2	0.06	0.08
(1,4940)	1:B:55:ASN:HD21	1:B:57:ASP:HB2	2	0.07	0.11
(1,4940)	1:B:55:ASN:HD21	1:B:57:ASP:HB3	2	0.07	0.11
(1,4940)	1:B:55:ASN:HD22	1:B:57:ASP:HB2	2	0.07	0.11
(1,4940)	1:B:55:ASN:HD22	1:B:57:ASP:HB3	2	0.07	0.11
(1,4935)	1:B:54:LYS:HD2	1:B:55:ASN:HD21	2	0.02	0.03
(1,4935)	1:B:54:LYS:HD2	1:B:55:ASN:HD22	2	0.02	0.03
(1,4935)	1:B:54:LYS:HD3	1:B:55:ASN:HD21	2	0.02	0.03
(1,4935)	1:B:54:LYS:HD3	1:B:55:ASN:HD22	2	0.02	0.03



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,4889)	1:B:37:VAL:HG21	1:B:48:ASN:HD21	2	0.01	0.01
(1,4889)	1:B:37:VAL:HG21	1:B:48:ASN:HD22	2	0.01	0.01
(1,4889)	1:B:37:VAL:HG22	1:B:48:ASN:HD21	2	0.01	0.01
(1,4889)	1:B:37:VAL:HG22	1:B:48:ASN:HD22	2	0.01	0.01
(1,4889)	1:B:37:VAL:HG23	1:B:48:ASN:HD21	2	0.01	0.01
(1,4889)	1:B:37:VAL:HG23	1:B:48:ASN:HD22	2	0.01	0.01
(1,4869)	1:B:34:ARG:HB2	1:B:51:ILE:H	2	0.04	0.05
(1,4869)	1:B:34:ARG:HB3	1:B:51:ILE:H	2	0.04	0.05
(1,4828)	1:B:27:SER:HG	1:B:28:LYS:HD2	2	0.01	0.02
(1,4828)	1:B:27:SER:HG	1:B:28:LYS:HD3	2	0.01	0.02
(1,4771)	1:B:15:LYS:HD2	1:B:16:ASN:HD21	2	0.03	0.03
(1,4771)	1:B:15:LYS:HD2	1:B:16:ASN:HD22	2	0.03	0.03
(1,4771)	1:B:15:LYS:HD3	1:B:16:ASN:HD21	2	0.03	0.03
(1,4771)	1:B:15:LYS:HD3	1:B:16:ASN:HD22	2	0.03	0.03
(1,4770)	1:B:15:LYS:HD2	1:B:16:ASN:HB2	2	0.08	0.11
(1,4770)	1:B:15:LYS:HD2	1:B:16:ASN:HB3	2	0.08	0.11
(1,4770)	1:B:15:LYS:HD3	1:B:16:ASN:HB2	2	0.08	0.11
(1,4770)	1:B:15:LYS:HD3	1:B:16:ASN:HB3	2	0.08	0.11
(1,4765)	1:B:15:LYS:HB2	1:B:18:MET:HG2	2	0.07	0.09
(1,4765)	1:B:15:LYS:HB2	1:B:18:MET:HG3	2	0.07	0.09
(1,4745)	1:B:9:ARG:HG2	1:B:11:VAL:HG21	2	0.1	0.15
(1,4745)	1:B:9:ARG:HG2	1:B:11:VAL:HG22	2	0.1	0.15
(1,4745)	1:B:9:ARG:HG2	1:B:11:VAL:HG23	2	0.1	0.15
(1,4745)	1:B:9:ARG:HG3	1:B:11:VAL:HG21	2	0.1	0.15
(1,4745)	1:B:9:ARG:HG3	1:B:11:VAL:HG22	2	0.1	0.15
(1,4745)	1:B:9:ARG:HG3	1:B:11:VAL:HG23	2	0.1	0.15
(1,4660)	1:A:58:LYS:HE2	1:A:62:LEU:H	2	0.01	0.02
(1,4660)	1:A:58:LYS:HE3	1:A:62:LEU:H	2	0.01	0.02
(1,4642)	1:A:54:LYS:HD2	1:A:55:ASN:HD21	2	0.05	0.05
(1,4642)	1:A:54:LYS:HD2	1:A:55:ASN:HD22	2	0.05	0.05
(1,4642)	1:A:54:LYS:HD3	1:A:55:ASN:HD21	2	0.05	0.05
(1,4642)	1:A:54:LYS:HD3	1:A:55:ASN:HD22	2	0.05	0.05
(1,4638)	1:A:54:LYS:HB2	1:A:55:ASN:HD21	2	0.04	0.05
(1,4638)	1:A:54:LYS:HB2	1:A:55:ASN:HD22	2	0.04	0.05
(1,4638)	1:A:54:LYS:HB3	1:A:55:ASN:HD21	2	0.04	0.05
(1,4638)	1:A:54:LYS:HB3	1:A:55:ASN:HD22	2	0.04	0.05
(1,4635)	1:A:54:LYS:H	1:A:54:LYS:HG2	2	0.01	0.01
(1,4635)	1:A:54:LYS:H	1:A:54:LYS:HG3	2	0.01	0.01
(1,462)	1:B:25:VAL:HB	1:B:27:SER:H	2	0.01	0.01
(1,4604)	1:A:39:ASN:HD21	1:A:41:LYS:HE2	2	0.03	0.03
(1,4604)	1:A:39:ASN:HD21	1:A:41:LYS:HE3	2	0.03	0.03
(1,4604)	1:A:39:ASN:HD22	1:A:41:LYS:HE2	2	0.03	0.03



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,4604)	1:A:39:ASN:HD22	1:A:41:LYS:HE3	2	0.03	0.03
(1,4595)	1:A:37:VAL:HG21	1:A:48:ASN:HD21	2	0.01	0.02
(1,4595)	1:A:37:VAL:HG21	1:A:48:ASN:HD22	2	0.01	0.02
(1,4595)	1:A:37:VAL:HG22	1:A:48:ASN:HD21	2	0.01	0.02
(1,4595)	1:A:37:VAL:HG22	1:A:48:ASN:HD22	2	0.01	0.02
(1,4595)	1:A:37:VAL:HG23	1:A:48:ASN:HD21	2	0.01	0.02
(1,4595)	1:A:37:VAL:HG23	1:A:48:ASN:HD22	2	0.01	0.02
(1,4577)	1:A:34:ARG:HG2	1:A:52:PHE:HD1	2	0.05	0.08
(1,4577)	1:A:34:ARG:HG2	1:A:52:PHE:HD2	2	0.05	0.08
(1,4577)	1:A:34:ARG:HG3	1:A:52:PHE:HD1	2	0.05	0.08
(1,4577)	1:A:34:ARG:HG3	1:A:52:PHE:HD2	2	0.05	0.08
(1,4478)	1:A:18:MET:HB2	1:A:18:MET:HE1	2	0.01	0.01
(1,4478)	1:A:18:MET:HB2	1:A:18:MET:HE2	2	0.01	0.01
(1,4478)	1:A:18:MET:HB2	1:A:18:MET:HE3	2	0.01	0.01
(1,4478)	1:A:18:MET:HB3	1:A:18:MET:HE1	2	0.01	0.01
(1,4478)	1:A:18:MET:HB3	1:A:18:MET:HE2	2	0.01	0.01
(1,4478)	1:A:18:MET:HB3	1:A:18:MET:HE3	2	0.01	0.01
(1,4468)	1:A:16:ASN:HB2	1:A:17:GLY:H	2	0.04	0.04
(1,4468)	1:A:16:ASN:HB3	1:A:17:GLY:H	2	0.04	0.04
(1,4464)	1:A:15:LYS:HE2	1:A:16:ASN:HD21	2	0.03	0.04
(1,4464)	1:A:15:LYS:HE2	1:A:16:ASN:HD22	2	0.03	0.04
(1,4464)	1:A:15:LYS:HE3	1:A:16:ASN:HD21	2	0.03	0.04
(1,4464)	1:A:15:LYS:HE3	1:A:16:ASN:HD22	2	0.03	0.04
(1,4458)	1:A:15:LYS:HB2	1:A:18:MET:HG2	2	0.06	0.1
(1,4458)	1:A:15:LYS:HB2	1:A:18:MET:HG3	2	0.06	0.1
(1,4458)	1:A:15:LYS:HB3	1:A:18:MET:HG2	2	0.06	0.1
(1,4458)	1:A:15:LYS:HB3	1:A:18:MET:HG3	2	0.06	0.1
(1,4407)	1:A:3:ASP:HB2	1:A:52:PHE:HD1	2	0.07	0.09
(1,4407)	1:A:3:ASP:HB2	1:A:52:PHE:HD2	2	0.07	0.09
(1,4407)	1:A:3:ASP:HB3	1:A:52:PHE:HD1	2	0.07	0.09
(1,4407)	1:A:3:ASP:HB3	1:A:52:PHE:HD2	2	0.07	0.09
(1,4405)	1:A:3:ASP:HB2	1:A:4:PHE:H	2	0.13	0.16
(1,4405)	1:A:3:ASP:HB3	1:A:4:PHE:H	2	0.13	0.16
(1,4380)	1:A:5:LEU:HD21	1:A:83:HIS:HD2	2	0.01	0.01
(1,4380)	1:A:5:LEU:HD22	1:A:83:HIS:HD2	2	0.01	0.01
(1,4380)	1:A:5:LEU:HD23	1:A:83:HIS:HD2	2	0.01	0.01
(1,4217)	1:B:26:ILE:HG21	1:B:29:PHE:HZ	2	0.02	0.02
(1,4217)	1:B:26:ILE:HG22	1:B:29:PHE:HZ	2	0.02	0.02
(1,4217)	1:B:26:ILE:HG23	1:B:29:PHE:HZ	2	0.02	0.02
(1,4164)	1:A:4:PHE:HE1	1:A:55:ASN:HA	2	0.07	0.07
(1,4164)	1:A:4:PHE:HE2	1:A:55:ASN:HA	2	0.07	0.07
(1,4147)	1:B:4:PHE:H	1:B:4:PHE:HD1	2	0.03	0.03



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,4147)	1:B:4:PHE:H	1:B:4:PHE:HD2	2	0.03	0.03
(1,4127)	1:B:83:HIS:HA	1:B:83:HIS:HB3	2	0.07	0.12
(1,4110)	1:A:79:SER:HA	1:A:81:LEU:HG	2	0.03	0.03
(1,4108)	1:A:79:SER:HA	1:A:81:LEU:HD21	2	0.02	0.03
(1,4108)	1:A:79:SER:HA	1:A:81:LEU:HD22	2	0.02	0.03
(1,4108)	1:A:79:SER:HA	1:A:81:LEU:HD23	2	0.02	0.03
(1,4091)	1:B:73:PHE:HA	1:B:73:PHE:HD1	2	0.01	0.02
(1,4091)	1:B:73:PHE:HA	1:B:73:PHE:HD2	2	0.01	0.02
(1,4086)	1:A:73:PHE:HA	1:A:75:VAL:HG21	2	0.02	0.03
(1,4086)	1:A:73:PHE:HA	1:A:75:VAL:HG22	2	0.02	0.03
(1,4086)	1:A:73:PHE:HA	1:A:75:VAL:HG23	2	0.02	0.03
(1,4072)	1:A:60:THR:HB	1:A:61:THR:H	2	0.11	0.11
(1,4050)	1:A:41:LYS:HA	1:A:42:ASP:H	2	0.23	0.39
(1,4048)	1:A:41:LYS:HA	1:A:41:LYS:HD2	2	0.01	0.02
(1,4048)	1:A:41:LYS:HA	1:A:41:LYS:HD3	2	0.01	0.02
(1,3927)	1:B:23:THR:H	1:B:26:ILE:HD11	2	0.03	0.04
(1,3927)	1:B:23:THR:H	1:B:26:ILE:HD12	2	0.03	0.04
(1,3927)	1:B:23:THR:H	1:B:26:ILE:HD13	2	0.03	0.04
(1,3917)	1:A:18:MET:HE1	1:A:21:GLN:HE21	2	0.04	0.07
(1,3917)	1:A:18:MET:HE2	1:A:21:GLN:HE21	2	0.04	0.07
(1,3917)	1:A:18:MET:HE3	1:A:21:GLN:HE21	2	0.04	0.07
(1,3913)	1:A:18:MET:HE1	1:A:69:VAL:HG11	2	0.01	0.01
(1,3913)	1:A:18:MET:HE1	1:A:69:VAL:HG12	2	0.01	0.01
(1,3913)	1:A:18:MET:HE1	1:A:69:VAL:HG13	2	0.01	0.01
(1,3913)	1:A:18:MET:HE2	1:A:69:VAL:HG11	2	0.01	0.01
(1,3913)	1:A:18:MET:HE2	1:A:69:VAL:HG12	2	0.01	0.01
(1,3913)	1:A:18:MET:HE2	1:A:69:VAL:HG13	2	0.01	0.01
(1,3913)	1:A:18:MET:HE3	1:A:69:VAL:HG11	2	0.01	0.01
(1,3913)	1:A:18:MET:HE3	1:A:69:VAL:HG12	2	0.01	0.01
(1,3913)	1:A:18:MET:HE3	1:A:69:VAL:HG13	2	0.01	0.01
(1,3876)	1:B:50:MET:HG3	1:B:81:LEU:HD21	2	0.01	0.02
(1,3876)	1:B:50:MET:HG3	1:B:81:LEU:HD22	2	0.01	0.02
(1,3876)	1:B:50:MET:HG3	1:B:81:LEU:HD23	2	0.01	0.02
(1,3846)	1:B:80:ASN:HB3	1:B:81:LEU:HD21	2	0.04	0.08
(1,3846)	1:B:80:ASN:HB3	1:B:81:LEU:HD22	2	0.04	0.08
(1,3846)	1:B:80:ASN:HB3	1:B:81:LEU:HD23	2	0.04	0.08
(1,3839)	1:A:78:LEU:H	1:A:79:SER:HB2	2	0.09	0.1
(1,3839)	1:A:78:LEU:H	1:A:79:SER:HB3	2	0.09	0.1
(1,3809)	1:A:48:ASN:HD21	1:A:78:LEU:HD11	2	0.03	0.03
(1,3809)	1:A:48:ASN:HD21	1:A:78:LEU:HD12	2	0.03	0.03
(1,3809)	1:A:48:ASN:HD21	1:A:78:LEU:HD13	2	0.03	0.03
(1,3797)	1:A:9:ARG:HD2	1:A:78:LEU:HD11	2	0.03	0.04



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,3797)	1:A:9:ARG:HD2	1:A:78:LEU:HD12	2	0.03	0.04
(1,3797)	1:A:9:ARG:HD2	1:A:78:LEU:HD13	2	0.03	0.04
(1,3797)	1:A:9:ARG:HD3	1:A:78:LEU:HD11	2	0.03	0.04
(1,3797)	1:A:9:ARG:HD3	1:A:78:LEU:HD12	2	0.03	0.04
(1,3797)	1:A:9:ARG:HD3	1:A:78:LEU:HD13	2	0.03	0.04
(1,3792)	1:B:50:MET:HE1	1:B:78:LEU:HD11	2	0.04	0.04
(1,3792)	1:B:50:MET:HE1	1:B:78:LEU:HD12	2	0.04	0.04
(1,3792)	1:B:50:MET:HE1	1:B:78:LEU:HD13	2	0.04	0.04
(1,3792)	1:B:50:MET:HE2	1:B:78:LEU:HD11	2	0.04	0.04
(1,3792)	1:B:50:MET:HE2	1:B:78:LEU:HD12	2	0.04	0.04
(1,3792)	1:B:50:MET:HE2	1:B:78:LEU:HD13	2	0.04	0.04
(1,3792)	1:B:50:MET:HE3	1:B:78:LEU:HD11	2	0.04	0.04
(1,3792)	1:B:50:MET:HE3	1:B:78:LEU:HD12	2	0.04	0.04
(1,3792)	1:B:50:MET:HE3	1:B:78:LEU:HD13	2	0.04	0.04
(1,3768)	1:B:77:ARG:HD2	1:B:78:LEU:H	2	0.01	0.02
(1,3768)	1:B:77:ARG:HD3	1:B:78:LEU:H	2	0.01	0.02
(1,3738)	1:B:59:LEU:HD11	1:B:77:ARG:HG2	2	0.03	0.04
(1,3738)	1:B:59:LEU:HD12	1:B:77:ARG:HG2	2	0.03	0.04
(1,3738)	1:B:59:LEU:HD13	1:B:77:ARG:HG2	2	0.03	0.04
(1,3732)	1:B:9:ARG:HB2	1:B:76:GLU:HG2	2	0.02	0.02
(1,3732)	1:B:9:ARG:HB2	1:B:76:GLU:HG3	2	0.02	0.02
(1,3732)	1:B:9:ARG:HB3	1:B:76:GLU:HG2	2	0.02	0.02
(1,3732)	1:B:9:ARG:HB3	1:B:76:GLU:HG3	2	0.02	0.02
(1,3606)	1:B:69:VAL:HG11	1:B:70:GLN:HB2	2	0.07	0.13
(1,3606)	1:B:69:VAL:HG11	1:B:70:GLN:HB3	2	0.07	0.13
(1,3606)	1:B:69:VAL:HG12	1:B:70:GLN:HB2	2	0.07	0.13
(1,3606)	1:B:69:VAL:HG12	1:B:70:GLN:HB3	2	0.07	0.13
(1,3606)	1:B:69:VAL:HG13	1:B:70:GLN:HB2	2	0.07	0.13
(1,3606)	1:B:69:VAL:HG13	1:B:70:GLN:HB3	2	0.07	0.13
(1,3530)	1:B:68:LYS:HA	1:B:68:LYS:HG3	2	0.01	0.01
(1,3516)	1:B:67:ARG:HD2	1:B:75:VAL:HG11	2	0.03	0.04
(1,3516)	1:B:67:ARG:HD2	1:B:75:VAL:HG12	2	0.03	0.04
(1,3516)	1:B:67:ARG:HD2	1:B:75:VAL:HG13	2	0.03	0.04
(1,3516)	1:B:67:ARG:HD3	1:B:75:VAL:HG11	2	0.03	0.04
(1,3516)	1:B:67:ARG:HD3	1:B:75:VAL:HG12	2	0.03	0.04
(1,3516)	1:B:67:ARG:HD3	1:B:75:VAL:HG13	2	0.03	0.04
(1,349)	1:B:18:MET:HE1	1:B:21:GLN:HE22	2	0.01	0.02
(1,349)	1:B:18:MET:HE2	1:B:21:GLN:HE22	2	0.01	0.02
(1,349)	1:B:18:MET:HE3	1:B:21:GLN:HE22	2	0.01	0.02
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE1	2	0.19	0.22
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE2	2	0.19	0.22
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE3	2	0.19	0.22



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE1	2	0.19	0.22
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE2	2	0.19	0.22
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE3	2	0.19	0.22
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE1	2	0.19	0.22
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE2	2	0.19	0.22
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE3	2	0.19	0.22
(1,3360)	1:A:30:ASP:H	1:A:62:LEU:HD11	2	0.08	0.08
(1,3360)	1:A:30:ASP:H	1:A:62:LEU:HD12	2	0.08	0.08
(1,3360)	1:A:30:ASP:H	1:A:62:LEU:HD13	2	0.08	0.08
(1,3293)	1:A:58:LYS:HZ1	1:A:61:THR:HG21	2	0.01	0.02
(1,3293)	1:A:58:LYS:HZ1	1:A:61:THR:HG22	2	0.01	0.02
(1,3293)	1:A:58:LYS:HZ1	1:A:61:THR:HG23	2	0.01	0.02
(1,3293)	1:A:58:LYS:HZ2	1:A:61:THR:HG21	2	0.01	0.02
(1,3293)	1:A:58:LYS:HZ2	1:A:61:THR:HG22	2	0.01	0.02
(1,3293)	1:A:58:LYS:HZ2	1:A:61:THR:HG23	2	0.01	0.02
(1,3293)	1:A:58:LYS:HZ3	1:A:61:THR:HG21	2	0.01	0.02
(1,3293)	1:A:58:LYS:HZ3	1:A:61:THR:HG22	2	0.01	0.02
(1,3293)	1:A:58:LYS:HZ3	1:A:61:THR:HG23	2	0.01	0.02
(1,3257)	1:A:60:THR:HA	1:A:60:THR:HG21	2	0.05	0.05
(1,3257)	1:A:60:THR:HA	1:A:60:THR:HG22	2	0.05	0.05
(1,3257)	1:A:60:THR:HA	1:A:60:THR:HG23	2	0.05	0.05
(1,3102)	1:B:54:LYS:HA	1:B:54:LYS:HE2	2	0.06	0.08
(1,3102)	1:B:54:LYS:HA	1:B:54:LYS:HE3	2	0.06	0.08
(1,3100)	1:B:54:LYS:H	1:B:54:LYS:HD2	2	0.1	0.14
(1,3100)	1:B:54:LYS:H	1:B:54:LYS:HD3	2	0.1	0.14
(1,3097)	1:A:15:LYS:HD2	1:A:16:ASN:HD21	2	0.07	0.1
(1,3097)	1:A:15:LYS:HD3	1:A:16:ASN:HD21	2	0.07	0.1
(1,3094)	1:B:15:LYS:HD2	1:B:16:ASN:HD22	2	0.07	0.07
(1,3094)	1:B:15:LYS:HD3	1:B:16:ASN:HD22	2	0.07	0.07
(1,3)	1:A:2:THR:HG21	1:A:4:PHE:H	2	0.08	0.08
(1,3)	1:A:2:THR:HG22	1:A:4:PHE:H	2	0.08	0.08
(1,3)	1:A:2:THR:HG23	1:A:4:PHE:H	2	0.08	0.08
(1,2901)	1:A:20:ASN:HD22	1:B:51:ILE:HG21	2	0.08	0.1
(1,2901)	1:A:20:ASN:HD22	1:B:51:ILE:HG22	2	0.08	0.1
(1,2901)	1:A:20:ASN:HD22	1:B:51:ILE:HG23	2	0.08	0.1
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG21	2	0.14	0.16
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG22	2	0.14	0.16
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG23	2	0.14	0.16
(1,2580)	1:B:42:ASP:HB2	1:B:44:ILE:HD11	2	0.03	0.05
(1,2580)	1:B:42:ASP:HB2	1:B:44:ILE:HD12	2	0.03	0.05
(1,2580)	1:B:42:ASP:HB2	1:B:44:ILE:HD13	2	0.03	0.05
(1,2572)	1:B:14:ASP:H	1:B:44:ILE:HG21	2	0.04	0.06



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2572)	1:B:14:ASP:H	1:B:44:ILE:HG22	2	0.04	0.06
(1,2572)	1:B:14:ASP:H	1:B:44:ILE:HG23	2	0.04	0.06
(1,2524)	1:B:14:ASP:HB3	1:B:43:GLY:HA3	2	0.02	0.03
(1,2522)	1:B:14:ASP:HB2	1:B:43:GLY:HA3	2	0.09	0.1
(1,2521)	1:A:14:ASP:HB2	1:A:43:GLY:HA3	2	0.05	0.09
(1,2400)	1:B:38:LEU:HD11	1:B:47:CYS:HG	2	0.03	0.03
(1,2400)	1:B:38:LEU:HD12	1:B:47:CYS:HG	2	0.03	0.03
(1,2400)	1:B:38:LEU:HD13	1:B:47:CYS:HG	2	0.03	0.03
(1,2334)	1:B:37:VAL:HB	1:B:48:ASN:HB2	2	0.01	0.01
(1,2284)	1:A:36:ILE:HG21	1:B:39:ASN:HB2	2	0.1	0.11
(1,2284)	1:A:36:ILE:HG21	1:B:39:ASN:HB3	2	0.1	0.11
(1,2284)	1:A:36:ILE:HG22	1:B:39:ASN:HB2	2	0.1	0.11
(1,2284)	1:A:36:ILE:HG22	1:B:39:ASN:HB3	2	0.1	0.11
(1,2284)	1:A:36:ILE:HG23	1:B:39:ASN:HB2	2	0.1	0.11
(1,2284)	1:A:36:ILE:HG23	1:B:39:ASN:HB3	2	0.1	0.11
(1,2247)	1:A:33:ILE:HD11	1:A:34:ARG:H	2	0.03	0.03
(1,2247)	1:A:33:ILE:HD12	1:A:34:ARG:H	2	0.03	0.03
(1,2247)	1:A:33:ILE:HD13	1:A:34:ARG:H	2	0.03	0.03
(1,2245)	1:A:33:ILE:H	1:A:33:ILE:HD11	2	0.01	0.01
(1,2245)	1:A:33:ILE:H	1:A:33:ILE:HD12	2	0.01	0.01
(1,2245)	1:A:33:ILE:H	1:A:33:ILE:HD13	2	0.01	0.01
(1,2242)	1:A:33:ILE:HD11	1:B:20:ASN:HD22	2	0.01	0.02
(1,2242)	1:A:33:ILE:HD12	1:B:20:ASN:HD22	2	0.01	0.02
(1,2242)	1:A:33:ILE:HD13	1:B:20:ASN:HD22	2	0.01	0.02
(1,2241)	1:A:20:ASN:HD22	1:B:33:ILE:HD11	2	0.01	0.02
(1,2241)	1:A:20:ASN:HD22	1:B:33:ILE:HD12	2	0.01	0.02
(1,2241)	1:A:20:ASN:HD22	1:B:33:ILE:HD13	2	0.01	0.02
(1,2237)	1:A:20:ASN:HA	1:B:33:ILE:HD11	2	0.02	0.02
(1,2237)	1:A:20:ASN:HA	1:B:33:ILE:HD12	2	0.02	0.02
(1,2237)	1:A:20:ASN:HA	1:B:33:ILE:HD13	2	0.02	0.02
(1,2176)	1:B:25:VAL:HA	1:B:28:LYS:HE2	2	0.04	0.04
(1,2176)	1:B:25:VAL:HA	1:B:28:LYS:HE3	2	0.04	0.04
(1,2174)	1:B:68:LYS:HA	1:B:68:LYS:HD2	2	0.1	0.14
(1,2164)	1:B:27:SER:HG	1:B:28:LYS:HG2	2	0.11	0.12
(1,2163)	1:A:27:SER:HG	1:A:28:LYS:HG2	2	0.07	0.07
(1,2094)	1:B:22:ILE:HA	1:B:25:VAL:HG21	2	0.04	0.05
(1,2094)	1:B:22:ILE:HA	1:B:25:VAL:HG22	2	0.04	0.05
(1,2094)	1:B:22:ILE:HA	1:B:25:VAL:HG23	2	0.04	0.05
(1,2051)	1:A:67:ARG:HE	1:A:75:VAL:HG11	2	0.06	0.09
(1,2051)	1:A:67:ARG:HE	1:A:75:VAL:HG12	2	0.06	0.09
(1,2051)	1:A:67:ARG:HE	1:A:75:VAL:HG13	2	0.06	0.09
(1,1940)	1:A:22:ILE:HB	1:A:47:CYS:HG	2	0.01	0.01



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1838)	1:B:18:MET:HA	1:B:21:GLN:HG2	2	0.01	0.01
(1,1838)	1:B:18:MET:HA	1:B:21:GLN:HG3	2	0.01	0.01
(1,1811)	1:B:41:LYS:HE2	1:B:44:ILE:HD11	2	0.04	0.05
(1,1811)	1:B:41:LYS:HE2	1:B:44:ILE:HD12	2	0.04	0.05
(1,1811)	1:B:41:LYS:HE2	1:B:44:ILE:HD13	2	0.04	0.05
(1,1811)	1:B:41:LYS:HE3	1:B:44:ILE:HD11	2	0.04	0.05
(1,1811)	1:B:41:LYS:HE3	1:B:44:ILE:HD12	2	0.04	0.05
(1,1811)	1:B:41:LYS:HE3	1:B:44:ILE:HD13	2	0.04	0.05
(1,1810)	1:A:41:LYS:HE2	1:A:44:ILE:HD11	2	0.06	0.07
(1,1810)	1:A:41:LYS:HE2	1:A:44:ILE:HD12	2	0.06	0.07
(1,1810)	1:A:41:LYS:HE2	1:A:44:ILE:HD13	2	0.06	0.07
(1,1810)	1:A:41:LYS:HE3	1:A:44:ILE:HD11	2	0.06	0.07
(1,1810)	1:A:41:LYS:HE3	1:A:44:ILE:HD12	2	0.06	0.07
(1,1810)	1:A:41:LYS:HE3	1:A:44:ILE:HD13	2	0.06	0.07
(1,1808)	1:A:11:VAL:HG21	1:A:41:LYS:HE2	2	0.08	0.12
(1,1808)	1:A:11:VAL:HG21	1:A:41:LYS:HE3	2	0.08	0.12
(1,1808)	1:A:11:VAL:HG22	1:A:41:LYS:HE2	2	0.08	0.12
(1,1808)	1:A:11:VAL:HG22	1:A:41:LYS:HE3	2	0.08	0.12
(1,1808)	1:A:11:VAL:HG23	1:A:41:LYS:HE2	2	0.08	0.12
(1,1808)	1:A:11:VAL:HG23	1:A:41:LYS:HE3	2	0.08	0.12
(1,1792)	1:B:13:GLU:HG2	1:B:15:LYS:HB3	2	0.02	0.02
(1,1792)	1:B:13:GLU:HG3	1:B:15:LYS:HB3	2	0.02	0.02
(1,1791)	1:A:13:GLU:HG2	1:A:15:LYS:HB3	2	0.02	0.02
(1,1791)	1:A:13:GLU:HG3	1:A:15:LYS:HB3	2	0.02	0.02
(1,176)	1:B:15:LYS:H	1:B:18:MET:HG2	2	0.13	0.24
(1,1690)	1:A:11:VAL:HG21	1:A:46:THR:HB	2	0.03	0.03
(1,1690)	1:A:11:VAL:HG22	1:A:46:THR:HB	2	0.03	0.03
(1,1690)	1:A:11:VAL:HG23	1:A:46:THR:HB	2	0.03	0.03
(1,168)	1:B:15:LYS:H	1:B:18:MET:HE1	2	0.04	0.07
(1,168)	1:B:15:LYS:H	1:B:18:MET:HE2	2	0.04	0.07
(1,168)	1:B:15:LYS:H	1:B:18:MET:HE3	2	0.04	0.07
(1,1572)	1:B:9:ARG:HG3	1:B:10:ILE:H	2	0.04	0.04
(1,1557)	1:A:24:GLY:H	1:A:26:ILE:HD11	2	0.01	0.02
(1,1557)	1:A:24:GLY:H	1:A:26:ILE:HD12	2	0.01	0.02
(1,1557)	1:A:24:GLY:H	1:A:26:ILE:HD13	2	0.01	0.02
(1,1551)	1:A:8:ILE:HD11	1:A:77:ARG:HA	2	0.03	0.03
(1,1551)	1:A:8:ILE:HD12	1:A:77:ARG:HA	2	0.03	0.03
(1,1551)	1:A:8:ILE:HD13	1:A:77:ARG:HA	2	0.03	0.03
(1,1377)	1:A:40:ALA:H	1:A:41:LYS:HD2	2	0.1	0.14
(1,1377)	1:A:40:ALA:H	1:A:41:LYS:HD3	2	0.1	0.14
(1,1318)	1:B:77:ARG:HG2	1:B:78:LEU:H	2	0.09	0.11
(1,1310)	1:B:77:ARG:H	1:B:77:ARG:HD2	2	0.01	0.02



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1310)	1:B:77:ARG:H	1:B:77:ARG:HD3	2	0.01	0.02
(1,1302)	1:B:77:ARG:H	1:B:77:ARG:HB2	2	0.07	0.08
(1,1266)	1:B:74:THR:HG21	1:B:75:VAL:H	2	0.01	0.02
(1,1266)	1:B:74:THR:HG22	1:B:75:VAL:H	2	0.01	0.02
(1,1266)	1:B:74:THR:HG23	1:B:75:VAL:H	2	0.01	0.02
(1,1227)	1:A:70:GLN:HA	1:A:72:VAL:H	2	0.02	0.02
(1,1223)	1:A:69:VAL:HG21	1:A:72:VAL:H	2	0.03	0.04
(1,1223)	1:A:69:VAL:HG22	1:A:72:VAL:H	2	0.03	0.04
(1,1223)	1:A:69:VAL:HG23	1:A:72:VAL:H	2	0.03	0.04
(1,1158)	1:B:68:LYS:H	1:B:75:VAL:HG21	2	0.02	0.03
(1,1158)	1:B:68:LYS:H	1:B:75:VAL:HG22	2	0.02	0.03
(1,1158)	1:B:68:LYS:H	1:B:75:VAL:HG23	2	0.02	0.03
(1,1149)	1:A:67:ARG:HE	1:A:75:VAL:HB	2	0.02	0.03
(1,1094)	1:B:65:LYS:H	1:B:68:LYS:HE2	2	0.07	0.1
(1,1094)	1:B:65:LYS:H	1:B:68:LYS:HE3	2	0.07	0.1
(1,1066)	1:A:64:ASP:H	1:A:75:VAL:HG11	2	0.01	0.01
(1,1066)	1:A:64:ASP:H	1:A:75:VAL:HG12	2	0.01	0.01
(1,1066)	1:A:64:ASP:H	1:A:75:VAL:HG13	2	0.01	0.01
(1,956)	1:A:53:VAL:HG21	1:A:58:LYS:H	1	0.01	0.01
(1,956)	1:A:53:VAL:HG22	1:A:58:LYS:H	1	0.01	0.01
(1,956)	1:A:53:VAL:HG23	1:A:58:LYS:H	1	0.01	0.01
(1,938)	1:A:54:LYS:HE2	1:A:55:ASN:HD22	1	0.04	0.04
(1,938)	1:A:54:LYS:HE3	1:A:55:ASN:HD22	1	0.04	0.04
(1,928)	1:A:55:ASN:H	1:A:56:THR:HG21	1	0.08	0.08
(1,928)	1:A:55:ASN:H	1:A:56:THR:HG22	1	0.08	0.08
(1,928)	1:A:55:ASN:H	1:A:56:THR:HG23	1	0.08	0.08
(1,84)	1:A:9:ARG:HE	1:A:10:ILE:H	1	0.02	0.02
(1,771)	1:B:44:ILE:HB	1:B:45:PHE:H	1	0.02	0.02
(1,760)	1:A:43:GLY:H	1:A:44:ILE:H	1	0.01	0.01
(1,745)	1:B:44:ILE:H	1:B:44:ILE:HG21	1	0.01	0.01
(1,745)	1:B:44:ILE:H	1:B:44:ILE:HG22	1	0.01	0.01
(1,745)	1:B:44:ILE:H	1:B:44:ILE:HG23	1	0.01	0.01
(1,736)	1:A:41:LYS:HG2	1:A:43:GLY:H	1	0.07	0.07
(1,736)	1:A:41:LYS:HG3	1:A:43:GLY:H	1	0.07	0.07
(1,735)	1:B:40:ALA:HB1	1:B:43:GLY:H	1	0.08	0.08
(1,735)	1:B:40:ALA:HB2	1:B:43:GLY:H	1	0.08	0.08
(1,735)	1:B:40:ALA:HB3	1:B:43:GLY:H	1	0.08	0.08
(1,727)	1:B:41:LYS:HB2	1:B:42:ASP:H	1	0.12	0.12
(1,727)	1:B:41:LYS:HB3	1:B:42:ASP:H	1	0.12	0.12
(1,725)	1:B:41:LYS:HG2	1:B:42:ASP:H	1	0.04	0.04
(1,725)	1:B:41:LYS:HG3	1:B:42:ASP:H	1	0.04	0.04
(1,723)	1:B:41:LYS:H	1:B:43:GLY:H	1	0.01	0.01



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,697)	1:B:41:LYS:H	1:B:41:LYS:HG2	1	0.09	0.09
(1,697)	1:B:41:LYS:H	1:B:41:LYS:HG3	1	0.09	0.09
(1,696)	1:A:41:LYS:H	1:A:41:LYS:HG2	1	0.07	0.07
(1,696)	1:A:41:LYS:H	1:A:41:LYS:HG3	1	0.07	0.07
(1,695)	1:B:41:LYS:H	1:B:44:ILE:HG21	1	0.01	0.01
(1,695)	1:B:41:LYS:H	1:B:44:ILE:HG22	1	0.01	0.01
(1,695)	1:B:41:LYS:H	1:B:44:ILE:HG23	1	0.01	0.01
(1,577)	1:A:32:ASN:HD22	1:B:17:GLY:H	1	0.01	0.01
(1,570)	1:A:32:ASN:HD22	1:B:16:ASN:HA	1	0.03	0.03
(1,548)	1:A:31:THR:H	1:B:20:ASN:HD21	1	0.05	0.05
(1,5013)	1:B:80:ASN:HB2	1:B:81:LEU:HD21	1	0.03	0.03
(1,5013)	1:B:80:ASN:HB2	1:B:81:LEU:HD22	1	0.03	0.03
(1,5013)	1:B:80:ASN:HB2	1:B:81:LEU:HD23	1	0.03	0.03
(1,5013)	1:B:80:ASN:HB3	1:B:81:LEU:HD21	1	0.03	0.03
(1,5013)	1:B:80:ASN:HB3	1:B:81:LEU:HD22	1	0.03	0.03
(1,5013)	1:B:80:ASN:HB3	1:B:81:LEU:HD23	1	0.03	0.03
(1,5007)	1:B:77:ARG:HB2	1:B:77:ARG:HE	1	0.01	0.01
(1,5007)	1:B:77:ARG:HB3	1:B:77:ARG:HE	1	0.01	0.01
(1,4989)	1:B:67:ARG:H	1:B:67:ARG:HG2	1	0.01	0.01
(1,4989)	1:B:67:ARG:H	1:B:67:ARG:HG3	1	0.01	0.01
(1,4988)	1:B:66:LEU:HB2	1:B:75:VAL:HG11	1	0.03	0.03
(1,4988)	1:B:66:LEU:HB2	1:B:75:VAL:HG12	1	0.03	0.03
(1,4988)	1:B:66:LEU:HB2	1:B:75:VAL:HG13	1	0.03	0.03
(1,4988)	1:B:66:LEU:HB3	1:B:75:VAL:HG11	1	0.03	0.03
(1,4988)	1:B:66:LEU:HB3	1:B:75:VAL:HG12	1	0.03	0.03
(1,4988)	1:B:66:LEU:HB3	1:B:75:VAL:HG13	1	0.03	0.03
(1,4961)	1:B:59:LEU:HD21	1:B:77:ARG:HG2	1	0.01	0.01
(1,4961)	1:B:59:LEU:HD21	1:B:77:ARG:HG3	1	0.01	0.01
(1,4961)	1:B:59:LEU:HD22	1:B:77:ARG:HG2	1	0.01	0.01
(1,4961)	1:B:59:LEU:HD22	1:B:77:ARG:HG3	1	0.01	0.01
(1,4961)	1:B:59:LEU:HD23	1:B:77:ARG:HG2	1	0.01	0.01
(1,4961)	1:B:59:LEU:HD23	1:B:77:ARG:HG3	1	0.01	0.01
(1,4934)	1:B:54:LYS:HD2	1:B:55:ASN:HB2	1	0.06	0.06
(1,4934)	1:B:54:LYS:HD2	1:B:55:ASN:HB3	1	0.06	0.06
(1,4934)	1:B:54:LYS:HD3	1:B:55:ASN:HB2	1	0.06	0.06
(1,4934)	1:B:54:LYS:HD3	1:B:55:ASN:HB3	1	0.06	0.06
(1,4928)	1:B:54:LYS:H	1:B:54:LYS:HG2	1	0.04	0.04
(1,4928)	1:B:54:LYS:H	1:B:54:LYS:HG3	1	0.04	0.04
(1,4926)	1:B:53:VAL:HG21	1:B:54:LYS:HG2	1	0.04	0.04
(1,4926)	1:B:53:VAL:HG21	1:B:54:LYS:HG3	1	0.04	0.04
(1,4926)	1:B:53:VAL:HG22	1:B:54:LYS:HG2	1	0.04	0.04
(1,4926)	1:B:53:VAL:HG22	1:B:54:LYS:HG3	1	0.04	0.04



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,4926)	1:B:53:VAL:HG23	1:B:54:LYS:HG2	1	0.04	0.04
(1,4926)	1:B:53:VAL:HG23	1:B:54:LYS:HG3	1	0.04	0.04
(1,4922)	1:B:53:VAL:HA	1:B:54:LYS:HB2	1	0.02	0.02
(1,4922)	1:B:53:VAL:HA	1:B:54:LYS:HB3	1	0.02	0.02
(1,4911)	1:B:46:THR:HG21	1:B:48:ASN:HD21	1	0.1	0.1
(1,4911)	1:B:46:THR:HG21	1:B:48:ASN:HD22	1	0.1	0.1
(1,4911)	1:B:46:THR:HG22	1:B:48:ASN:HD21	1	0.1	0.1
(1,4911)	1:B:46:THR:HG22	1:B:48:ASN:HD22	1	0.1	0.1
(1,4911)	1:B:46:THR:HG23	1:B:48:ASN:HD21	1	0.1	0.1
(1,4911)	1:B:46:THR:HG23	1:B:48:ASN:HD22	1	0.1	0.1
(1,4897)	1:B:39:ASN:HD21	1:B:41:LYS:HD2	1	0.05	0.05
(1,4897)	1:B:39:ASN:HD21	1:B:41:LYS:HD3	1	0.05	0.05
(1,4897)	1:B:39:ASN:HD22	1:B:41:LYS:HD2	1	0.05	0.05
(1,4897)	1:B:39:ASN:HD22	1:B:41:LYS:HD3	1	0.05	0.05
(1,4879)	1:B:36:ILE:HG12	1:B:37:VAL:HA	1	0.09	0.09
(1,4879)	1:B:36:ILE:HG13	1:B:37:VAL:HA	1	0.09	0.09
(1,4873)	1:B:34:ARG:HG2	1:B:52:PHE:HE1	1	0.02	0.02
(1,4873)	1:B:34:ARG:HG2	1:B:52:PHE:HE2	1	0.02	0.02
(1,4873)	1:B:34:ARG:HG3	1:B:52:PHE:HE1	1	0.02	0.02
(1,4873)	1:B:34:ARG:HG3	1:B:52:PHE:HE2	1	0.02	0.02
(1,4867)	1:B:34:ARG:HB2	1:B:50:MET:HG2	1	0.02	0.02
(1,4867)	1:B:34:ARG:HB3	1:B:50:MET:HG2	1	0.02	0.02
(1,4857)	1:B:32:ASN:HB2	1:B:33:ILE:HG12	1	0.01	0.01
(1,4857)	1:B:32:ASN:HB2	1:B:33:ILE:HG13	1	0.01	0.01
(1,4857)	1:B:32:ASN:HB3	1:B:33:ILE:HG12	1	0.01	0.01
(1,4857)	1:B:32:ASN:HB3	1:B:33:ILE:HG13	1	0.01	0.01
(1,4850)	1:B:29:PHE:HZ	1:B:65:LYS:HD2	1	0.03	0.03
(1,4850)	1:B:29:PHE:HZ	1:B:65:LYS:HD3	1	0.03	0.03
(1,4833)	1:B:28:LYS:HA	1:B:28:LYS:HG2	1	0.03	0.03
(1,4833)	1:B:28:LYS:HA	1:B:28:LYS:HG3	1	0.03	0.03
(1,4814)	1:B:25:VAL:HG11	1:B:28:LYS:HD2	1	0.02	0.02
(1,4814)	1:B:25:VAL:HG11	1:B:28:LYS:HD3	1	0.02	0.02
(1,4814)	1:B:25:VAL:HG12	1:B:28:LYS:HD2	1	0.02	0.02
(1,4814)	1:B:25:VAL:HG12	1:B:28:LYS:HD3	1	0.02	0.02
(1,4814)	1:B:25:VAL:HG13	1:B:28:LYS:HD2	1	0.02	0.02
(1,4814)	1:B:25:VAL:HG13	1:B:28:LYS:HD3	1	0.02	0.02
(1,481)	1:A:23:THR:HG21	1:A:28:LYS:H	1	0.02	0.02
(1,481)	1:A:23:THR:HG22	1:A:28:LYS:H	1	0.02	0.02
(1,481)	1:A:23:THR:HG23	1:A:28:LYS:H	1	0.02	0.02
(1,4805)	1:B:24:GLY:HA2	1:B:28:LYS:HE2	1	0.02	0.02
(1,4805)	1:B:24:GLY:HA2	1:B:28:LYS:HE3	1	0.02	0.02
(1,4805)	1:B:24:GLY:HA3	1:B:28:LYS:HE2	1	0.02	0.02



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,4805)	1:B:24:GLY:HA3	1:B:28:LYS:HE3	1	0.02	0.02
(1,4792)	1:B:20:ASN:HB2	1:B:21:GLN:HE21	1	0.01	0.01
(1,4792)	1:B:20:ASN:HB3	1:B:21:GLN:HE21	1	0.01	0.01
(1,4731)	1:B:7:GLY:H	1:B:77:ARG:HG2	1	0.01	0.01
(1,4731)	1:B:7:GLY:H	1:B:77:ARG:HG3	1	0.01	0.01
(1,4719)	1:B:3:ASP:HB2	1:B:52:PHE:HD1	1	0.18	0.18
(1,4719)	1:B:3:ASP:HB2	1:B:52:PHE:HD2	1	0.18	0.18
(1,4719)	1:B:3:ASP:HB3	1:B:52:PHE:HD1	1	0.18	0.18
(1,4719)	1:B:3:ASP:HB3	1:B:52:PHE:HD2	1	0.18	0.18
(1,4695)	1:A:67:ARG:HG2	1:A:75:VAL:H	1	0.04	0.04
(1,4695)	1:A:67:ARG:HG3	1:A:75:VAL:H	1	0.04	0.04
(1,4689)	1:A:66:LEU:HB2	1:A:75:VAL:HG11	1	0.03	0.03
(1,4689)	1:A:66:LEU:HB2	1:A:75:VAL:HG12	1	0.03	0.03
(1,4689)	1:A:66:LEU:HB2	1:A:75:VAL:HG13	1	0.03	0.03
(1,4689)	1:A:66:LEU:HB3	1:A:75:VAL:HG11	1	0.03	0.03
(1,4689)	1:A:66:LEU:HB3	1:A:75:VAL:HG12	1	0.03	0.03
(1,4689)	1:A:66:LEU:HB3	1:A:75:VAL:HG13	1	0.03	0.03
(1,4679)	1:A:63:MET:HE1	1:A:77:ARG:HB2	1	0.03	0.03
(1,4679)	1:A:63:MET:HE1	1:A:77:ARG:HB3	1	0.03	0.03
(1,4679)	1:A:63:MET:HE2	1:A:77:ARG:HB2	1	0.03	0.03
(1,4679)	1:A:63:MET:HE2	1:A:77:ARG:HB3	1	0.03	0.03
(1,4679)	1:A:63:MET:HE3	1:A:77:ARG:HB2	1	0.03	0.03
(1,4679)	1:A:63:MET:HE3	1:A:77:ARG:HB3	1	0.03	0.03
(1,4647)	1:A:55:ASN:HD21	1:A:57:ASP:HB2	1	0.14	0.14
(1,4647)	1:A:55:ASN:HD21	1:A:57:ASP:HB3	1	0.14	0.14
(1,4647)	1:A:55:ASN:HD22	1:A:57:ASP:HB2	1	0.14	0.14
(1,4647)	1:A:55:ASN:HD22	1:A:57:ASP:HB3	1	0.14	0.14
(1,4633)	1:A:53:VAL:HG21	1:A:54:LYS:HG2	1	0.01	0.01
(1,4633)	1:A:53:VAL:HG21	1:A:54:LYS:HG3	1	0.01	0.01
(1,4633)	1:A:53:VAL:HG22	1:A:54:LYS:HG2	1	0.01	0.01
(1,4633)	1:A:53:VAL:HG22	1:A:54:LYS:HG3	1	0.01	0.01
(1,4633)	1:A:53:VAL:HG23	1:A:54:LYS:HG2	1	0.01	0.01
(1,4633)	1:A:53:VAL:HG23	1:A:54:LYS:HG3	1	0.01	0.01
(1,461)	1:A:25:VAL:HB	1:A:27:SER:H	1	0.01	0.01
(1,4607)	1:A:39:ASN:HD21	1:A:48:ASN:HD21	1	0.02	0.02
(1,4607)	1:A:39:ASN:HD21	1:A:48:ASN:HD22	1	0.02	0.02
(1,4607)	1:A:39:ASN:HD22	1:A:48:ASN:HD21	1	0.02	0.02
(1,4607)	1:A:39:ASN:HD22	1:A:48:ASN:HD22	1	0.02	0.02
(1,4585)	1:A:36:ILE:HG12	1:A:37:VAL:HA	1	0.09	0.09
(1,4585)	1:A:36:ILE:HG13	1:A:37:VAL:HA	1	0.09	0.09
(1,4574)	1:A:34:ARG:HB2	1:A:51:ILE:H	1	0.01	0.01
(1,4574)	1:A:34:ARG:HB3	1:A:51:ILE:H	1	0.01	0.01



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,4534)	1:A:27:SER:HB2	1:A:33:ILE:HD11	1	0.02	0.02
(1,4534)	1:A:27:SER:HB2	1:A:33:ILE:HD12	1	0.02	0.02
(1,4534)	1:A:27:SER:HB2	1:A:33:ILE:HD13	1	0.02	0.02
(1,4534)	1:A:27:SER:HB3	1:A:33:ILE:HD11	1	0.02	0.02
(1,4534)	1:A:27:SER:HB3	1:A:33:ILE:HD12	1	0.02	0.02
(1,4534)	1:A:27:SER:HB3	1:A:33:ILE:HD13	1	0.02	0.02
(1,4523)	1:A:25:VAL:HG11	1:A:28:LYS:HD2	1	0.01	0.01
(1,4523)	1:A:25:VAL:HG11	1:A:28:LYS:HD3	1	0.01	0.01
(1,4523)	1:A:25:VAL:HG12	1:A:28:LYS:HD2	1	0.01	0.01
(1,4523)	1:A:25:VAL:HG12	1:A:28:LYS:HD3	1	0.01	0.01
(1,4523)	1:A:25:VAL:HG13	1:A:28:LYS:HD2	1	0.01	0.01
(1,4523)	1:A:25:VAL:HG13	1:A:28:LYS:HD3	1	0.01	0.01
(1,4518)	1:A:25:VAL:HA	1:A:28:LYS:HB2	1	0.01	0.01
(1,4518)	1:A:25:VAL:HA	1:A:28:LYS:HB3	1	0.01	0.01
(1,4504)	1:A:23:THR:HG21	1:A:27:SER:HB2	1	0.01	0.01
(1,4504)	1:A:23:THR:HG21	1:A:27:SER:HB3	1	0.01	0.01
(1,4504)	1:A:23:THR:HG22	1:A:27:SER:HB2	1	0.01	0.01
(1,4504)	1:A:23:THR:HG22	1:A:27:SER:HB3	1	0.01	0.01
(1,4504)	1:A:23:THR:HG23	1:A:27:SER:HB2	1	0.01	0.01
(1,4504)	1:A:23:THR:HG23	1:A:27:SER:HB3	1	0.01	0.01
(1,4477)	1:A:18:MET:H	1:B:32:ASN:HD21	1	0.03	0.03
(1,4477)	1:A:18:MET:H	1:B:32:ASN:HD22	1	0.03	0.03
(1,4463)	1:A:15:LYS:HD2	1:A:16:ASN:HD21	1	0.08	0.08
(1,4463)	1:A:15:LYS:HD2	1:A:16:ASN:HD22	1	0.08	0.08
(1,4463)	1:A:15:LYS:HD3	1:A:16:ASN:HD21	1	0.08	0.08
(1,4463)	1:A:15:LYS:HD3	1:A:16:ASN:HD22	1	0.08	0.08
(1,4462)	1:A:15:LYS:HD2	1:A:16:ASN:HB2	1	0.04	0.04
(1,4462)	1:A:15:LYS:HD2	1:A:16:ASN:HB3	1	0.04	0.04
(1,4462)	1:A:15:LYS:HD3	1:A:16:ASN:HB2	1	0.04	0.04
(1,4462)	1:A:15:LYS:HD3	1:A:16:ASN:HB3	1	0.04	0.04
(1,4406)	1:A:3:ASP:HB2	1:A:52:PHE:HB2	1	0.01	0.01
(1,4406)	1:A:3:ASP:HB2	1:A:52:PHE:HB3	1	0.01	0.01
(1,4406)	1:A:3:ASP:HB3	1:A:52:PHE:HB2	1	0.01	0.01
(1,4406)	1:A:3:ASP:HB3	1:A:52:PHE:HB3	1	0.01	0.01
(1,4391)	1:B:50:MET:HE1	1:B:83:HIS:HD2	1	0.1	0.1
(1,4391)	1:B:50:MET:HE2	1:B:83:HIS:HD2	1	0.1	0.1
(1,4391)	1:B:50:MET:HE3	1:B:83:HIS:HD2	1	0.1	0.1
(1,4385)	1:B:81:LEU:HD11	1:B:83:HIS:HD2	1	0.01	0.01
(1,4385)	1:B:81:LEU:HD12	1:B:83:HIS:HD2	1	0.01	0.01
(1,4385)	1:B:81:LEU:HD13	1:B:83:HIS:HD2	1	0.01	0.01
(1,4370)	1:A:13:GLU:H	1:A:73:PHE:HZ	1	0.02	0.02
(1,4355)	1:B:44:ILE:HG12	1:B:73:PHE:HE1	1	0.02	0.02



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,4355)	1:B:44:ILE:HG12	1:B:73:PHE:HE2	1	0.02	0.02
(1,4354)	1:A:44:ILE:HG12	1:A:73:PHE:HE1	1	0.01	0.01
(1,4354)	1:A:44:ILE:HG12	1:A:73:PHE:HE2	1	0.01	0.01
(1,4342)	1:A:29:PHE:HE1	1:A:65:LYS:HE2	1	0.01	0.01
(1,4342)	1:A:29:PHE:HE1	1:A:65:LYS:HE3	1	0.01	0.01
(1,4342)	1:A:29:PHE:HE2	1:A:65:LYS:HE2	1	0.01	0.01
(1,4342)	1:A:29:PHE:HE2	1:A:65:LYS:HE3	1	0.01	0.01
(1,4325)	1:B:6:ALA:H	1:B:52:PHE:HD1	1	0.01	0.01
(1,4325)	1:B:6:ALA:H	1:B:52:PHE:HD2	1	0.01	0.01
(1,4324)	1:A:6:ALA:H	1:A:52:PHE:HD1	1	0.01	0.01
(1,4324)	1:A:6:ALA:H	1:A:52:PHE:HD2	1	0.01	0.01
(1,4300)	1:A:5:LEU:HD11	1:A:52:PHE:HD1	1	0.04	0.04
(1,4300)	1:A:5:LEU:HD11	1:A:52:PHE:HD2	1	0.04	0.04
(1,4300)	1:A:5:LEU:HD12	1:A:52:PHE:HD1	1	0.04	0.04
(1,4300)	1:A:5:LEU:HD12	1:A:52:PHE:HD2	1	0.04	0.04
(1,4300)	1:A:5:LEU:HD13	1:A:52:PHE:HD1	1	0.04	0.04
(1,4300)	1:A:5:LEU:HD13	1:A:52:PHE:HD2	1	0.04	0.04
(1,4297)	1:B:45:PHE:HZ	1:B:71:GLY:HA3	1	0.03	0.03
(1,4296)	1:A:45:PHE:HZ	1:A:71:GLY:HA3	1	0.02	0.02
(1,4245)	1:B:14:ASP:HA	1:B:45:PHE:HD1	1	0.02	0.02
(1,4245)	1:B:14:ASP:HA	1:B:45:PHE:HD2	1	0.02	0.02
(1,4241)	1:B:18:MET:HE1	1:B:45:PHE:HD1	1	0.01	0.01
(1,4241)	1:B:18:MET:HE1	1:B:45:PHE:HD2	1	0.01	0.01
(1,4241)	1:B:18:MET:HE2	1:B:45:PHE:HD1	1	0.01	0.01
(1,4241)	1:B:18:MET:HE2	1:B:45:PHE:HD2	1	0.01	0.01
(1,4241)	1:B:18:MET:HE3	1:B:45:PHE:HD1	1	0.01	0.01
(1,4241)	1:B:18:MET:HE3	1:B:45:PHE:HD2	1	0.01	0.01
(1,4237)	1:B:40:ALA:HB1	1:B:45:PHE:HD1	1	0.01	0.01
(1,4237)	1:B:40:ALA:HB1	1:B:45:PHE:HD2	1	0.01	0.01
(1,4237)	1:B:40:ALA:HB2	1:B:45:PHE:HD1	1	0.01	0.01
(1,4237)	1:B:40:ALA:HB2	1:B:45:PHE:HD2	1	0.01	0.01
(1,4237)	1:B:40:ALA:HB3	1:B:45:PHE:HD1	1	0.01	0.01
(1,4237)	1:B:40:ALA:HB3	1:B:45:PHE:HD2	1	0.01	0.01
(1,4210)	1:A:29:PHE:H	1:A:29:PHE:HD1	1	0.01	0.01
(1,4210)	1:A:29:PHE:H	1:A:29:PHE:HD2	1	0.01	0.01
(1,4182)	1:A:4:PHE:HZ	1:A:56:THR:HA	1	0.02	0.02
(1,4179)	1:B:4:PHE:HZ	1:B:59:LEU:HD21	1	0.01	0.01
(1,4179)	1:B:4:PHE:HZ	1:B:59:LEU:HD22	1	0.01	0.01
(1,4179)	1:B:4:PHE:HZ	1:B:59:LEU:HD23	1	0.01	0.01
(1,4165)	1:B:4:PHE:HE1	1:B:55:ASN:HA	1	0.04	0.04
(1,4165)	1:B:4:PHE:HE2	1:B:55:ASN:HA	1	0.04	0.04
(1,4162)	1:A:4:PHE:HE1	1:A:56:THR:HA	1	0.07	0.07



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,4162)	1:A:4:PHE:HE2	1:A:56:THR:HA	1	0.07	0.07
(1,4139)	1:B:4:PHE:HD1	1:B:54:LYS:HA	1	0.01	0.01
(1,4139)	1:B:4:PHE:HD2	1:B:54:LYS:HA	1	0.01	0.01
(1,4115)	1:B:77:ARG:HG2	1:B:79:SER:HA	1	0.02	0.02
(1,4109)	1:B:79:SER:HA	1:B:81:LEU:HD21	1	0.02	0.02
(1,4109)	1:B:79:SER:HA	1:B:81:LEU:HD22	1	0.02	0.02
(1,4109)	1:B:79:SER:HA	1:B:81:LEU:HD23	1	0.02	0.02
(1,4093)	1:B:74:THR:HA	1:B:75:VAL:HG21	1	0.01	0.01
(1,4093)	1:B:74:THR:HA	1:B:75:VAL:HG22	1	0.01	0.01
(1,4093)	1:B:74:THR:HA	1:B:75:VAL:HG23	1	0.01	0.01
(1,4087)	1:B:73:PHE:HA	1:B:75:VAL:HG21	1	0.05	0.05
(1,4087)	1:B:73:PHE:HA	1:B:75:VAL:HG22	1	0.05	0.05
(1,4087)	1:B:73:PHE:HA	1:B:75:VAL:HG23	1	0.05	0.05
(1,4073)	1:B:60:THR:HB	1:B:61:THR:H	1	0.12	0.12
(1,4051)	1:B:41:LYS:HA	1:B:42:ASP:H	1	0.37	0.37
(1,3986)	1:A:81:LEU:HD11	1:A:83:HIS:HB3	1	0.04	0.04
(1,3986)	1:A:81:LEU:HD12	1:A:83:HIS:HB3	1	0.04	0.04
(1,3986)	1:A:81:LEU:HD13	1:A:83:HIS:HB3	1	0.04	0.04
(1,3954)	1:A:41:LYS:HE2	1:A:44:ILE:HB	1	0.05	0.05
(1,3954)	1:A:41:LYS:HE3	1:A:44:ILE:HB	1	0.05	0.05
(1,3928)	1:A:23:THR:H	1:B:33:ILE:HD11	1	0.01	0.01
(1,3928)	1:A:23:THR:H	1:B:33:ILE:HD12	1	0.01	0.01
(1,3928)	1:A:23:THR:H	1:B:33:ILE:HD13	1	0.01	0.01
(1,3886)	1:B:79:SER:H	1:B:81:LEU:HD21	1	0.01	0.01
(1,3886)	1:B:79:SER:H	1:B:81:LEU:HD22	1	0.01	0.01
(1,3886)	1:B:79:SER:H	1:B:81:LEU:HD23	1	0.01	0.01
(1,3873)	1:A:6:ALA:H	1:A:81:LEU:HD11	1	0.05	0.05
(1,3873)	1:A:6:ALA:H	1:A:81:LEU:HD12	1	0.05	0.05
(1,3873)	1:A:6:ALA:H	1:A:81:LEU:HD13	1	0.05	0.05
(1,3860)	1:B:50:MET:HG3	1:B:81:LEU:HD11	1	0.02	0.02
(1,3860)	1:B:50:MET:HG3	1:B:81:LEU:HD12	1	0.02	0.02
(1,3860)	1:B:50:MET:HG3	1:B:81:LEU:HD13	1	0.02	0.02
(1,3858)	1:B:50:MET:HG2	1:B:81:LEU:HD11	1	0.03	0.03
(1,3858)	1:B:50:MET:HG2	1:B:81:LEU:HD12	1	0.03	0.03
(1,3858)	1:B:50:MET:HG2	1:B:81:LEU:HD13	1	0.03	0.03
(1,3857)	1:A:50:MET:HG2	1:A:81:LEU:HD11	1	0.01	0.01
(1,3857)	1:A:50:MET:HG2	1:A:81:LEU:HD12	1	0.01	0.01
(1,3857)	1:A:50:MET:HG2	1:A:81:LEU:HD13	1	0.01	0.01
(1,3845)	1:A:80:ASN:HB3	1:A:81:LEU:HD21	1	0.03	0.03
(1,3845)	1:A:80:ASN:HB3	1:A:81:LEU:HD22	1	0.03	0.03
(1,3845)	1:A:80:ASN:HB3	1:A:81:LEU:HD23	1	0.03	0.03
(1,3841)	1:A:80:ASN:HB2	1:A:81:LEU:HD21	1	0.04	0.04



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,3841)	1:A:80:ASN:HB2	1:A:81:LEU:HD22	1	0.04	0.04
(1,3841)	1:A:80:ASN:HB2	1:A:81:LEU:HD23	1	0.04	0.04
(1,3836)	1:B:9:ARG:H	1:B:78:LEU:HD21	1	0.01	0.01
(1,3836)	1:B:9:ARG:H	1:B:78:LEU:HD22	1	0.01	0.01
(1,3836)	1:B:9:ARG:H	1:B:78:LEU:HD23	1	0.01	0.01
(1,3810)	1:B:48:ASN:HD21	1:B:78:LEU:HD11	1	0.03	0.03
(1,3810)	1:B:48:ASN:HD21	1:B:78:LEU:HD12	1	0.03	0.03
(1,3810)	1:B:48:ASN:HD21	1:B:78:LEU:HD13	1	0.03	0.03
(1,3791)	1:A:50:MET:HE1	1:A:78:LEU:HD11	1	0.03	0.03
(1,3791)	1:A:50:MET:HE1	1:A:78:LEU:HD12	1	0.03	0.03
(1,3791)	1:A:50:MET:HE1	1:A:78:LEU:HD13	1	0.03	0.03
(1,3791)	1:A:50:MET:HE2	1:A:78:LEU:HD11	1	0.03	0.03
(1,3791)	1:A:50:MET:HE2	1:A:78:LEU:HD12	1	0.03	0.03
(1,3791)	1:A:50:MET:HE2	1:A:78:LEU:HD13	1	0.03	0.03
(1,3791)	1:A:50:MET:HE3	1:A:78:LEU:HD11	1	0.03	0.03
(1,3791)	1:A:50:MET:HE3	1:A:78:LEU:HD12	1	0.03	0.03
(1,3791)	1:A:50:MET:HE3	1:A:78:LEU:HD13	1	0.03	0.03
(1,3757)	1:A:6:ALA:HB1	1:A:77:ARG:HD2	1	0.01	0.01
(1,3757)	1:A:6:ALA:HB1	1:A:77:ARG:HD3	1	0.01	0.01
(1,3757)	1:A:6:ALA:HB2	1:A:77:ARG:HD2	1	0.01	0.01
(1,3757)	1:A:6:ALA:HB2	1:A:77:ARG:HD3	1	0.01	0.01
(1,3757)	1:A:6:ALA:HB3	1:A:77:ARG:HD2	1	0.01	0.01
(1,3757)	1:A:6:ALA:HB3	1:A:77:ARG:HD3	1	0.01	0.01
(1,3755)	1:A:59:LEU:HD21	1:A:77:ARG:HD2	1	0.02	0.02
(1,3755)	1:A:59:LEU:HD21	1:A:77:ARG:HD3	1	0.02	0.02
(1,3755)	1:A:59:LEU:HD22	1:A:77:ARG:HD2	1	0.02	0.02
(1,3755)	1:A:59:LEU:HD22	1:A:77:ARG:HD3	1	0.02	0.02
(1,3755)	1:A:59:LEU:HD23	1:A:77:ARG:HD2	1	0.02	0.02
(1,3755)	1:A:59:LEU:HD23	1:A:77:ARG:HD3	1	0.02	0.02
(1,3737)	1:A:59:LEU:HD11	1:A:77:ARG:HG2	1	0.01	0.01
(1,3737)	1:A:59:LEU:HD12	1:A:77:ARG:HG2	1	0.01	0.01
(1,3737)	1:A:59:LEU:HD13	1:A:77:ARG:HG2	1	0.01	0.01
(1,3731)	1:A:9:ARG:HB2	1:A:76:GLU:HG2	1	0.01	0.01
(1,3731)	1:A:9:ARG:HB2	1:A:76:GLU:HG3	1	0.01	0.01
(1,3731)	1:A:9:ARG:HB3	1:A:76:GLU:HG2	1	0.01	0.01
(1,3731)	1:A:9:ARG:HB3	1:A:76:GLU:HG3	1	0.01	0.01
(1,3695)	1:A:73:PHE:HA	1:A:74:THR:HG21	1	0.04	0.04
(1,3695)	1:A:73:PHE:HA	1:A:74:THR:HG22	1	0.04	0.04
(1,3695)	1:A:73:PHE:HA	1:A:74:THR:HG23	1	0.04	0.04
(1,3688)	1:B:74:THR:HB	1:B:75:VAL:H	1	0.02	0.02
(1,3685)	1:A:10:ILE:HA	1:A:74:THR:HB	1	0.01	0.01
(1,3660)	1:B:66:LEU:HA	1:B:72:VAL:HG21	1	0.01	0.01



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,3660)	1:B:66:LEU:HA	1:B:72:VAL:HG22	1	0.01	0.01
(1,3660)	1:B:66:LEU:HA	1:B:72:VAL:HG23	1	0.01	0.01
(1,3659)	1:A:66:LEU:HA	1:A:72:VAL:HG21	1	0.02	0.02
(1,3659)	1:A:66:LEU:HA	1:A:72:VAL:HG22	1	0.02	0.02
(1,3659)	1:A:66:LEU:HA	1:A:72:VAL:HG23	1	0.02	0.02
(1,3628)	1:B:70:GLN:HG2	1:B:72:VAL:H	1	0.04	0.04
(1,3628)	1:B:70:GLN:HG3	1:B:72:VAL:H	1	0.04	0.04
(1,3627)	1:A:70:GLN:HG2	1:A:72:VAL:H	1	0.05	0.05
(1,3627)	1:A:70:GLN:HG3	1:A:72:VAL:H	1	0.05	0.05
(1,3621)	1:A:69:VAL:HA	1:A:70:GLN:HG2	1	0.13	0.13
(1,3621)	1:A:69:VAL:HA	1:A:70:GLN:HG3	1	0.13	0.13
(1,3605)	1:A:69:VAL:HG11	1:A:70:GLN:HB2	1	0.02	0.02
(1,3605)	1:A:69:VAL:HG11	1:A:70:GLN:HB3	1	0.02	0.02
(1,3605)	1:A:69:VAL:HG12	1:A:70:GLN:HB2	1	0.02	0.02
(1,3605)	1:A:69:VAL:HG12	1:A:70:GLN:HB3	1	0.02	0.02
(1,3605)	1:A:69:VAL:HG13	1:A:70:GLN:HB2	1	0.02	0.02
(1,3605)	1:A:69:VAL:HG13	1:A:70:GLN:HB3	1	0.02	0.02
(1,3563)	1:A:67:ARG:H	1:A:68:LYS:HE2	1	0.03	0.03
(1,3563)	1:A:67:ARG:H	1:A:68:LYS:HE3	1	0.03	0.03
(1,3552)	1:B:68:LYS:HA	1:B:68:LYS:HE2	1	0.02	0.02
(1,3552)	1:B:68:LYS:HA	1:B:68:LYS:HE3	1	0.02	0.02
(1,3551)	1:A:68:LYS:HA	1:A:68:LYS:HE2	1	0.06	0.06
(1,3551)	1:A:68:LYS:HA	1:A:68:LYS:HE3	1	0.06	0.06
(1,3531)	1:A:68:LYS:HA	1:A:68:LYS:HD3	1	0.01	0.01
(1,353)	1:B:21:GLN:HE22	1:B:69:VAL:HA	1	0.04	0.04
(1,3529)	1:A:68:LYS:HA	1:A:68:LYS:HG3	1	0.03	0.03
(1,3515)	1:A:67:ARG:HD2	1:A:75:VAL:HG11	1	0.02	0.02
(1,3515)	1:A:67:ARG:HD2	1:A:75:VAL:HG12	1	0.02	0.02
(1,3515)	1:A:67:ARG:HD2	1:A:75:VAL:HG13	1	0.02	0.02
(1,3515)	1:A:67:ARG:HD3	1:A:75:VAL:HG11	1	0.02	0.02
(1,3515)	1:A:67:ARG:HD3	1:A:75:VAL:HG12	1	0.02	0.02
(1,3515)	1:A:67:ARG:HD3	1:A:75:VAL:HG13	1	0.02	0.02
(1,3511)	1:A:64:ASP:HA	1:A:67:ARG:HG3	1	0.02	0.02
(1,3480)	1:B:65:LYS:HA	1:B:65:LYS:HE2	1	0.14	0.14
(1,3480)	1:B:65:LYS:HA	1:B:65:LYS:HE3	1	0.14	0.14
(1,348)	1:A:18:MET:HE1	1:A:21:GLN:HE22	1	0.02	0.02
(1,348)	1:A:18:MET:HE2	1:A:21:GLN:HE22	1	0.02	0.02
(1,348)	1:A:18:MET:HE3	1:A:21:GLN:HE22	1	0.02	0.02
(1,346)	1:A:21:GLN:HE22	1:A:69:VAL:HG21	1	0.04	0.04
(1,346)	1:A:21:GLN:HE22	1:A:69:VAL:HG22	1	0.04	0.04
(1,346)	1:A:21:GLN:HE22	1:A:69:VAL:HG23	1	0.04	0.04
(1,342)	1:A:21:GLN:HE22	1:A:69:VAL:HG11	1	0.03	0.03



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,342)	1:A:21:GLN:HE22	1:A:69:VAL:HG12	1	0.03	0.03
(1,342)	1:A:21:GLN:HE22	1:A:69:VAL:HG13	1	0.03	0.03
(1,3397)	1:B:60:THR:HG21	1:B:63:MET:HE1	1	0.23	0.23
(1,3397)	1:B:60:THR:HG21	1:B:63:MET:HE2	1	0.23	0.23
(1,3397)	1:B:60:THR:HG21	1:B:63:MET:HE3	1	0.23	0.23
(1,3397)	1:B:60:THR:HG22	1:B:63:MET:HE1	1	0.23	0.23
(1,3397)	1:B:60:THR:HG22	1:B:63:MET:HE2	1	0.23	0.23
(1,3397)	1:B:60:THR:HG22	1:B:63:MET:HE3	1	0.23	0.23
(1,3397)	1:B:60:THR:HG23	1:B:63:MET:HE1	1	0.23	0.23
(1,3397)	1:B:60:THR:HG23	1:B:63:MET:HE2	1	0.23	0.23
(1,3397)	1:B:60:THR:HG23	1:B:63:MET:HE3	1	0.23	0.23
(1,3386)	1:A:58:LYS:HZ1	1:A:62:LEU:HD21	1	0.01	0.01
(1,3386)	1:A:58:LYS:HZ1	1:A:62:LEU:HD22	1	0.01	0.01
(1,3386)	1:A:58:LYS:HZ1	1:A:62:LEU:HD23	1	0.01	0.01
(1,3386)	1:A:58:LYS:HZ2	1:A:62:LEU:HD21	1	0.01	0.01
(1,3386)	1:A:58:LYS:HZ2	1:A:62:LEU:HD22	1	0.01	0.01
(1,3386)	1:A:58:LYS:HZ2	1:A:62:LEU:HD23	1	0.01	0.01
(1,3386)	1:A:58:LYS:HZ3	1:A:62:LEU:HD21	1	0.01	0.01
(1,3386)	1:A:58:LYS:HZ3	1:A:62:LEU:HD22	1	0.01	0.01
(1,3386)	1:A:58:LYS:HZ3	1:A:62:LEU:HD23	1	0.01	0.01
(1,3343)	1:B:62:LEU:HD11	1:B:63:MET:HA	1	0.02	0.02
(1,3343)	1:B:62:LEU:HD12	1:B:63:MET:HA	1	0.02	0.02
(1,3343)	1:B:62:LEU:HD13	1:B:63:MET:HA	1	0.02	0.02
(1,3334)	1:A:58:LYS:HE2	1:A:62:LEU:HD11	1	0.02	0.02
(1,3334)	1:A:58:LYS:HE2	1:A:62:LEU:HD12	1	0.02	0.02
(1,3334)	1:A:58:LYS:HE2	1:A:62:LEU:HD13	1	0.02	0.02
(1,3258)	1:B:60:THR:HA	1:B:60:THR:HG21	1	0.05	0.05
(1,3258)	1:B:60:THR:HA	1:B:60:THR:HG22	1	0.05	0.05
(1,3258)	1:B:60:THR:HA	1:B:60:THR:HG23	1	0.05	0.05
(1,3183)	1:A:58:LYS:HD2	1:A:62:LEU:H	1	0.1	0.1
(1,3183)	1:A:58:LYS:HD3	1:A:62:LEU:H	1	0.1	0.1
(1,3149)	1:A:55:ASN:H	1:A:58:LYS:HB2	1	0.11	0.11
(1,3106)	1:B:54:LYS:H	1:B:54:LYS:HE2	1	0.16	0.16
(1,3106)	1:B:54:LYS:H	1:B:54:LYS:HE3	1	0.16	0.16
(1,3105)	1:A:54:LYS:H	1:A:54:LYS:HE2	1	0.03	0.03
(1,3105)	1:A:54:LYS:H	1:A:54:LYS:HE3	1	0.03	0.03
(1,3041)	1:A:5:LEU:HA	1:A:53:VAL:HG21	1	0.02	0.02
(1,3041)	1:A:5:LEU:HA	1:A:53:VAL:HG22	1	0.02	0.02
(1,3041)	1:A:5:LEU:HA	1:A:53:VAL:HG23	1	0.02	0.02
(1,3037)	1:A:53:VAL:HG21	1:A:58:LYS:HA	1	0.04	0.04
(1,3037)	1:A:53:VAL:HG22	1:A:58:LYS:HA	1	0.04	0.04
(1,3037)	1:A:53:VAL:HG23	1:A:58:LYS:HA	1	0.04	0.04



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,3034)	1:B:53:VAL:HG21	1:B:59:LEU:HA	1	0.01	0.01
(1,3034)	1:B:53:VAL:HG22	1:B:59:LEU:HA	1	0.01	0.01
(1,3034)	1:B:53:VAL:HG23	1:B:59:LEU:HA	1	0.01	0.01
(1,3008)	1:B:52:PHE:H	1:B:53:VAL:HG11	1	0.01	0.01
(1,3008)	1:B:52:PHE:H	1:B:53:VAL:HG12	1	0.01	0.01
(1,3008)	1:B:52:PHE:H	1:B:53:VAL:HG13	1	0.01	0.01
(1,3007)	1:A:52:PHE:H	1:A:53:VAL:HG11	1	0.01	0.01
(1,3007)	1:A:52:PHE:H	1:A:53:VAL:HG12	1	0.01	0.01
(1,3007)	1:A:52:PHE:H	1:A:53:VAL:HG13	1	0.01	0.01
(1,3006)	1:B:53:VAL:HG11	1:B:55:ASN:H	1	0.03	0.03
(1,3006)	1:B:53:VAL:HG12	1:B:55:ASN:H	1	0.03	0.03
(1,3006)	1:B:53:VAL:HG13	1:B:55:ASN:H	1	0.03	0.03
(1,3005)	1:A:53:VAL:HG11	1:A:55:ASN:H	1	0.01	0.01
(1,3005)	1:A:53:VAL:HG12	1:A:55:ASN:H	1	0.01	0.01
(1,3005)	1:A:53:VAL:HG13	1:A:55:ASN:H	1	0.01	0.01
(1,2972)	1:B:53:VAL:HG11	1:B:62:LEU:HD21	1	0.02	0.02
(1,2972)	1:B:53:VAL:HG11	1:B:62:LEU:HD22	1	0.02	0.02
(1,2972)	1:B:53:VAL:HG11	1:B:62:LEU:HD23	1	0.02	0.02
(1,2972)	1:B:53:VAL:HG12	1:B:62:LEU:HD21	1	0.02	0.02
(1,2972)	1:B:53:VAL:HG12	1:B:62:LEU:HD22	1	0.02	0.02
(1,2972)	1:B:53:VAL:HG12	1:B:62:LEU:HD23	1	0.02	0.02
(1,2972)	1:B:53:VAL:HG13	1:B:62:LEU:HD21	1	0.02	0.02
(1,2972)	1:B:53:VAL:HG13	1:B:62:LEU:HD22	1	0.02	0.02
(1,2972)	1:B:53:VAL:HG13	1:B:62:LEU:HD23	1	0.02	0.02
(1,294)	1:A:33:ILE:HG13	1:B:20:ASN:HD22	1	0.14	0.14
(1,289)	1:A:33:ILE:HG13	1:B:20:ASN:HD21	1	0.08	0.08
(1,2871)	1:A:15:LYS:HG2	1:A:16:ASN:H	1	0.08	0.08
(1,2871)	1:A:15:LYS:HG3	1:A:16:ASN:H	1	0.08	0.08
(1,2833)	1:A:6:ALA:HA	1:A:50:MET:HE1	1	0.02	0.02
(1,2833)	1:A:6:ALA:HA	1:A:50:MET:HE2	1	0.02	0.02
(1,2833)	1:A:6:ALA:HA	1:A:50:MET:HE3	1	0.02	0.02
(1,2830)	1:B:50:MET:HE1	1:B:81:LEU:HA	1	0.02	0.02
(1,2830)	1:B:50:MET:HE2	1:B:81:LEU:HA	1	0.02	0.02
(1,2830)	1:B:50:MET:HE3	1:B:81:LEU:HA	1	0.02	0.02
(1,2829)	1:A:50:MET:HE1	1:A:81:LEU:HA	1	0.01	0.01
(1,2829)	1:A:50:MET:HE2	1:A:81:LEU:HA	1	0.01	0.01
(1,2829)	1:A:50:MET:HE3	1:A:81:LEU:HA	1	0.01	0.01
(1,2812)	1:B:50:MET:HE1	1:B:81:LEU:HD21	1	0.02	0.02
(1,2812)	1:B:50:MET:HE1	1:B:81:LEU:HD22	1	0.02	0.02
(1,2812)	1:B:50:MET:HE1	1:B:81:LEU:HD23	1	0.02	0.02
(1,2812)	1:B:50:MET:HE2	1:B:81:LEU:HD21	1	0.02	0.02
(1,2812)	1:B:50:MET:HE2	1:B:81:LEU:HD22	1	0.02	0.02



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2812)	1:B:50:MET:HE2	1:B:81:LEU:HD23	1	0.02	0.02
(1,2812)	1:B:50:MET:HE3	1:B:81:LEU:HD21	1	0.02	0.02
(1,2812)	1:B:50:MET:HE3	1:B:81:LEU:HD22	1	0.02	0.02
(1,2812)	1:B:50:MET:HE3	1:B:81:LEU:HD23	1	0.02	0.02
(1,2773)	1:B:50:MET:HG3	1:B:78:LEU:HD11	1	0.01	0.01
(1,2773)	1:B:50:MET:HG3	1:B:78:LEU:HD12	1	0.01	0.01
(1,2773)	1:B:50:MET:HG3	1:B:78:LEU:HD13	1	0.01	0.01
(1,2680)	1:B:9:ARG:HG2	1:B:48:ASN:HA	1	0.09	0.09
(1,2679)	1:A:9:ARG:HG2	1:A:48:ASN:HA	1	0.14	0.14
(1,2638)	1:B:10:ILE:H	1:B:46:THR:HG21	1	0.02	0.02
(1,2638)	1:B:10:ILE:H	1:B:46:THR:HG22	1	0.02	0.02
(1,2638)	1:B:10:ILE:H	1:B:46:THR:HG23	1	0.02	0.02
(1,2637)	1:A:10:ILE:H	1:A:46:THR:HG21	1	0.02	0.02
(1,2637)	1:A:10:ILE:H	1:A:46:THR:HG22	1	0.02	0.02
(1,2637)	1:A:10:ILE:H	1:A:46:THR:HG23	1	0.02	0.02
(1,2615)	1:A:41:LYS:HE2	1:A:46:THR:HG21	1	0.02	0.02
(1,2615)	1:A:41:LYS:HE2	1:A:46:THR:HG22	1	0.02	0.02
(1,2615)	1:A:41:LYS:HE2	1:A:46:THR:HG23	1	0.02	0.02
(1,2615)	1:A:41:LYS:HE3	1:A:46:THR:HG21	1	0.02	0.02
(1,2615)	1:A:41:LYS:HE3	1:A:46:THR:HG22	1	0.02	0.02
(1,2615)	1:A:41:LYS:HE3	1:A:46:THR:HG23	1	0.02	0.02
(1,2591)	1:A:44:ILE:HD11	1:A:73:PHE:HZ	1	0.03	0.03
(1,2591)	1:A:44:ILE:HD12	1:A:73:PHE:HZ	1	0.03	0.03
(1,2591)	1:A:44:ILE:HD13	1:A:73:PHE:HZ	1	0.03	0.03
(1,2587)	1:A:44:ILE:HA	1:A:44:ILE:HD11	1	0.01	0.01
(1,2587)	1:A:44:ILE:HA	1:A:44:ILE:HD12	1	0.01	0.01
(1,2587)	1:A:44:ILE:HA	1:A:44:ILE:HD13	1	0.01	0.01
(1,2571)	1:A:14:ASP:H	1:A:44:ILE:HG21	1	0.03	0.03
(1,2571)	1:A:14:ASP:H	1:A:44:ILE:HG22	1	0.03	0.03
(1,2571)	1:A:14:ASP:H	1:A:44:ILE:HG23	1	0.03	0.03
(1,2537)	1:A:44:ILE:HG12	1:A:45:PHE:H	1	0.04	0.04
(1,2527)	1:A:12:GLY:H	1:A:44:ILE:HB	1	0.01	0.01
(1,2502)	1:B:15:LYS:H	1:B:40:ALA:HB1	1	0.07	0.07
(1,2502)	1:B:15:LYS:H	1:B:40:ALA:HB2	1	0.07	0.07
(1,2502)	1:B:15:LYS:H	1:B:40:ALA:HB3	1	0.07	0.07
(1,2418)	1:B:38:LEU:HD11	1:B:45:PHE:HZ	1	0.02	0.02
(1,2418)	1:B:38:LEU:HD12	1:B:45:PHE:HZ	1	0.02	0.02
(1,2418)	1:B:38:LEU:HD13	1:B:45:PHE:HZ	1	0.02	0.02
(1,2399)	1:A:38:LEU:HD11	1:A:47:CYS:HG	1	0.01	0.01
(1,2399)	1:A:38:LEU:HD12	1:A:47:CYS:HG	1	0.01	0.01
(1,2399)	1:A:38:LEU:HD13	1:A:47:CYS:HG	1	0.01	0.01
(1,2385)	1:A:37:VAL:HG21	1:A:48:ASN:H	1	0.02	0.02



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2385)	1:A:37:VAL:HG22	1:A:48:ASN:H	1	0.02	0.02
(1,2385)	1:A:37:VAL:HG23	1:A:48:ASN:H	1	0.02	0.02
(1,237)	1:B:19:THR:H	1:B:40:ALA:HB1	1	0.02	0.02
(1,237)	1:B:19:THR:H	1:B:40:ALA:HB2	1	0.02	0.02
(1,237)	1:B:19:THR:H	1:B:40:ALA:HB3	1	0.02	0.02
(1,2365)	1:A:37:VAL:HG21	1:A:48:ASN:HB3	1	0.01	0.01
(1,2365)	1:A:37:VAL:HG22	1:A:48:ASN:HB3	1	0.01	0.01
(1,2365)	1:A:37:VAL:HG23	1:A:48:ASN:HB3	1	0.01	0.01
(1,2346)	1:B:37:VAL:HG11	1:B:48:ASN:HB3	1	0.03	0.03
(1,2346)	1:B:37:VAL:HG12	1:B:48:ASN:HB3	1	0.03	0.03
(1,2346)	1:B:37:VAL:HG13	1:B:48:ASN:HB3	1	0.03	0.03
(1,2345)	1:A:37:VAL:HG11	1:A:48:ASN:HB3	1	0.04	0.04
(1,2345)	1:A:37:VAL:HG12	1:A:48:ASN:HB3	1	0.04	0.04
(1,2345)	1:A:37:VAL:HG13	1:A:48:ASN:HB3	1	0.04	0.04
(1,2330)	1:B:36:ILE:HD11	1:B:38:LEU:H	1	0.07	0.07
(1,2330)	1:B:36:ILE:HD12	1:B:38:LEU:H	1	0.07	0.07
(1,2330)	1:B:36:ILE:HD13	1:B:38:LEU:H	1	0.07	0.07
(1,2329)	1:A:36:ILE:HD11	1:A:38:LEU:H	1	0.02	0.02
(1,2329)	1:A:36:ILE:HD12	1:A:38:LEU:H	1	0.02	0.02
(1,2329)	1:A:36:ILE:HD13	1:A:38:LEU:H	1	0.02	0.02
(1,2326)	1:B:23:THR:H	1:B:36:ILE:HD11	1	0.01	0.01
(1,2326)	1:B:23:THR:H	1:B:36:ILE:HD12	1	0.01	0.01
(1,2326)	1:B:23:THR:H	1:B:36:ILE:HD13	1	0.01	0.01
(1,2316)	1:B:23:THR:HG1	1:B:36:ILE:HD11	1	0.06	0.06
(1,2316)	1:B:23:THR:HG1	1:B:36:ILE:HD12	1	0.06	0.06
(1,2316)	1:B:23:THR:HG1	1:B:36:ILE:HD13	1	0.06	0.06
(1,2288)	1:B:35:THR:HB	1:B:36:ILE:HG21	1	0.02	0.02
(1,2288)	1:B:35:THR:HB	1:B:36:ILE:HG22	1	0.02	0.02
(1,2288)	1:B:35:THR:HB	1:B:36:ILE:HG23	1	0.02	0.02
(1,2287)	1:A:35:THR:HB	1:A:36:ILE:HG21	1	0.01	0.01
(1,2287)	1:A:35:THR:HB	1:A:36:ILE:HG22	1	0.01	0.01
(1,2287)	1:A:35:THR:HB	1:A:36:ILE:HG23	1	0.01	0.01
(1,2243)	1:A:20:ASN:HD21	1:B:33:ILE:HD11	1	0.03	0.03
(1,2243)	1:A:20:ASN:HD21	1:B:33:ILE:HD12	1	0.03	0.03
(1,2243)	1:A:20:ASN:HD21	1:B:33:ILE:HD13	1	0.03	0.03
(1,2238)	1:A:33:ILE:HD11	1:B:20:ASN:HA	1	0.01	0.01
(1,2238)	1:A:33:ILE:HD12	1:B:20:ASN:HA	1	0.01	0.01
(1,2238)	1:A:33:ILE:HD13	1:B:20:ASN:HA	1	0.01	0.01
(1,2201)	1:A:31:THR:HG21	1:A:52:PHE:H	1	0.01	0.01
(1,2201)	1:A:31:THR:HG22	1:A:52:PHE:H	1	0.01	0.01
(1,2201)	1:A:31:THR:HG23	1:A:52:PHE:H	1	0.01	0.01
(1,2188)	1:B:31:THR:HG21	1:B:51:ILE:HD11	1	0.03	0.03



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(1,2188) 1:B:31:THR:HG21 1:B:51:ILE:HD13 1 0.03 0.03 (1,2188) 1:B:31:THR:HG22 1:B:51:ILE:HD11 1 0.03 0.03 (1,2188) 1:B:31:THR:HG22 1:B:51:ILE:HD12 1 0.03 0.03 (1,2188) 1:B:31:THR:HG22 1:B:51:ILE:HD13 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD11 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD13 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD13 1 0.03 0.03 (1,2178) 1:B:28:LYS:HA 1:B:28:LYS:HB2 1 0.16 0.16 (1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HB2 1 0.01 0.01 (1,2167) 1:A:28:LYS:HA 1:A:28:LYS:HB3 1 0.01 0.01 (1,2167) 1:A:28:LYS:HA 1:A:28:LYS:HG3 1 0.01 0.01 (1,2167) 1:A:28:LYS:HA 1:A:28:LYS:HB3 1 0.01	Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2188) 1:B:31:THR:HG22 1:B:51:ILE:HD11 1 0.03 0.03 (1,2188) 1:B:31:THR:HG22 1:B:51:ILE:HD12 1 0.03 0.03 (1,2188) 1:B:31:THR:HG22 1:B:51:ILE:HD13 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD11 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD11 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD11 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD12 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD13 1 0.03 0.03 (1,2188) 1:B:32:TYR:HG23 1:B:51:ILE:HD13 1 0.03 0.03 (1,2178) 1:B:28:LYS:HA 1:B:28:LYS:HE2 1 0.16 0.16 0.16 (1,2177) 1:A:28:LYS:HA 1:B:28:LYS:HE2 1 0.16 0.16 0.16 (1,2177) 1:A:28:LYS:HA 1:B:28:LYS:HE2 1 0.01 0.01 0.01 (1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HE3 1 0.01 0.01 0.01 (1,2167) 1:A:27:SER:HG 1:A:28:LYS:HG3 1 0.01 0.01 (1,2167) 1:A:28:LYS:HA 1:B:28:LYS:HG3 1 0.06 0.16 (1,2162) 1:B:28:LYS:HA 1:B:28:LYS:HG3 1 0.06 0.16 (1,2162) 1:B:28:LYS:HA 1:B:28:LYS:HG2 1 0.24 0.24 (1,216) 1:A:38:MET:H 1:A:18:MET:HG3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG21 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.00 0.00 (1,2147) 1:A:23:THR:HG22 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.00 0.00 0.00 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.00 0.00 0.00 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.00 0.00 0.00 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.00 0.00 0.00 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.00 0.00 0.00 (1,2009) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.00 0.00 0.00 0.00 (1,2009) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00	(1,2188)	1:B:31:THR:HG21	1:B:51:ILE:HD12	1	0.03	0.03
(1,2188) 1:B:31:THR:HG22 1:B:51:ILE:HD12 1 0.03 0.03 (1,2188) 1:B:31:THR:HG22 1:B:51:ILE:HD13 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD11 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD12 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD13 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD13 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD13 1 0.06 0.06 (1,2178) 1:B:28:IVS:HA 1:B:28:IVS:HE2 1 0.16 0.16 0.16 (1,2178) 1:B:28:IVS:HA 1:B:28:IVS:HE3 1 0.16 0.16 0.16 (1,2177) 1:A:28:IVS:HA 1:B:28:IVS:HE3 1 0.16 0.16 0.16 (1,2177) 1:A:28:IVS:HA 1:A:28:IVS:HE3 1 0.01 0.01 (1,2177) 1:A:28:IVS:HA 1:A:28:IVS:HE3 1 0.01 0.01 (1,2167) 1:A:27:SER:HG 1:A:28:IVS:HG3 1 0.16 0.16 (1,2162) 1:B:28:IVS:HA 1:B:28:IVS:HG3 1 0.01 0.01 (1,2161) 1:A:28:IWS:HA 1:A:28:IVS:HG3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG21 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG21 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.00 0.00 (1,2140) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.09 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.09 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:IVS:HE3 1 0.09 0.09 0.	(1,2188)	1:B:31:THR:HG21	1:B:51:ILE:HD13	1	0.03	0.03
(1,2188) 1:B:31:THR:HG22 1:B:51:ILE:HD13 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD11 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD12 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD12 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD13 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD13 1 0.06 0.06 (1,2178) 1:B:28:LYS:HA 1:B:28:LYS:HE2 1 0.16 0.16 0.16 (1,2178) 1:B:28:LYS:HA 1:B:28:LYS:HE3 1 0.16 0.16 (1,2177) 1:A:28:I.YS:HA 1:B:28:LYS:HE3 1 0.01 0.01 (1,2177) 1:A:28:I.YS:HA 1:A:28:I.YS:HE3 1 0.01 0.01 (1,2177) 1:A:28:I.YS:HA 1:A:28:I.YS:HE3 1 0.01 0.01 (1,2167) 1:A:27:SER:HG 1:A:28:I.YS:HG3 1 0.01 0.01 (1,2167) 1:A:27:SER:HG 1:A:28:I.YS:HG3 1 0.01 0.01 (1,2162) 1:B:28:LYS:HA 1:B:28:LYS:HG2 1 0.24 0.24 (1,216) 1:A:18:MET:H 1:A:18:MET:HG3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG21 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG22 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD2 1 0.00 0.00 0.00 (1,2009) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.00 0.00 0.00 (1,2009) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00	(1,2188)	1:B:31:THR:HG22	1:B:51:ILE:HD11	1	0.03	0.03
(1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD11 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD12 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD13 1 0.03 0.03 (1,2178) 1:B:28:LYS:HA 1:B:28:LYS:HE2 1 0.16 0.16 (1,2178) 1:B:28:LYS:HA 1:B:28:LYS:HE2 1 0.16 0.16 (1,2178) 1:B:28:LYS:HA 1:B:28:LYS:HE2 1 0.01 0.01 (1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HE2 1 0.01 0.01 (1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HE2 1 0.01 0.01 (1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HE2 1 0.01 0.01 (1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HE3 1 0.01 0.01 (1,2167) 1:A:28:LYS:HA 1:A:28:LYS:HG3 1 0.16 0.16 (1,2162) 1:B:28:LYS:HA 1:B:28:LYS:HG3 1 0.16 0.16 (1,2162) 1:B:28:LYS:HA 1:B:28:LYS:HG2 1 0.24 0.24 (1,216) 1:A:28:MET:H 1:A:18:MET:HG3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG21 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD1 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:29:PHE:HD1 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:29:PHE:HD1 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:29:PHE:HD2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE3	(1,2188)	1:B:31:THR:HG22	1:B:51:ILE:HD12	1	0.03	0.03
(1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD12 1 0.03 0.03 (1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD13 1 0.03 0.03 (1,2178) 1:B:28:LYS:HA 1:B:28:LYS:HE2 1 0.16 0.16 (1,2177) 1:B:28:LYS:HA 1:B:28:LYS:HE2 1 0.16 0.16 (1,2177) 1:A:28:LYS:HA 1:B:28:LYS:HE3 1 0.16 0.16 (1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HE3 1 0.01 0.01 (1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HE3 1 0.01 0.01 (1,2167) 1:A:28:LYS:HA 1:A:28:LYS:HG3 1 0.16 0.16 (1,2167) 1:A:28:LYS:HA 1:A:28:LYS:HG3 1 0.16 0.16 (1,2162) 1:B:28:LYS:HA 1:B:28:LYS:HG3 1 0.16 0.16 (1,2162) 1:B:28:LYS:HA 1:B:28:LYS:HG2 1 0.24 0.24 0.24 (1,216) 1:A:18:MET:H 1:A:18:MET:HG3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG21 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG22 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG22 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2143) 1:A:20:ASN:HD22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.00 0.00 (1,2009) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.00 0.00 (1,2009) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.00 0.00 0.00 (1,2009) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.00 0.00 0.00 (1,2009) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00	(1,2188)	1:B:31:THR:HG22	1:B:51:ILE:HD13	1	0.03	0.03
(1,2188) 1:B:31:THR:HG23 1:B:51:ILE:HD13 1 0.03 0.03 (1,2178) 1:B:28:LYS:HA 1:B:28:LYS:HE2 1 0.16 0.16 (1,2178) 1:B:28:LYS:HA 1:B:28:LYS:HE3 1 0.16 0.16 (1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HE3 1 0.16 0.16 (1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HE3 1 0.01 0.01 (1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HE3 1 0.01 0.01 (1,2167) 1:A:28:LYS:HA 1:A:28:LYS:HE3 1 0.01 0.01 (1,2167) 1:A:28:LYS:HA 1:A:28:LYS:HG3 1 0.16 0.16 (1,2162) 1:B:28:LYS:HA 1:B:28:LYS:HG2 1 0.24 0.24 (1,216) 1:A:18:MET:H 1:A:18:MET:HG3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG21 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG22 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.00 0.00 0.00 (1,2089) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00	(1,2188)	1:B:31:THR:HG23	1:B:51:ILE:HD11	1	0.03	0.03
(1,2178) 1:B:28:LYS:HA 1:B:28:LYS:HE2 1 0.16 0.16 (1,2178) 1:B:28:LYS:HA 1:B:28:LYS:HB3 1 0.16 0.16 (1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HB3 1 0.01 0.01 (1,2167) 1:A:27:SER:HG 1:A:28:LYS:HG3 1 0.16 0.16 (1,2162) 1:B:28:LYS:HA 1:B:28:LYS:HG2 1 0.24 0.24 (1,216) 1:A:38:MET:H 1:A:18:MET:HG3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG21 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.00 0.00 0.00 (1,2089) 1:A:25:VAL:HG23 1:A:28:LVS:HE3 1 0.00 0.00 0.00 (1,2089) 1:A:25:VAL:HG23 1:A:28:LVS:HE3 1 0.00 0.00 0.0	(1,2188)	1:B:31:THR:HG23	1:B:51:ILE:HD12	1	0.03	0.03
(1,2178) 1:B:28:LYS:HA 1:B:28:LYS:HE3 1 0.16 0.16 (1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HE2 1 0.01 0.01 (1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HE3 1 0.01 0.01 (1,2167) 1:A:28:LYS:HG 1:A:28:LYS:HG3 1 0.16 0.16 (1,2162) 1:B:28:LYS:HA 1:B:28:LYS:HG3 1 0.01 0.01 (1,2161) 1:A:18:MET:H 1:A:18:MET:HG3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG21 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG21 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG22 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG22 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG22 1:A:27:SER:HB2 1 0.04 0	(1,2188)	1:B:31:THR:HG23	1:B:51:ILE:HD13	1	0.03	0.03
(1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HE2 1 0.01 0.01 (1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HE3 1 0.01 0.01 (1,2167) 1:A:27:SER:HG 1:A:28:LYS:HG3 1 0.16 0.16 (1,2162) 1:B:28:LYS:HA 1:B:28:LYS:HG2 1 0.24 0.24 (1,216) 1:A:18:MET;H 1:A:18:MET;HG3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG21 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG21 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:29:THE:HG23 1:A:27:SER:HB2 1 0.04	(1,2178)	1:B:28:LYS:HA	1:B:28:LYS:HE2	1	0.16	0.16
(1,2177) 1:A:28:LYS:HA 1:A:28:LYS:HE3 1 0.01 0.01 (1,2167) 1:A:27:SER:HG 1:A:28:LYS:HG3 1 0.16 0.16 (1,2162) 1:B:28:LYS:HA 1:B:28:LYS:HG2 1 0.24 0.24 (1,216) 1:A:18:MET:H 1:A:18:MET:HG3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG21 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG21 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 <t< td=""><td>(1,2178)</td><td>1:B:28:LYS:HA</td><td>1:B:28:LYS:HE3</td><td>1</td><td>0.16</td><td>0.16</td></t<>	(1,2178)	1:B:28:LYS:HA	1:B:28:LYS:HE3	1	0.16	0.16
(1,2167) 1:A:27:SER:HG 1:A:28:LYS:HG3 1 0.16 0.16 (1,2162) 1:B:28:LYS:HA 1:B:28:LYS:HG2 1 0.24 0.24 (1,216) 1:A:18:MET:H 1:A:18:MET:HG3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG21 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG21 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG22 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG22 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2140) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02	(1,2177)	1:A:28:LYS:HA	1:A:28:LYS:HE2	1	0.01	0.01
(1,2162) 1:B:28:LYS:HA 1:B:28:LYS:HG2 1 0.24 0.24 (1,216) 1:A:18:MET:H 1:A:18:MET:HG3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG21 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG21 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG22 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02	(1,2177)	1:A:28:LYS:HA	1:A:28:LYS:HE3	1	0.01	0.01
(1,216) 1:A:18:MET:H 1:A:18:MET:HG3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG21 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG21 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG22 1:B:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG22 1:B:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:B:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:B:29:PHE:HD1 1 0.02	(1,2167)	1:A:27:SER:HG	1:A:28:LYS:HG3	1	0.16	0.16
(1,2151) 1:A:23:THR:HG21 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG21 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG22 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2143) 1:A:20:ASN:HD22 1:B:27:SER:HB2 1 0.04 0.04 (1,2143) 1:A:20:ASN:HD22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD2 1 0.02 0.02 (1,2000) 1:B:25:VAL:HG23 1:B:29:PHE:HD2 1 0.02	(1,2162)	1:B:28:LYS:HA	1:B:28:LYS:HG2	1	0.24	0.24
(1,2151) 1:A:23:THR:HG22 1:A:27:SER:HB3 1 0.01 0.01 (1,2151) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG21 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG22 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2143) 1:A:20:ASN:HD22 1:B:27:SER:HB2 1 0.04 0.04 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2099) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD1 1 0.03	(1,216)	1:A:18:MET:H	1:A:18:MET:HG3	1	0.01	0.01
(1,2151) 1:A:23:THR:HG23 1:A:27:SER:HB3 1 0.01 0.01 (1,2147) 1:A:23:THR:HG21 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG22 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2143) 1:A:20:ASN:HD22 1:B:27:SER:HA 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2099) 1:A:25:VAL:HG23 1:B:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD1 1 0.03	(1,2151)	1:A:23:THR:HG21	1:A:27:SER:HB3	1	0.01	0.01
(1,2147) 1:A:23:THR:HG21 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG22 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2143) 1:A:20:ASN:HD22 1:B:25:SER:HA 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2000) 1:B:25:VAL:HG23 1:B:29:PHE:HD2 1 0.02 0.02 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD1 1 0.03	(1,2151)	1:A:23:THR:HG22	1:A:27:SER:HB3	1	0.01	0.01
(1,2147) 1:A:23:THR:HG22 1:A:27:SER:HB2 1 0.04 0.04 (1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2143) 1:A:20:ASN:HD22 1:B:27:SER:HA 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD2 1 0.02 0.02 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03	(1,2151)	1:A:23:THR:HG23	1:A:27:SER:HB3	1	0.01	0.01
(1,2147) 1:A:23:THR:HG23 1:A:27:SER:HB2 1 0.04 0.04 (1,2143) 1:A:20:ASN:HD22 1:B:27:SER:HA 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD2 1 0.02 0.02 (1,2099) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03	(1,2147)	1:A:23:THR:HG21	1:A:27:SER:HB2	1	0.04	0.04
(1,2143) 1:A:20:ASN:HD22 1:B:27:SER:HA 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD2 1 0.02 0.02 (1,2099) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03	(1,2147)	1:A:23:THR:HG22	1:A:27:SER:HB2	1	0.04	0.04
(1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD2 1 0.02 0.02 (1,2099) 1:A:25:VAL:HG23 1:B:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03	(1,2147)	1:A:23:THR:HG23	1:A:27:SER:HB2	1	0.04	0.04
(1,2100) 1:B:25:VAL:HG21 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD2 1 0.02 0.02 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD2 1 0.03 0.03 (1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE2 1 0.09	(1,2143)	1:A:20:ASN:HD22	1:B:27:SER:HA	1	0.02	0.02
(1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD2 1 0.02 0.02 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD2 1 0.03 0.03 (1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE3 1 0.09	(1,2100)	1:B:25:VAL:HG21	1:B:29:PHE:HD1	1	0.02	0.02
(1,2100) 1:B:25:VAL:HG22 1:B:29:PHE:HD2 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD2 1 0.02 0.02 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD2 1 0.03 0.03 (1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09	(1,2100)	1:B:25:VAL:HG21	1:B:29:PHE:HD2	1	0.02	0.02
(1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD1 1 0.02 0.02 (1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD2 1 0.02 0.02 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09	(1,2100)	1:B:25:VAL:HG22	1:B:29:PHE:HD1	1	0.02	0.02
(1,2100) 1:B:25:VAL:HG23 1:B:29:PHE:HD2 1 0.02 0.02 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD2 1 0.03 0.03 (1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09	(1,2100)	1:B:25:VAL:HG22	1:B:29:PHE:HD2	1	0.02	0.02
(1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD2 1 0.03 0.03 (1,2089) 1:A:25:VAL:HG23 1:A:29:PHE:HD2 1 0.03 0.03 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09	(1,2100)	1:B:25:VAL:HG23	1:B:29:PHE:HD1	1	0.02	0.02
(1,2099) 1:A:25:VAL:HG21 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD2 1 0.03 0.03 (1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2084) 1:B:25:VAL:HG11 1:B:69:VAL:H 1 0.01 0.01	(1,2100)	1:B:25:VAL:HG23	1:B:29:PHE:HD2	1	0.02	0.02
(1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD2 1 0.03 0.03 (1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2084) 1:B:25:VAL:HG11 1:B:69:VAL:H 1 0.01 0.01	(1,2099)	1:A:25:VAL:HG21	1:A:29:PHE:HD1	1	0.03	0.03
(1,2099) 1:A:25:VAL:HG22 1:A:29:PHE:HD2 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD2 1 0.03 0.03 (1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2084) 1:B:25:VAL:HG11 1:B:69:VAL:H 1 0.01 0.01	(1,2099)	1:A:25:VAL:HG21	1:A:29:PHE:HD2	1	0.03	0.03
(1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD1 1 0.03 0.03 (1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD2 1 0.03 0.03 (1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2084) 1:B:25:VAL:HG11 1:B:69:VAL:H 1 0.01 0.01	(1,2099)	1:A:25:VAL:HG22	1:A:29:PHE:HD1	1	0.03	0.03
(1,2099) 1:A:25:VAL:HG23 1:A:29:PHE:HD2 1 0.03 0.03 (1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2084) 1:B:25:VAL:HG11 1:B:69:VAL:H 1 0.01 0.01	(1,2099)	1:A:25:VAL:HG22	1:A:29:PHE:HD2	1	0.03	0.03
(1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2084) 1:B:25:VAL:HG11 1:B:69:VAL:H 1 0.01 0.01	(1,2099)	1:A:25:VAL:HG23	1:A:29:PHE:HD1	1	0.03	0.03
(1,2089) 1:A:25:VAL:HG21 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2084) 1:B:25:VAL:HG11 1:B:69:VAL:H 1 0.01 0.01	(1,2099)	1:A:25:VAL:HG23	1:A:29:PHE:HD2	1	0.03	0.03
(1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2084) 1:B:25:VAL:HG11 1:B:69:VAL:H 1 0.01 0.01	(1,2089)	1:A:25:VAL:HG21	1:A:28:LYS:HE2	1	0.09	0.09
(1,2089) 1:A:25:VAL:HG22 1:A:28:LYS:HE3 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2084) 1:B:25:VAL:HG11 1:B:69:VAL:H 1 0.01 0.01	(1,2089)	1:A:25:VAL:HG21	1:A:28:LYS:HE3	1	0.09	0.09
(1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE2 1 0.09 0.09 (1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2084) 1:B:25:VAL:HG11 1:B:69:VAL:H 1 0.01 0.01	(1,2089)	1:A:25:VAL:HG22	1:A:28:LYS:HE2	1	0.09	0.09
(1,2089) 1:A:25:VAL:HG23 1:A:28:LYS:HE3 1 0.09 0.09 (1,2084) 1:B:25:VAL:HG11 1:B:69:VAL:H 1 0.01 0.01	(1,2089)	1:A:25:VAL:HG22	1:A:28:LYS:HE3	1	0.09	0.09
(1,2084) 1:B:25:VAL:HG11 1:B:69:VAL:H 1 0.01 0.01	(1,2089)	1:A:25:VAL:HG23	1:A:28:LYS:HE2	1	0.09	0.09
	(1,2089)	1:A:25:VAL:HG23	1:A:28:LYS:HE3	1	0.09	0.09
(1,2084) 1:B:25:VAL:HG12 1:B:69:VAL:H 1 0.01 0.01	(1,2084)	1:B:25:VAL:HG11	1:B:69:VAL:H	1	0.01	0.01
	(1,2084)	1:B:25:VAL:HG12	1:B:69:VAL:H	1	0.01	0.01



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2084)	1:B:25:VAL:HG13	1:B:69:VAL:H	1	0.01	0.01
(1,2067)	1:A:25:VAL:HG11	1:A:28:LYS:HD3	1	0.02	0.02
(1,2067)	1:A:25:VAL:HG12	1:A:28:LYS:HD3	1	0.02	0.02
(1,2067)	1:A:25:VAL:HG13	1:A:28:LYS:HD3	1	0.02	0.02
(1,2052)	1:B:67:ARG:HE	1:B:75:VAL:HG11	1	0.09	0.09
(1,2052)	1:B:67:ARG:HE	1:B:75:VAL:HG12	1	0.09	0.09
(1,2052)	1:B:67:ARG:HE	1:B:75:VAL:HG13	1	0.09	0.09
(1,2019)	1:A:22:ILE:HA	1:A:22:ILE:HD11	1	0.01	0.01
(1,2019)	1:A:22:ILE:HA	1:A:22:ILE:HD12	1	0.01	0.01
(1,2019)	1:A:22:ILE:HA	1:A:22:ILE:HD13	1	0.01	0.01
(1,2007)	1:A:22:ILE:HD11	1:A:69:VAL:HG21	1	0.03	0.03
(1,2007)	1:A:22:ILE:HD11	1:A:69:VAL:HG22	1	0.03	0.03
(1,2007)	1:A:22:ILE:HD11	1:A:69:VAL:HG23	1	0.03	0.03
(1,2007)	1:A:22:ILE:HD12	1:A:69:VAL:HG21	1	0.03	0.03
(1,2007)	1:A:22:ILE:HD12	1:A:69:VAL:HG22	1	0.03	0.03
(1,2007)	1:A:22:ILE:HD12	1:A:69:VAL:HG23	1	0.03	0.03
(1,2007)	1:A:22:ILE:HD13	1:A:69:VAL:HG21	1	0.03	0.03
(1,2007)	1:A:22:ILE:HD13	1:A:69:VAL:HG22	1	0.03	0.03
(1,2007)	1:A:22:ILE:HD13	1:A:69:VAL:HG23	1	0.03	0.03
(1,1937)	1:B:19:THR:HG21	1:B:22:ILE:HB	1	0.02	0.02
(1,1937)	1:B:19:THR:HG22	1:B:22:ILE:HB	1	0.02	0.02
(1,1937)	1:B:19:THR:HG23	1:B:22:ILE:HB	1	0.02	0.02
(1,1936)	1:A:19:THR:HG21	1:A:22:ILE:HB	1	0.03	0.03
(1,1936)	1:A:19:THR:HG22	1:A:22:ILE:HB	1	0.03	0.03
(1,1936)	1:A:19:THR:HG23	1:A:22:ILE:HB	1	0.03	0.03
(1,1873)	1:B:18:MET:HE1	1:B:70:GLN:H	1	0.02	0.02
(1,1873)	1:B:18:MET:HE2	1:B:70:GLN:H	1	0.02	0.02
(1,1873)	1:B:18:MET:HE3	1:B:70:GLN:H	1	0.02	0.02
(1,1864)	1:A:18:MET:HE1	1:A:45:PHE:HE1	1	0.01	0.01
(1,1864)	1:A:18:MET:HE1	1:A:45:PHE:HE2	1	0.01	0.01
(1,1864)	1:A:18:MET:HE2	1:A:45:PHE:HE1	1	0.01	0.01
(1,1864)	1:A:18:MET:HE2	1:A:45:PHE:HE2	1	0.01	0.01
(1,1864)	1:A:18:MET:HE3	1:A:45:PHE:HE1	1	0.01	0.01
(1,1864)	1:A:18:MET:HE3	1:A:45:PHE:HE2	1	0.01	0.01
(1,1844)	1:B:17:GLY:H	1:B:18:MET:HG3	1	0.01	0.01
(1,1825)	1:B:15:LYS:HA	1:B:15:LYS:HE2	1	0.01	0.01
(1,1825)	1:B:15:LYS:HA	1:B:15:LYS:HE3	1	0.01	0.01
(1,1816)	1:A:15:LYS:HG2	1:A:15:LYS:HE2	1	0.02	0.02
(1,1816)	1:A:15:LYS:HG2	1:A:15:LYS:HE3	1	0.02	0.02
(1,1816)	1:A:15:LYS:HG3	1:A:15:LYS:HE2	1	0.02	0.02
(1,1816)	1:A:15:LYS:HG3	1:A:15:LYS:HE3	1	0.02	0.02
	1:B:15:LYS:HD2	1:B:71:GLY:HA2	1	0.02	0.02



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1807)	1:B:15:LYS:HD3	1:B:71:GLY:HA2	1	0.02	0.02
(1,1795)	1:B:14:ASP:HA	1:B:15:LYS:HB3	1	0.11	0.11
(1,1793)	1:B:15:LYS:HB3	1:B:16:ASN:HB2	1	0.03	0.03
(1,1775)	1:B:13:GLU:HG2	1:B:44:ILE:HA	1	0.03	0.03
(1,1775)	1:B:13:GLU:HG3	1:B:44:ILE:HA	1	0.03	0.03
(1,1774)	1:A:13:GLU:HG2	1:A:44:ILE:HA	1	0.01	0.01
(1,1774)	1:A:13:GLU:HG3	1:A:44:ILE:HA	1	0.01	0.01
(1,1707)	1:B:11:VAL:HG11	1:B:41:LYS:HE2	1	0.02	0.02
(1,1707)	1:B:11:VAL:HG11	1:B:41:LYS:HE3	1	0.02	0.02
(1,1707)	1:B:11:VAL:HG12	1:B:41:LYS:HE2	1	0.02	0.02
(1,1707)	1:B:11:VAL:HG12	1:B:41:LYS:HE3	1	0.02	0.02
(1,1707)	1:B:11:VAL:HG13	1:B:41:LYS:HE2	1	0.02	0.02
(1,1707)	1:B:11:VAL:HG13	1:B:41:LYS:HE3	1	0.02	0.02
(1,170)	1:B:15:LYS:H	1:B:18:MET:HB2	1	0.02	0.02
(1,170)	1:B:15:LYS:H	1:B:18:MET:HB3	1	0.02	0.02
(1,1691)	1:B:11:VAL:HG21	1:B:46:THR:HB	1	0.05	0.05
(1,1691)	1:B:11:VAL:HG22	1:B:46:THR:HB	1	0.05	0.05
(1,1691)	1:B:11:VAL:HG23	1:B:46:THR:HB	1	0.05	0.05
(1,1677)	1:B:10:ILE:HD11	1:B:49:LEU:H	1	0.01	0.01
(1,1677)	1:B:10:ILE:HD12	1:B:49:LEU:H	1	0.01	0.01
(1,1677)	1:B:10:ILE:HD13	1:B:49:LEU:H	1	0.01	0.01
(1,1676)	1:A:10:ILE:HD11	1:A:49:LEU:H	1	0.01	0.01
(1,1676)	1:A:10:ILE:HD12	1:A:49:LEU:H	1	0.01	0.01
(1,1676)	1:A:10:ILE:HD13	1:A:49:LEU:H	1	0.01	0.01
(1,1667)	1:B:10:ILE:HD11	1:B:11:VAL:H	1	0.01	0.01
(1,1667)	1:B:10:ILE:HD12	1:B:11:VAL:H	1	0.01	0.01
(1,1667)	1:B:10:ILE:HD13	1:B:11:VAL:H	1	0.01	0.01
(1,1666)	1:A:10:ILE:HD11	1:A:11:VAL:H	1	0.03	0.03
(1,1666)	1:A:10:ILE:HD12	1:A:11:VAL:H	1	0.03	0.03
(1,1666)	1:A:10:ILE:HD13	1:A:11:VAL:H	1	0.03	0.03
(1,1631)	1:B:9:ARG:HA	1:B:10:ILE:HG21	1	0.02	0.02
(1,1631)	1:B:9:ARG:HA	1:B:10:ILE:HG22	1	0.02	0.02
(1,1631)	1:B:9:ARG:HA	1:B:10:ILE:HG23	1	0.02	0.02
(1,161)	1:B:13:GLU:H	1:B:73:PHE:H	1	0.05	0.05
(1,160)	1:A:13:GLU:H	1:A:73:PHE:H	1	0.01	0.01
(1,1579)	1:B:9:ARG:HD2	1:B:76:GLU:HG2	1	0.05	0.05
(1,1579)	1:B:9:ARG:HD2	1:B:76:GLU:HG3	1	0.05	0.05
(1,1579)	1:B:9:ARG:HD3	1:B:76:GLU:HG2	1	0.05	0.05
(1,1579)	1:B:9:ARG:HD3	1:B:76:GLU:HG3	1	0.05	0.05
(1,1550)	1:B:23:THR:HA	1:B:26:ILE:HD11	1	0.01	0.01
(1,1550)	1:B:23:THR:HA	1:B:26:ILE:HD12	1	0.01	0.01
(1,1550)	1:B:23:THR:HA	1:B:26:ILE:HD13	1	0.01	0.01



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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1517)	1:A:8:ILE:HG21	1:A:63:MET:HG2	1	0.01	0.01
(1,1517)	1:A:8:ILE:HG21	1:A:63:MET:HG3	1	0.01	0.01
(1,1517)	1:A:8:ILE:HG22	1:A:63:MET:HG2	1	0.01	0.01
(1,1517)	1:A:8:ILE:HG22	1:A:63:MET:HG3	1	0.01	0.01
(1,1517)	1:A:8:ILE:HG23	1:A:63:MET:HG2	1	0.01	0.01
(1,1517)	1:A:8:ILE:HG23	1:A:63:MET:HG3	1	0.01	0.01
(1,151)	1:B:13:GLU:H	1:B:44:ILE:HA	1	0.01	0.01
(1,1477)	1:A:5:LEU:HD21	1:A:51:ILE:HA	1	0.01	0.01
(1,1477)	1:A:5:LEU:HD22	1:A:51:ILE:HA	1	0.01	0.01
(1,1477)	1:A:5:LEU:HD23	1:A:51:ILE:HA	1	0.01	0.01
(1,144)	1:A:13:GLU:H	1:A:13:GLU:HG2	1	0.01	0.01
(1,144)	1:A:13:GLU:H	1:A:13:GLU:HG3	1	0.01	0.01
(1,1429)	1:A:5:LEU:HG	1:A:52:PHE:HE1	1	0.01	0.01
(1,1429)	1:A:5:LEU:HG	1:A:52:PHE:HE2	1	0.01	0.01
(1,1358)	1:B:81:LEU:HA	1:B:82:GLU:H	1	0.05	0.05
(1,1339)	1:A:81:LEU:H	1:A:81:LEU:HD11	1	0.02	0.02
(1,1339)	1:A:81:LEU:H	1:A:81:LEU:HD12	1	0.02	0.02
(1,1339)	1:A:81:LEU:H	1:A:81:LEU:HD13	1	0.02	0.02
(1,1309)	1:A:77:ARG:H	1:A:77:ARG:HD2	1	0.04	0.04
(1,1309)	1:A:77:ARG:H	1:A:77:ARG:HD3	1	0.04	0.04
(1,13)	1:A:4:PHE:H	1:A:54:LYS:HA	1	0.05	0.05
(1,1265)	1:A:74:THR:HG21	1:A:75:VAL:H	1	0.01	0.01
(1,1265)	1:A:74:THR:HG22	1:A:75:VAL:H	1	0.01	0.01
(1,1265)	1:A:74:THR:HG23	1:A:75:VAL:H	1	0.01	0.01
(1,1245)	1:A:74:THR:H	1:A:75:VAL:HG21	1	0.03	0.03
(1,1245)	1:A:74:THR:H	1:A:75:VAL:HG22	1	0.03	0.03
(1,1245)	1:A:74:THR:H	1:A:75:VAL:HG23	1	0.03	0.03
(1,1224)	1:B:69:VAL:HG21	1:B:72:VAL:H	1	0.03	0.03
(1,1224)	1:B:69:VAL:HG22	1:B:72:VAL:H	1	0.03	0.03
(1,1224)	1:B:69:VAL:HG23	1:B:72:VAL:H	1	0.03	0.03
(1,1156)	1:B:67:ARG:HE	1:B:75:VAL:H	1	0.1	0.1
(1,1139)	1:A:67:ARG:H	1:A:67:ARG:HE	1	0.01	0.01
(1,1134)	1:B:67:ARG:H	1:B:67:ARG:HD2	1	0.08	0.08
(1,1134)	1:B:67:ARG:H	1:B:67:ARG:HD3	1	0.08	0.08
(1,1123)	1:A:67:ARG:H	1:A:69:VAL:HG21	1	0.02	0.02
(1,1123)	1:A:67:ARG:H	1:A:69:VAL:HG22	1	0.02	0.02
(1,1123)	1:A:67:ARG:H	1:A:69:VAL:HG23	1	0.02	0.02
(1,1047)	1:B:58:LYS:HZ1	1:B:62:LEU:H	1	0.01	0.01
(1,1047)	1:B:58:LYS:HZ2	1:B:62:LEU:H	1	0.01	0.01
(1,1047)	1:B:58:LYS:HZ3	1:B:62:LEU:H	1	0.01	0.01
(1,1046)	1:A:58:LYS:HZ1	1:A:62:LEU:H	1	0.02	0.02
(1,1046)	1:A:58:LYS:HZ2	1:A:62:LEU:H	1	0.02	0.02



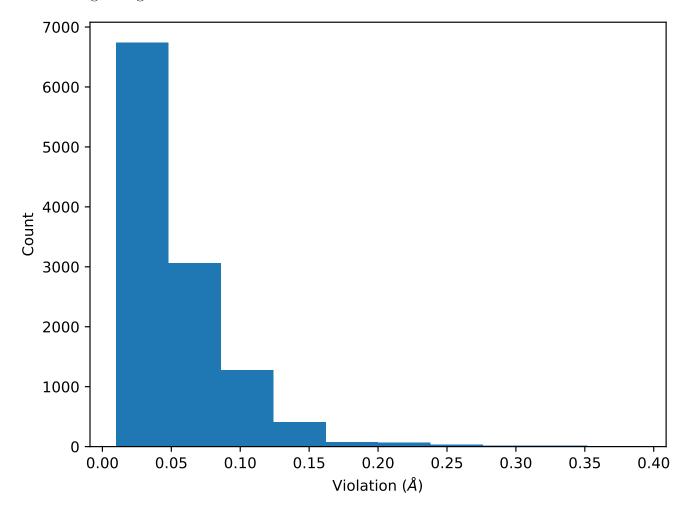
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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1046)	1:A:58:LYS:HZ3	1:A:62:LEU:H	1	0.02	0.02

8.8 All distance violations

8.8.1 Histogram : Distribution of distance violations

The following histogram shows the distribution of violations in the ensemble.



8.8.2 Table : All distance violations

The following table lists the violations in the ensemble sorted by violation value

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4050)	1:A:41:LYS:HA	1:A:42:ASP:H	1	0.39
(1,4051)	1:B:41:LYS:HA	1:B:42:ASP:H	13	0.37



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4715)	1:A:81:LEU:H	1:A:82:GLU:HG2	2	0.36
(1,4715)	1:A:81:LEU:H	1:A:82:GLU:HG3	2	0.36
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	5	0.36
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE2	18	0.34
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE3	18	0.34
(1,4715)	1:A:81:LEU:H	1:A:82:GLU:HG2	18	0.33
(1,4715)	1:A:81:LEU:H	1:A:82:GLU:HG3	18	0.33
(1,4036)	1:A:15:LYS:HA	1:A:17:GLY:H	18	0.33
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	1	0.33
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	1	0.33
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	19	0.33
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	19	0.33
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE2	15	0.33
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE3	15	0.33
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	3	0.32
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	3	0.32
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	3	0.32
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	3	0.32
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	10	0.3
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	10	0.3
(1,4036)	1:A:15:LYS:HA	1:A:17:GLY:H	20	0.29
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	8	0.29
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	8	0.29
(1,4715)	1:A:81:LEU:H	1:A:82:GLU:HG2	14	0.28
(1,4715)	1:A:81:LEU:H	1:A:82:GLU:HG3	14	0.28
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	14	0.28
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	14	0.28
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	14	0.28
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	14	0.28
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE2	8	0.28
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE3	8	0.28
(1,4036)	1:A:15:LYS:HA	1:A:17:GLY:H	1	0.27
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	16	0.27
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	16	0.27
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	1	0.27
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	1	0.27
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	1	0.26
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	1	0.26
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	1	0.26
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	1	0.26
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	8	0.26
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG11	15	0.26



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG12	15	0.26
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG13	15	0.26
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG11	15	0.26
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG12	15	0.26
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG13	15	0.26
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	3	0.26
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	3	0.26
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	10	0.26
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	10	0.26
(1,5014)	1:B:81:LEU:H	1:B:82:GLU:HG2	7	0.25
(1,5014)	1:B:81:LEU:H	1:B:82:GLU:HG3	7	0.25
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	15	0.25
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	15	0.25
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	15	0.25
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	15	0.25
(1,3622)	1:B:69:VAL:HA	1:B:70:GLN:HG2	7	0.25
(1,3622)	1:B:69:VAL:HA	1:B:70:GLN:HG3	7	0.25
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	11	0.24
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	11	0.24
(1,2162)	1:B:28:LYS:HA	1:B:28:LYS:HG2	12	0.24
(1,176)	1:B:15:LYS:H	1:B:18:MET:HG2	14	0.24
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	7	0.23
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	7	0.23
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	7	0.23
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	7	0.23
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	15	0.23
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	15	0.23
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	15	0.23
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	15	0.23
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	18	0.23
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	18	0.23
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	18	0.23
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	18	0.23
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	19	0.23
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	19	0.23
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	19	0.23
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	19	0.23
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	2	0.23
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	2	0.23
(1,3397)	1:B:60:THR:HG21	1:B:63:MET:HE1	3	0.23
(1,3397)	1:B:60:THR:HG21	1:B:63:MET:HE2	3	0.23
(1,3397)	1:B:60:THR:HG21	1:B:63:MET:HE3	3	0.23



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Key		Atom-2	Model	Violation (Å)
(1,3397)	1:B:60:THR:HG22	1:B:63:MET:HE1	3	0.23
(1,3397)	1:B:60:THR:HG22	1:B:63:MET:HE2	3	0.23
(1,3397)	1:B:60:THR:HG22	1:B:63:MET:HE3	3	0.23
(1,3397)	1:B:60:THR:HG23	1:B:63:MET:HE1	3	0.23
(1,3397)	1:B:60:THR:HG23	1:B:63:MET:HE2	3	0.23
(1,3397)	1:B:60:THR:HG23	1:B:63:MET:HE3	3	0.23
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	1	0.22
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE1	14	0.22
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE2	14	0.22
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE3	14	0.22
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE1	14	0.22
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE2	14	0.22
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE3	14	0.22
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE1	14	0.22
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE2	14	0.22
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE3	14	0.22
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	13	0.21
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	5	0.21
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	5	0.21
(1,3103)	1:A:54:LYS:HE2	1:A:55:ASN:HD21	19	0.21
(1,3103)	1:A:54:LYS:HE3	1:A:55:ASN:HD21	19	0.21
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	6	0.21
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	6	0.21
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	6	0.21
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	13	0.21
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	13	0.21
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	13	0.21
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	4	0.21
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	4	0.21
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	4	0.21
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	4	0.2
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	4	0.2
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	4	0.2
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	4	0.2
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	14	0.2
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	14	0.2
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	14	0.2
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	14	0.2
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE2	1	0.2
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE3	1	0.2
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	3	0.2
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	3	0.2



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	3	0.2
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	1	0.19
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	1	0.19
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	1	0.19
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	1	0.19
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	11	0.19
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	11	0.19
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	11	0.19
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	11	0.19
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	6	0.19
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	6	0.19
(1,3484)	1:B:41:LYS:HE2	1:B:44:ILE:H	2	0.19
(1,3484)	1:B:41:LYS:HE3	1:B:44:ILE:H	2	0.19
(1,277)	1:A:20:ASN:H	1:A:20:ASN:HD22	13	0.19
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	8	0.19
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	8	0.19
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	8	0.19
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	10	0.19
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	10	0.19
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	10	0.19
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	12	0.19
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	12	0.19
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	12	0.19
(1,545)	1:A:29:PHE:HD1	1:A:31:THR:H	4	0.18
(1,545)	1:A:29:PHE:HD2	1:A:31:THR:H	4	0.18
(1,545)	1:A:29:PHE:HD1	1:A:31:THR:H	17	0.18
(1,545)	1:A:29:PHE:HD2	1:A:31:THR:H	17	0.18
(1,4719)	1:B:3:ASP:HB2	1:B:52:PHE:HD1	12	0.18
(1,4719)	1:B:3:ASP:HB2	1:B:52:PHE:HD2	12	0.18
(1,4719)	1:B:3:ASP:HB3	1:B:52:PHE:HD1	12	0.18
(1,4719)	1:B:3:ASP:HB3	1:B:52:PHE:HD2	12	0.18
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG11	14	0.18
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG12	14	0.18
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG13	14	0.18
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG11	14	0.18
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG12	14	0.18
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG13	14	0.18
(1,278)	1:B:20:ASN:H	1:B:20:ASN:HD22	7	0.18
(1,277)	1:A:20:ASN:H	1:A:20:ASN:HD22	14	0.18
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG21	14	0.18
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG22	14	0.18
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG23	14	0.18



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	6	0.18
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	6	0.18
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	6	0.18
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	8	0.18
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	8	0.18
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	8	0.18
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	3	0.18
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	3	0.18
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	3	0.18
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	15	0.18
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	15	0.18
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	15	0.18
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	11	0.17
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	11	0.17
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	11	0.17
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	7	0.17
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	7	0.17
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	7	0.17
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	7	0.17
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	7	0.17
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	7	0.17
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	7	0.17
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	7	0.17
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	7	0.17
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG21	6	0.17
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG22	6	0.17
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG23	6	0.17
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	19	0.17
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	7	0.17
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	7	0.17
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	7	0.17
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG21	17	0.17
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG22	17	0.17
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG23	17	0.17
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG21	17	0.17
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG22	17	0.17
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG23	17	0.17
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB2	7	0.16
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB3	7	0.16
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB2	7	0.16
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB3	7	0.16
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	16	0.16



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	16	0.16
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	16	0.16
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	16	0.16
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	20	0.16
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	20	0.16
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	20	0.16
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	20	0.16
(1,4405)	1:A:3:ASP:HB2	1:A:4:PHE:H	17	0.16
(1,4405)	1:A:3:ASP:HB3	1:A:4:PHE:H	17	0.16
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE1	2	0.16
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE2	2	0.16
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE3	2	0.16
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE1	2	0.16
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE2	2	0.16
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE3	2	0.16
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE1	2	0.16
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE2	2	0.16
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE3	2	0.16
(1,3106)	1:B:54:LYS:H	1:B:54:LYS:HE2	12	0.16
(1,3106)	1:B:54:LYS:H	1:B:54:LYS:HE3	12	0.16
(1,278)	1:B:20:ASN:H	1:B:20:ASN:HD22	12	0.16
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG21	5	0.16
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG22	5	0.16
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG23	5	0.16
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	9	0.16
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	9	0.16
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	9	0.16
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	7	0.16
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	7	0.16
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	7	0.16
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	9	0.16
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	1	0.16
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	1	0.16
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	1	0.16
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	18	0.16
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	18	0.16
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	18	0.16
(1,2178)	1:B:28:LYS:HA	1:B:28:LYS:HE2	12	0.16
(1,2178)	1:B:28:LYS:HA	1:B:28:LYS:HE3	12	0.16
(1,2167)	1:A:27:SER:HG	1:A:28:LYS:HG3	20	0.16
(1,1814)	1:A:68:LYS:HE2	1:A:69:VAL:HG21	1	0.16
(1,1814)	1:A:68:LYS:HE2	1:A:69:VAL:HG22	1	0.16



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(1,1814) 1:A:68:LYS:HE2 1:A:69:VAL:HG23 1 0.16 (1,1814) 1:A:68:LYS:HE3 1:A:69:VAL:HG21 1 0.16 (1,1814) 1:A:68:LYS:HE3 1:A:69:VAL:HG22 1 0.16 (1,1814) 1:A:68:LYS:HE3 1:A:69:VAL:HG23 1 0.16 (1,1814) 1:A:68:LYS:HE3 1:A:69:VAL:HG23 1 0.16 (1,1837) 1:A:8:ILE:HD11 1:A:62:LEU:HD21 4 0.16 (1,1537) 1:A:8:ILE:HD11 1:A:62:LEU:HD23 4 0.16 (1,1537) 1:A:8:ILE:HD12 1:A:62:LEU:HD21 4 0.16 (1,1537) 1:A:8:ILE:HD12 1:A:62:LEU:HD22 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD23 4 0.16 (1,1537) 1:B:58:LYS:HZ3 <th></th>	
(1,1814) 1:A:68:LYS:HE3 1:A:69:VAL:HG22 1 0.16 (1,1814) 1:A:68:LYS:HE3 1:A:69:VAL:HG23 1 0.16 (1,1537) 1:A:8:ILE:HD11 1:A:62:LEU:HD21 4 0.16 (1,1537) 1:A:8:ILE:HD11 1:A:62:LEU:HD22 4 0.16 (1,1537) 1:A:8:ILE:HD11 1:A:62:LEU:HD23 4 0.16 (1,1537) 1:A:8:ILE:HD12 1:A:62:LEU:HD21 4 0.16 (1,1537) 1:A:8:ILE:HD12 1:A:62:LEU:HD22 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD23 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD21 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD22 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD23 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD23 4 0.16 (1,1021) 1:B:58:LYS:HZ3 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ3 1:B:6	
(1,1814) 1:A:68:LYS:HE3 1:A:69:VAL:HG23 1 0.16 (1,1537) 1:A:8:ILE:HD11 1:A:62:LEU:HD21 4 0.16 (1,1537) 1:A:8:ILE:HD11 1:A:62:LEU:HD22 4 0.16 (1,1537) 1:A:8:ILE:HD11 1:A:62:LEU:HD23 4 0.16 (1,1537) 1:A:8:ILE:HD12 1:A:62:LEU:HD21 4 0.16 (1,1537) 1:A:8:ILE:HD12 1:A:62:LEU:HD22 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD23 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD21 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD22 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD23 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ1 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ2 1:B:61:THR:H 4 0.16 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG21 19 0.15 (1,4745) 1:B:9:ARG:HG2 <	
(1,1537) 1:A:8:ILE:HD11 1:A:62:LEU:HD21 4 0.16 (1,1537) 1:A:8:ILE:HD11 1:A:62:LEU:HD22 4 0.16 (1,1537) 1:A:8:ILE:HD11 1:A:62:LEU:HD23 4 0.16 (1,1537) 1:A:8:ILE:HD12 1:A:62:LEU:HD21 4 0.16 (1,1537) 1:A:8:ILE:HD12 1:A:62:LEU:HD22 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD23 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD21 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD22 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD22 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD23 4 0.16 (1,1021) 1:B:58:LYS:HZ1 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ2 1:B:61:THR:H 4 0.16 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG21 19 0.15 (1,4745) 1:B:9:ARG:HG2 1:B:11:VA	
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(1,1537) 1:A:8:ILE:HD12 1:A:62:LEU:HD22 4 0.16 (1,1537) 1:A:8:ILE:HD12 1:A:62:LEU:HD23 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD21 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD22 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD23 4 0.16 (1,1021) 1:B:58:LYS:HZ1 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ2 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ3 1:B:61:THR:H 4 0.16 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG21 19 0.15 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG22 19 0.15	
(1,1537) 1:A:8:ILE:HD12 1:A:62:LEU:HD23 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD21 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD22 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD23 4 0.16 (1,1021) 1:B:58:LYS:HZ1 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ2 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ3 1:B:61:THR:H 4 0.16 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG21 19 0.15 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG22 19 0.15	
(1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD21 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD22 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD23 4 0.16 (1,1021) 1:B:58:LYS:HZ1 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ2 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ3 1:B:61:THR:H 4 0.16 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG21 19 0.15 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG22 19 0.15	
(1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD22 4 0.16 (1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD23 4 0.16 (1,1021) 1:B:58:LYS:HZ1 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ2 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ3 1:B:61:THR:H 4 0.16 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG21 19 0.15 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG22 19 0.15	
(1,1537) 1:A:8:ILE:HD13 1:A:62:LEU:HD23 4 0.16 (1,1021) 1:B:58:LYS:HZ1 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ2 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ3 1:B:61:THR:H 4 0.16 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG21 19 0.15 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG22 19 0.15	
(1,1021) 1:B:58:LYS:HZ1 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ2 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ3 1:B:61:THR:H 4 0.16 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG21 19 0.15 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG22 19 0.15	
(1,1021) 1:B:58:LYS:HZ2 1:B:61:THR:H 4 0.16 (1,1021) 1:B:58:LYS:HZ3 1:B:61:THR:H 4 0.16 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG21 19 0.15 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG22 19 0.15	
(1,1021) 1:B:58:LYS:HZ3 1:B:61:THR:H 4 0.16 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG21 19 0.15 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG22 19 0.15	
(1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG21 19 0.15 (1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG22 19 0.15	
(1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG22 19 0.15	
(1,4745) 1:B:9:ARG:HG2 1:B:11:VAL:HG23 19 0.15	
(1,4745) 1:B:9:ARG:HG3 1:B:11:VAL:HG21 19 0.15	
(1,4745) 1:B:9:ARG:HG3 1:B:11:VAL:HG22 19 0.15	
(1,4745) 1:B:9:ARG:HG3 1:B:11:VAL:HG23 19 0.15	
(1,4643) 1:A:54:LYS:HE2 1:A:55:ASN:HD21 1 0.15	
(1,4643) 1:A:54:LYS:HE2 1:A:55:ASN:HD22 1 0.15	
(1,4643) 1:A:54:LYS:HE3 1:A:55:ASN:HD21 1 0.15	
(1,4643) 1:A:54:LYS:HE3 1:A:55:ASN:HD22 1 0.15	
(1,4591) 1:A:37:VAL:HG11 1:A:39:ASN:HD21 10 0.15	
(1,4591) 1:A:37:VAL:HG11 1:A:39:ASN:HD22 10 0.15	
(1,4591) 1:A:37:VAL:HG12 1:A:39:ASN:HD21 10 0.15	
(1,4591) 1:A:37:VAL:HG12 1:A:39:ASN:HD22 10 0.15	
(1,4591) 1:A:37:VAL:HG13 1:A:39:ASN:HD21 10 0.15	
(1,4591) 1:A:37:VAL:HG13 1:A:39:ASN:HD22 10 0.15	
(1,4397) 1:B:82:GLU:HA 1:B:83:HIS:HD2 5 0.15	
(1,4037) 1:B:15:LYS:HA 1:B:17:GLY:H 17 0.15	
(1,3994) 1:A:82:GLU:H 1:A:83:HIS:HB3 2 0.15	
(1,3569) 1:A:15:LYS:HD2 1:A:69:VAL:HG11 19 0.15	
(1,3569) 1:A:15:LYS:HD2 1:A:69:VAL:HG12 19 0.15	
(1,3569) 1:A:15:LYS:HD2 1:A:69:VAL:HG13 19 0.15	
(1,3569) 1:A:15:LYS:HD3 1:A:69:VAL:HG11 19 0.15	
(1,3569) 1:A:15:LYS:HD3 1:A:69:VAL:HG12 19 0.15	
(1,3569) 1:A:15:LYS:HD3 1:A:69:VAL:HG13 19 0.15	
(1,3103) 1:A:54:LYS:HE2 1:A:55:ASN:HD21 20 0.15	



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3103)	1:A:54:LYS:HE3	1:A:55:ASN:HD21	20	0.15
(1,3099)	1:A:54:LYS:H	1:A:54:LYS:HD2	15	0.15
(1,3099)	1:A:54:LYS:H	1:A:54:LYS:HD3	15	0.15
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	10	0.15
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	10	0.15
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	10	0.15
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	10	0.15
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	10	0.15
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	10	0.15
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	10	0.15
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	10	0.15
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	10	0.15
(1,278)	1:B:20:ASN:H	1:B:20:ASN:HD22	14	0.15
, ,	1:B:44:ILE:HD11	1:B:45:PHE:H	10	0.15
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	10	0.15
	1:B:44:ILE:HD13	1:B:45:PHE:H	10	0.15
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	18	0.15
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	18	0.15
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	18	0.15
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	4	0.15
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	4	0.15
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	4	0.15
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	11	0.15
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	11	0.15
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	11	0.15
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	2	0.15
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	3	0.15
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	17	0.15
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	17	0.15
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	3	0.15
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	3	0.15
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	3	0.15
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	14	0.15
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	14	0.15
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	14	0.15
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	14	0.15
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	14	0.15
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	14	0.15
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	15	0.15
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	15	0.15
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	15	0.15
(1,1378)	1:B:40:ALA:H	1:B:41:LYS:HD2	13	0.15



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1378)	1:B:40:ALA:H	1:B:41:LYS:HD3	13	0.15
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	2	0.14
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	2	0.14
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	2	0.14
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	2	0.14
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	17	0.14
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	17	0.14
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	17	0.14
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	17	0.14
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	18	0.14
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	18	0.14
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	18	0.14
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	18	0.14
	1:A:55:ASN:HD21	1:A:57:ASP:HB2	15	0.14
(1,4647)	1:A:55:ASN:HD21	1:A:57:ASP:HB3	15	0.14
(1,4647)	1:A:55:ASN:HD22	1:A:57:ASP:HB2	15	0.14
(1,4647)	1:A:55:ASN:HD22	1:A:57:ASP:HB3	15	0.14
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD21	2	0.14
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD22	2	0.14
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD21	2	0.14
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD22	2	0.14
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD21	2	0.14
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD22	2	0.14
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	9	0.14
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	9	0.14
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	9	0.14
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	9	0.14
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	10	0.14
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	10	0.14
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	10	0.14
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	10	0.14
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	6	0.14
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	14	0.14
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	14	0.14
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	14	0.14
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	14	0.14
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	16	0.14
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	16	0.14
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	16	0.14
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	17	0.14
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	17	0.14
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	17	0.14



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	10	0.14
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	10	0.14
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	10	0.14
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB2	9	0.14
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB3	9	0.14
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	12	0.14
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	12	0.14
(1,3480)	1:B:65:LYS:HA	1:B:65:LYS:HE2	15	0.14
(1,3480)	1:B:65:LYS:HA	1:B:65:LYS:HE3	15	0.14
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	2	0.14
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	2	0.14
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	2	0.14
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE1	1	0.14
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE2	1	0.14
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE3	1	0.14
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE1	12	0.14
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE2	12	0.14
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE3	12	0.14
(1,3100)	1:B:54:LYS:H	1:B:54:LYS:HD2	4	0.14
(1,3100)	1:B:54:LYS:H	1:B:54:LYS:HD3	4	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	13	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	13	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	13	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	13	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	13	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	13	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	13	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	13	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	13	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	14	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	14	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	14	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	14	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	14	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	14	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	14	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	14	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	14	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	19	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	19	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	19	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	19	0.14



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	19	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	19	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	19	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	19	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	19	0.14
(1,294)	1:A:33:ILE:HG13	1:B:20:ASN:HD22	15	0.14
(1,278)	1:B:20:ASN:H	1:B:20:ASN:HD22	11	0.14
(1,277)	1:A:20:ASN:H	1:A:20:ASN:HD22	16	0.14
(1,2679)	1:A:9:ARG:HG2	1:A:48:ASN:HA	9	0.14
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG21	19	0.14
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG22	19	0.14
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG23	19	0.14
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	3	0.14
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	3	0.14
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	3	0.14
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	13	0.14
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	13	0.14
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	13	0.14
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	17	0.14
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	17	0.14
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	17	0.14
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	18	0.14
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	18	0.14
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	18	0.14
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	20	0.14
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	5	0.14
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	7	0.14
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	7	0.14
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	7	0.14
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	2	0.14
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	2	0.14
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	2	0.14
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	12	0.14
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	12	0.14
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	12	0.14
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	8	0.14
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	8	0.14
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	8	0.14
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	13	0.14
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	13	0.14
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	13	0.14
(1,2174)	1:B:68:LYS:HA	1:B:68:LYS:HD2	15	0.14



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	9	0.14
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	18	0.14
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	14	0.14
(1,1809)	1:B:11:VAL:HG21	1:B:41:LYS:HE2	15	0.14
(1,1809)	1:B:11:VAL:HG21	1:B:41:LYS:HE3	15	0.14
(1,1809)	1:B:11:VAL:HG22	1:B:41:LYS:HE2	15	0.14
(1,1809)	1:B:11:VAL:HG22	1:B:41:LYS:HE3	15	0.14
(1,1809)	1:B:11:VAL:HG23	1:B:41:LYS:HE2	15	0.14
(1,1809)	1:B:11:VAL:HG23	1:B:41:LYS:HE3	15	0.14
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG11	4	0.14
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG12	4	0.14
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG13	4	0.14
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG11	4	0.14
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG12	4	0.14
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG13	4	0.14
(1,175)	1:A:15:LYS:H	1:A:18:MET:HG2	2	0.14
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	19	0.14
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	19	0.14
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	19	0.14
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	19	0.14
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	19	0.14
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	19	0.14
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	19	0.14
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	19	0.14
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	19	0.14
(1,1377)	1:A:40:ALA:H	1:A:41:LYS:HD2	1	0.14
(1,1377)	1:A:40:ALA:H	1:A:41:LYS:HD3	1	0.14
(1,545)	1:A:29:PHE:HD1	1:A:31:THR:H	20	0.13
(1,545)	1:A:29:PHE:HD2	1:A:31:THR:H	20	0.13
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	12	0.13
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	12	0.13
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	12	0.13
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	12	0.13
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	12	0.13
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	12	0.13
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	12	0.13
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	12	0.13
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	12	0.13
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	12	0.13
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	17	0.13
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	17	0.13
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	17	0.13



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	2	0.13
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	2	0.13
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	2	0.13
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	4	0.13
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	4	0.13
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	4	0.13
(1,4053)	1:B:41:LYS:HG2	1:B:42:ASP:HA	14	0.13
(1,4053)	1:B:41:LYS:HG3	1:B:42:ASP:HA	14	0.13
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	18	0.13
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	10	0.13
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	10	0.13
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	10	0.13
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	5	0.13
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	5	0.13
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	5	0.13
(1,3622)	1:B:69:VAL:HA	1:B:70:GLN:HG2	13	0.13
(1,3622)	1:B:69:VAL:HA	1:B:70:GLN:HG3	13	0.13
(1,3621)	1:A:69:VAL:HA	1:A:70:GLN:HG2	7	0.13
(1,3621)	1:A:69:VAL:HA	1:A:70:GLN:HG3	7	0.13
(1,3606)	1:B:69:VAL:HG11	1:B:70:GLN:HB2	14	0.13
(1,3606)	1:B:69:VAL:HG11	1:B:70:GLN:HB3	14	0.13
(1,3606)	1:B:69:VAL:HG12	1:B:70:GLN:HB2	14	0.13
(1,3606)	1:B:69:VAL:HG12	1:B:70:GLN:HB3	14	0.13
(1,3606)	1:B:69:VAL:HG13	1:B:70:GLN:HB2	14	0.13
(1,3606)	1:B:69:VAL:HG13	1:B:70:GLN:HB3	14	0.13
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG11	17	0.13
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG12	17	0.13
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG13	17	0.13
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG11	17	0.13
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG12	17	0.13
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG13	17	0.13
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG11	20	0.13
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG12	20	0.13
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG13	20	0.13
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG11	20	0.13
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG12	20	0.13
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG13	20	0.13
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	10	0.13
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	10	0.13
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	10	0.13
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	18	0.13
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	18	0.13



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	18	0.13
, ,	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	18	0.13
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	18	0.13
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	18	0.13
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	18	0.13
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	18	0.13
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	18	0.13
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	2	0.13
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	2	0.13
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	2	0.13
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	2	0.13
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	2	0.13
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	2	0.13
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	2	0.13
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	2	0.13
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	2	0.13
(1,277)	1:A:20:ASN:H	1:A:20:ASN:HD22	7	0.13
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	20	0.13
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	20	0.13
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	20	0.13
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	5	0.13
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	7	0.13
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	9	0.13
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	11	0.13
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	12	0.13
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	13	0.13
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	15	0.13
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	4	0.13
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	20	0.13
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	20	0.13
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	20	0.13
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	10	0.13
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	10	0.13
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	10	0.13
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	20	0.13
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	20	0.13
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	20	0.13
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	7	0.13
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	7	0.13
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	7	0.13
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	15	0.13
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	15	0.13



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	15	0.13
(1,2173)	1:A:68:LYS:HA	1:A:68:LYS:HD2	10	0.13
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	17	0.13
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	17	0.13
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	17	0.13
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	13	0.13
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	16	0.13
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	19	0.13
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	8	0.13
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG21	1	0.13
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG22	1	0.13
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG23	1	0.13
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG21	1	0.13
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG22	1	0.13
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG23	1	0.13
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	5	0.13
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	5	0.13
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	5	0.13
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	13	0.13
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	13	0.13
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	13	0.13
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	13	0.13
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	13	0.13
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	13	0.13
(1,1020)	1:A:58:LYS:HZ1	1:A:61:THR:H	3	0.13
(1,1020)	1:A:58:LYS:HZ2	1:A:61:THR:H	3	0.13
(1,1020)	1:A:58:LYS:HZ3	1:A:61:THR:H	3	0.13
(1,82)	1:A:9:ARG:HE	1:A:11:VAL:HG21	10	0.12
(1,82)	1:A:9:ARG:HE	1:A:11:VAL:HG22	10	0.12
(1,82)	1:A:9:ARG:HE	1:A:11:VAL:HG23	10	0.12
(1,727)	1:B:41:LYS:HB2	1:B:42:ASP:H	13	0.12
(1,727)	1:B:41:LYS:HB3	1:B:42:ASP:H	13	0.12
(1,563)	1:A:32:ASN:HD21	1:A:33:ILE:HB	15	0.12
(1,5002)	1:B:69:VAL:HG11	1:B:70:GLN:HE21	17	0.12
(1,5002)	1:B:69:VAL:HG11	1:B:70:GLN:HE22	17	0.12
(1,5002)	1:B:69:VAL:HG12	1:B:70:GLN:HE21	17	0.12
(1,5002)	1:B:69:VAL:HG12	1:B:70:GLN:HE22	17	0.12
(1,5002)	1:B:69:VAL:HG13	1:B:70:GLN:HE21	17	0.12
(1,5002)	1:B:69:VAL:HG13	1:B:70:GLN:HE22	17	0.12
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE1	8	0.12
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE2	8	0.12
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE3	8	0.12



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE1	8	0.12
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE2	8	0.12
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE3	8	0.12
(1,4851)	1:B:31:THR:HG21	1:B:58:LYS:HE2	20	0.12
(1,4851)	1:B:31:THR:HG21	1:B:58:LYS:HE3	20	0.12
(1,4851)	1:B:31:THR:HG22	1:B:58:LYS:HE2	20	0.12
(1,4851)	1:B:31:THR:HG22	1:B:58:LYS:HE3	20	0.12
(1,4851)	1:B:31:THR:HG23	1:B:58:LYS:HE2	20	0.12
(1,4851)	1:B:31:THR:HG23	1:B:58:LYS:HE3	20	0.12
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	5	0.12
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	5	0.12
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	5	0.12
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	5	0.12
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	13	0.12
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	13	0.12
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	13	0.12
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	13	0.12
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD21	11	0.12
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD22	11	0.12
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD21	11	0.12
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD22	11	0.12
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD21	11	0.12
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD22	11	0.12
(1,4560)	1:A:31:THR:HG21	1:A:58:LYS:HE2	14	0.12
(1,4560)	1:A:31:THR:HG21	1:A:58:LYS:HE3	14	0.12
(1,4560)	1:A:31:THR:HG22	1:A:58:LYS:HE2	14	0.12
(1,4560)	1:A:31:THR:HG22	1:A:58:LYS:HE3	14	0.12
(1,4560)	1:A:31:THR:HG23	1:A:58:LYS:HE2	14	0.12
(1,4560)	1:A:31:THR:HG23	1:A:58:LYS:HE3	14	0.12
(1,4538)	1:A:27:SER:HG	1:A:28:LYS:HD2	2	0.12
(1,4538)	1:A:27:SER:HG	1:A:28:LYS:HD3	2	0.12
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	16	0.12
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	16	0.12
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	16	0.12
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	16	0.12
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	16	0.12
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	16	0.12
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	5	0.12
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	5	0.12
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	5	0.12
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	5	0.12
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	15	0.12



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	15	0.12
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	15	0.12
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	1	0.12
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	1	0.12
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	1	0.12
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	11	0.12
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	11	0.12
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	11	0.12
(1,4127)	1:B:83:HIS:HA	1:B:83:HIS:HB3	5	0.12
(1,4073)	1:B:60:THR:HB	1:B:61:THR:H	3	0.12
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	20	0.12
(1,3994)	1:A:82:GLU:H	1:A:83:HIS:HB3	17	0.12
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	6	0.12
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	6	0.12
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	6	0.12
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	7	0.12
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	7	0.12
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	7	0.12
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	9	0.12
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	9	0.12
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	9	0.12
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	18	0.12
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	18	0.12
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	18	0.12
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	12	0.12
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	12	0.12
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	12	0.12
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	20	0.12
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	20	0.12
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	20	0.12
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB2	11	0.12
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB3	11	0.12
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG11	4	0.12
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG12	4	0.12
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG13	4	0.12
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG11	4	0.12
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG12	4	0.12
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG13	4	0.12
(1,3560)	1:B:15:LYS:HE2	1:B:16:ASN:HD21	6	0.12
(1,3560)	1:B:15:LYS:HE3	1:B:16:ASN:HD21	6	0.12
(1,3559)	1:A:15:LYS:HE2	1:A:16:ASN:HD21	7	0.12
(1,3559)	1:A:15:LYS:HE3	1:A:16:ASN:HD21	7	0.12



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3484)	1:B:41:LYS:HE2	1:B:44:ILE:H	9	0.12
(1,3484)	1:B:41:LYS:HE3	1:B:44:ILE:H	9	0.12
(1,3410)	1:A:63:MET:HE1	1:A:77:ARG:HA	4	0.12
(1,3410)	1:A:63:MET:HE2	1:A:77:ARG:HA	4	0.12
(1,3410)	1:A:63:MET:HE3	1:A:77:ARG:HA	4	0.12
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	15	0.12
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	15	0.12
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	15	0.12
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG21	2	0.12
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG22	2	0.12
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG23	2	0.12
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG21	2	0.12
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG22	2	0.12
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG23	2	0.12
(1,3098)	1:B:15:LYS:HD2	1:B:16:ASN:HD21	13	0.12
(1,3098)	1:B:15:LYS:HD3	1:B:16:ASN:HD21	13	0.12
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	3	0.12
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	3	0.12
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	3	0.12
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	3	0.12
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	3	0.12
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	3	0.12
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	3	0.12
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	3	0.12
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	3	0.12
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	5	0.12
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	5	0.12
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	5	0.12
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	5	0.12
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	5	0.12
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	5	0.12
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	5	0.12
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	5	0.12
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	5	0.12
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	17	0.12
(1,278)	1:B:20:ASN:H	1:B:20:ASN:HD22	4	0.12
(1,278)	1:B:20:ASN:H	1:B:20:ASN:HD22	18	0.12
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG21	12	0.12
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG22	12	0.12
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG23	12	0.12
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	4	0.12
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	4	0.12



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	4	0.12
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	19	0.12
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	19	0.12
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	19	0.12
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	10	0.12
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	15	0.12
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	19	0.12
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	4	0.12
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	4	0.12
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	4	0.12
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	18	0.12
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	18	0.12
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	18	0.12
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	10	0.12
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	10	0.12
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	10	0.12
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	5	0.12
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	5	0.12
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	5	0.12
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	7	0.12
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	7	0.12
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	7	0.12
(1,2164)	1:B:27:SER:HG	1:B:28:LYS:HG2	5	0.12
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	1	0.12
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	5	0.12
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	15	0.12
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	9	0.12
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	13	0.12
(1,1813)	1:B:25:VAL:HG21	1:B:65:LYS:HE2	15	0.12
(1,1813)	1:B:25:VAL:HG21	1:B:65:LYS:HE3	15	0.12
(1,1813)	1:B:25:VAL:HG22	1:B:65:LYS:HE2	15	0.12
(1,1813)	1:B:25:VAL:HG22	1:B:65:LYS:HE3	15	0.12
(1,1813)	1:B:25:VAL:HG23	1:B:65:LYS:HE2	15	0.12
(1,1813)	1:B:25:VAL:HG23	1:B:65:LYS:HE3	15	0.12
(1,1808)	1:A:11:VAL:HG21	1:A:41:LYS:HE2	11	0.12
(1,1808)	1:A:11:VAL:HG21	1:A:41:LYS:HE3	11	0.12
(1,1808)	1:A:11:VAL:HG22	1:A:41:LYS:HE2	11	0.12
(1,1808)	1:A:11:VAL:HG22	1:A:41:LYS:HE3	11	0.12
(1,1808)	1:A:11:VAL:HG23	1:A:41:LYS:HE2	11	0.12
(1,1808)	1:A:11:VAL:HG23	1:A:41:LYS:HE3	11	0.12
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	2	0.12
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	2	0.12



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	2	0.12
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	3	0.12
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	3	0.12
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	3	0.12
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	18	0.12
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	18	0.12
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	18	0.12
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	18	0.12
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	18	0.12
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	18	0.12
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	18	0.12
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	18	0.12
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	18	0.12
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	10	0.12
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	10	0.12
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	10	0.12
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	10	0.12
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	10	0.12
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	10	0.12
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	10	0.12
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	10	0.12
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	10	0.12
(1,718)	1:A:41:LYS:H	1:A:46:THR:H	11	0.11
(1,545)	1:A:29:PHE:HD1	1:A:31:THR:H	3	0.11
(1,545)	1:A:29:PHE:HD2	1:A:31:THR:H	3	0.11
(1,4940)	1:B:55:ASN:HD21	1:B:57:ASP:HB2	10	0.11
(1,4940)	1:B:55:ASN:HD21	1:B:57:ASP:HB3	10	0.11
(1,4940)	1:B:55:ASN:HD22	1:B:57:ASP:HB2	10	0.11
(1,4940)	1:B:55:ASN:HD22	1:B:57:ASP:HB3	10	0.11
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB2	20	0.11
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB3	20	0.11
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB2	20	0.11
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB3	20	0.11
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD21	5	0.11
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD22	5	0.11
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD21	5	0.11
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD22	5	0.11
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD21	5	0.11
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD22	5	0.11
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD21	17	0.11
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD22	17	0.11
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD21	17	0.11



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD22	17	0.11
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD21	17	0.11
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD22	17	0.11
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG2	19	0.11
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	19	0.11
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	19	0.11
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG3	19	0.11
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	19	0.11
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	19	0.11
(1,4770)	1:B:15:LYS:HD2	1:B:16:ASN:HB2	9	0.11
(1,4770)	1:B:15:LYS:HD2	1:B:16:ASN:HB3	9	0.11
(1,4770)	1:B:15:LYS:HD3	1:B:16:ASN:HB2	9	0.11
(1,4770)	1:B:15:LYS:HD3	1:B:16:ASN:HB3	9	0.11
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE1	14	0.11
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE2	14	0.11
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE3	14	0.11
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE1	14	0.11
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE2	14	0.11
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE3	14	0.11
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB2	20	0.11
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB3	20	0.11
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB2	20	0.11
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB3	20	0.11
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD21	13	0.11
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD22	13	0.11
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD21	13	0.11
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD22	13	0.11
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD21	13	0.11
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD22	13	0.11
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	8	0.11
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	8	0.11
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	8	0.11
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	8	0.11
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	20	0.11
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	20	0.11
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	20	0.11
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	4	0.11
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	4	0.11
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	4	0.11
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	4	0.11
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	4	0.11
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	4	0.11



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE1	12	0.11
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE2	12	0.11
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE1	12	0.11
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE2	12	0.11
(1,4209)	1:B:29:PHE:HA	1:B:29:PHE:HD1	4	0.11
(1,4209)	1:B:29:PHE:HA	1:B:29:PHE:HD2	4	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	10	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	10	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	10	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	11	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	11	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	11	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	12	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	12	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	12	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	15	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	15	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	15	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	19	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	19	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	19	0.11
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	15	0.11
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	15	0.11
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	15	0.11
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	17	0.11
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	17	0.11
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	17	0.11
(1,4072)	1:A:60:THR:HB	1:A:61:THR:H	2	0.11
(1,4053)	1:B:41:LYS:HG2	1:B:42:ASP:HA	1	0.11
(1,4053)	1:B:41:LYS:HG3	1:B:42:ASP:HA	1	0.11
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	4	0.11
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	10	0.11
(1,4036)	1:A:15:LYS:HA	1:A:17:GLY:H	12	0.11
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	20	0.11
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	20	0.11
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	20	0.11
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	2	0.11
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	2	0.11
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	2	0.11
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	15	0.11
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	15	0.11
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	15	0.11



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Key	Atom-1	$\mathbf{Atom-2}$	Model	Violation (Å)
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	19	0.11
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	19	0.11
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	19	0.11
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	1	0.11
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	1	0.11
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	1	0.11
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	2	0.11
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	2	0.11
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	2	0.11
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	3	0.11
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	3	0.11
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	3	0.11
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	15	0.11
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	15	0.11
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	7	0.11
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	7	0.11
(1,3483)	1:A:41:LYS:HE2	1:A:44:ILE:H	1	0.11
(1,3483)	1:A:41:LYS:HE3	1:A:44:ILE:H	1	0.11
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	19	0.11
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	19	0.11
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	19	0.11
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE1	16	0.11
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE2	16	0.11
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE3	16	0.11
(1,3149)	1:A:55:ASN:H	1:A:58:LYS:HB2	6	0.11
(1,3103)	1:A:54:LYS:HE2	1:A:55:ASN:HD21	1	0.11
(1,3103)	1:A:54:LYS:HE3	1:A:55:ASN:HD21	1	0.11
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE2	17	0.11
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE3	17	0.11
(1,3099)	1:A:54:LYS:H	1:A:54:LYS:HD2	18	0.11
(1,3099)	1:A:54:LYS:H	1:A:54:LYS:HD3	18	0.11
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	15	0.11
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	15	0.11
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	15	0.11
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	15	0.11
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	15	0.11
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	15	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	2	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	2	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	2	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	2	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	2	0.11



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	2	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	2	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	2	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	2	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	7	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	7	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	7	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	7	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	7	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	7	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	7	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	7	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	7	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	8	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	8	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	8	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	8	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	8	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	8	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	8	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	8	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	8	0.11
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	19	0.11
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	19	0.11
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	19	0.11
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	19	0.11
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	19	0.11
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	19	0.11
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	19	0.11
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	19	0.11
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	19	0.11
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	1	0.11
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	1	0.11
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	1	0.11
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	15	0.11
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	15	0.11
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	15	0.11
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	8	0.11
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	8	0.11
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	8	0.11
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	12	0.11
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	12	0.11



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	12	0.11
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	4	0.11
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	18	0.11
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	3	0.11
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	6	0.11
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	16	0.11
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	18	0.11
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	4	0.11
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	4	0.11
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	4	0.11
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	5	0.11
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	5	0.11
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	5	0.11
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	9	0.11
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	9	0.11
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	9	0.11
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	15	0.11
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	15	0.11
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	15	0.11
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	16	0.11
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	16	0.11
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	16	0.11
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	8	0.11
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	8	0.11
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	8	0.11
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	7	0.11
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	7	0.11
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	7	0.11
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	12	0.11
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	12	0.11
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	12	0.11
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	18	0.11
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	18	0.11
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	18	0.11
(1,2284)	1:A:36:ILE:HG21	1:B:39:ASN:HB2	10	0.11
(1,2284)	1:A:36:ILE:HG21	1:B:39:ASN:HB3	10	0.11
(1,2284)	1:A:36:ILE:HG22	1:B:39:ASN:HB2	10	0.11
(1,2284)	1:A:36:ILE:HG22	1:B:39:ASN:HB3	10	0.11
(1,2284)	1:A:36:ILE:HG23	1:B:39:ASN:HB2	10	0.11
(1,2284)	1:A:36:ILE:HG23	1:B:39:ASN:HB3	10	0.11
(1,2173)	1:A:68:LYS:HA	1:A:68:LYS:HD2	6	0.11
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	8	0.11



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	12	0.11
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	1	0.11
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	5	0.11
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	7	0.11
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	12	0.11
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG21	20	0.11
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG22	20	0.11
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG23	20	0.11
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG21	20	0.11
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG22	20	0.11
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG23	20	0.11
(1,1795)	1:B:14:ASP:HA	1:B:15:LYS:HB3	8	0.11
(1,175)	1:A:15:LYS:H	1:A:18:MET:HG2	15	0.11
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	7	0.11
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	7	0.11
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	7	0.11
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	10	0.11
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	10	0.11
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	10	0.11
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	1	0.11
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	1	0.11
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	1	0.11
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	8	0.11
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	8	0.11
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	8	0.11
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	18	0.11
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	18	0.11
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	18	0.11
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	15	0.11
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	15	0.11
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	15	0.11
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	15	0.11
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	15	0.11
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	15	0.11
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	15	0.11
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	15	0.11
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	15	0.11
(1,1413)	1:A:3:ASP:HB2	1:A:53:VAL:H	1	0.11
(1,1318)	1:B:77:ARG:HG2	1:B:78:LEU:H	8	0.11
(1,1020)	1:A:58:LYS:HZ1	1:A:61:THR:H	20	0.11
(1,1020)	1:A:58:LYS:HZ2	1:A:61:THR:H	20	0.11
(1,1020)	1:A:58:LYS:HZ3	1:A:61:THR:H	20	0.11



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(1,822) 1:A:45:PHE:HZ 1:A:47:CYS:H 1 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 18 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 18 (1,546) 1:B:29:PHE:HD1 1:B:31:THR:H 15 (1,546) 1:B:29:PHE:HD2 1:B:31:THR:H 15 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB2 8 (1,4976) 1:B:63:MET:HE2 1:B:77:ARG:HB2 8 (1,4976) 1:B:63:MET:HE2 1:B:77:ARG:HB3 8 (1,4976) 1:B:63:MET:HE2 1:B:77:ARG:HB3 8	0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1
(1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 18 (1,546) 1:B:29:PHE:HD1 1:B:31:THR:H 15 (1,546) 1:B:29:PHE:HD2 1:B:31:THR:H 15 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB2 8 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB3 8 (1,4976) 1:B:63:MET:HE2 1:B:77:ARG:HB2 8	0.1 0.1 0.1 0.1 0.1 0.1 0.1
(1,546) 1:B:29:PHE:HD1 1:B:31:THR:H 15 (1,546) 1:B:29:PHE:HD2 1:B:31:THR:H 15 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB2 8 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB3 8 (1,4976) 1:B:63:MET:HE2 1:B:77:ARG:HB2 8	0.1 0.1 0.1 0.1 0.1 0.1
(1,546) 1:B:29:PHE:HD2 1:B:31:THR:H 15 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB2 8 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB3 8 (1,4976) 1:B:63:MET:HE2 1:B:77:ARG:HB2 8	0.1 0.1 0.1 0.1 0.1
(1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB2 8 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB3 8 (1,4976) 1:B:63:MET:HE2 1:B:77:ARG:HB2 8	0.1 0.1 0.1 0.1
(1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB3 8 (1,4976) 1:B:63:MET:HE2 1:B:77:ARG:HB2 8	0.1 0.1 0.1
(1,4976) 1:B:63:MET:HE2 1:B:77:ARG:HB2 8	0.1 0.1
	0.1
(1.4976) 1·B·63·MET·HE2 1·B·77·ABC·HB3 8	
(1,1010) 1.D.00.MID1.IID2 1.D.11.MIW.IID0 0	0.1
(1,4976) 1:B:63:MET:HE3 1:B:77:ARG:HB2 8	
(1,4976) 1:B:63:MET:HE3 1:B:77:ARG:HB3 8	0.1
(1,4911) 1:B:46:THR:HG21 1:B:48:ASN:HD21 11	0.1
(1,4911) 1:B:46:THR:HG21 1:B:48:ASN:HD22 11	0.1
(1,4911) 1:B:46:THR:HG22 1:B:48:ASN:HD21 11	0.1
(1,4911) 1:B:46:THR:HG22 1:B:48:ASN:HD22 11	0.1
(1,4911) 1:B:46:THR:HG23 1:B:48:ASN:HD21 11	0.1
(1,4911) 1:B:46:THR:HG23 1:B:48:ASN:HD22 11	0.1
(1,4896) 1:B:39:ASN:HD21 1:B:41:LYS:HB2 3	0.1
(1,4896) 1:B:39:ASN:HD21 1:B:41:LYS:HB3 3	0.1
(1,4896) 1:B:39:ASN:HD22 1:B:41:LYS:HB2 3	0.1
(1,4896) 1:B:39:ASN:HD22 1:B:41:LYS:HB3 3	0.1
(1,4885) 1:B:37:VAL:HG11 1:B:39:ASN:HD21 16	0.1
(1,4885) 1:B:37:VAL:HG11 1:B:39:ASN:HD22 16	0.1
(1,4885) 1:B:37:VAL:HG12 1:B:39:ASN:HD21 16	0.1
(1,4885) 1:B:37:VAL:HG12 1:B:39:ASN:HD22 16	0.1
(1,4885) 1:B:37:VAL:HG13 1:B:39:ASN:HD21 16	0.1
(1,4885) 1:B:37:VAL:HG13 1:B:39:ASN:HD22 16	0.1
(1,4861) 1:B:32:ASN:HD21 1:B:33:ILE:HB 16	0.1
(1,4861) 1:B:32:ASN:HD22 1:B:33:ILE:HB 16	0.1
(1,4851) 1:B:31:THR:HG21 1:B:58:LYS:HE2 3	0.1
(1,4851) 1:B:31:THR:HG21 1:B:58:LYS:HE3 3	0.1
(1,4851) 1:B:31:THR:HG22 1:B:58:LYS:HE2 3	0.1
(1,4851) 1:B:31:THR:HG22 1:B:58:LYS:HE3 3	0.1
(1,4851) 1:B:31:THR:HG23 1:B:58:LYS:HE2 3	0.1
(1,4851) 1:B:31:THR:HG23 1:B:58:LYS:HE3 3	0.1
(1,4815) 1:B:25:VAL:HG21 1:B:28:LYS:HG2 6	0.1
(1,4815) 1:B:25:VAL:HG21 1:B:28:LYS:HG3 6	0.1
(1,4815) 1:B:25:VAL:HG22 1:B:28:LYS:HG2 6	0.1
(1,4815) 1:B:25:VAL:HG22 1:B:28:LYS:HG3 6	0.1
(1,4815) 1:B:25:VAL:HG23 1:B:28:LYS:HG2 6	0.1
(1,4815) 1:B:25:VAL:HG23 1:B:28:LYS:HG3 6	0.1
(1,4815) 1:B:25:VAL:HG21 1:B:28:LYS:HG2 11	0.1



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	11	0.1
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	11	0.1
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG3	11	0.1
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	11	0.1
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	11	0.1
(1,4768)	1:B:15:LYS:HG2	1:B:16:ASN:HD21	11	0.1
(1,4768)	1:B:15:LYS:HG2	1:B:16:ASN:HD22	11	0.1
(1,4768)	1:B:15:LYS:HG3	1:B:16:ASN:HD21	11	0.1
(1,4768)	1:B:15:LYS:HG3	1:B:16:ASN:HD22	11	0.1
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	8	0.1
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	8	0.1
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	8	0.1
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	8	0.1
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE1	1	0.1
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE2	1	0.1
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE3	1	0.1
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE1	1	0.1
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE2	1	0.1
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE3	1	0.1
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB2	4	0.1
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB3	4	0.1
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB2	4	0.1
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB3	4	0.1
(1,4560)	1:A:31:THR:HG21	1:A:58:LYS:HE2	18	0.1
(1,4560)	1:A:31:THR:HG21	1:A:58:LYS:HE3	18	0.1
(1,4560)	1:A:31:THR:HG22	1:A:58:LYS:HE2	18	0.1
(1,4560)	1:A:31:THR:HG22	1:A:58:LYS:HE3	18	0.1
(1,4560)	1:A:31:THR:HG23	1:A:58:LYS:HE2	18	0.1
(1,4560)	1:A:31:THR:HG23	1:A:58:LYS:HE3	18	0.1
(1,4458)	1:A:15:LYS:HB2	1:A:18:MET:HG2	15	0.1
(1,4458)	1:A:15:LYS:HB2	1:A:18:MET:HG3	15	0.1
(1,4458)	1:A:15:LYS:HB3	1:A:18:MET:HG2	15	0.1
(1,4458)	1:A:15:LYS:HB3	1:A:18:MET:HG3	15	0.1
(1,4405)	1:A:3:ASP:HB2	1:A:4:PHE:H	1	0.1
(1,4405)	1:A:3:ASP:HB3	1:A:4:PHE:H	1	0.1
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	5	0.1
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	5	0.1
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	5	0.1
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	11	0.1
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	11	0.1
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	11	0.1
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	14	0.1
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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	14	0.1
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	14	0.1
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	18	0.1
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	18	0.1
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	18	0.1
(1,4391)	1:B:50:MET:HE1	1:B:83:HIS:HD2	17	0.1
(1,4391)	1:B:50:MET:HE2	1:B:83:HIS:HD2	17	0.1
(1,4391)	1:B:50:MET:HE3	1:B:83:HIS:HD2	17	0.1
(1,4353)	1:B:44:ILE:HG13	1:B:73:PHE:HE1	14	0.1
(1,4353)	1:B:44:ILE:HG13	1:B:73:PHE:HE2	14	0.1
(1,4343)	1:B:29:PHE:HE1	1:B:65:LYS:HE2	6	0.1
(1,4343)	1:B:29:PHE:HE1	1:B:65:LYS:HE3	6	0.1
(1,4343)	1:B:29:PHE:HE2	1:B:65:LYS:HE2	6	0.1
(1,4343)	1:B:29:PHE:HE2	1:B:65:LYS:HE3	6	0.1
(1,4205)	1:B:29:PHE:HD1	1:B:65:LYS:HD2	4	0.1
(1,4205)	1:B:29:PHE:HD2	1:B:65:LYS:HD2	4	0.1
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	1	0.1
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	1	0.1
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	1	0.1
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	4	0.1
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	4	0.1
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	4	0.1
(1,4118)	1:A:80:ASN:HA	1:A:81:LEU:HG	3	0.1
(1,4072)	1:A:60:THR:HB	1:A:61:THR:H	14	0.1
(1,4053)	1:B:41:LYS:HG2	1:B:42:ASP:HA	18	0.1
(1,4053)	1:B:41:LYS:HG3	1:B:42:ASP:HA	18	0.1
(1,4052)	1:A:41:LYS:HG2	1:A:42:ASP:HA	9	0.1
(1,4052)	1:A:41:LYS:HG3	1:A:42:ASP:HA	9	0.1
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	7	0.1
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	14	0.1
(1,3994)	1:A:82:GLU:H	1:A:83:HIS:HB3	14	0.1
(1,3889)	1:A:82:GLU:HA	1:A:83:HIS:HB2	14	0.1
(1,3839)	1:A:78:LEU:H	1:A:79:SER:HB2	7	0.1
(1,3839)	1:A:78:LEU:H	1:A:79:SER:HB3	7	0.1
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD11	3	0.1
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD12	3	0.1
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD13	3	0.1
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	7	0.1
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	7	0.1
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	7	0.1
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	11	0.1
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	11	0.1



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	11	0.1
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	19	0.1
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	19	0.1
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	19	0.1
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	4	0.1
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	4	0.1
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	4	0.1
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	19	0.1
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	19	0.1
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	19	0.1
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	20	0.1
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	20	0.1
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	20	0.1
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	13	0.1
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	13	0.1
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	13	0.1
(1,3622)	1:B:69:VAL:HA	1:B:70:GLN:HG2	10	0.1
(1,3622)	1:B:69:VAL:HA	1:B:70:GLN:HG3	10	0.1
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	13	0.1
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	13	0.1
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	13	0.1
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE1	5	0.1
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE2	5	0.1
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE3	5	0.1
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE1	20	0.1
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE2	20	0.1
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE3	20	0.1
(1,3183)	1:A:58:LYS:HD2	1:A:62:LEU:H	7	0.1
(1,3183)	1:A:58:LYS:HD3	1:A:62:LEU:H	7	0.1
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE2	7	0.1
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE3	7	0.1
(1,3097)	1:A:15:LYS:HD2	1:A:16:ASN:HD21	16	0.1
(1,3097)	1:A:15:LYS:HD3	1:A:16:ASN:HD21	16	0.1
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	9	0.1
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	9	0.1
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	9	0.1
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	9	0.1
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	9	0.1
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	9	0.1
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	10	0.1
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	10	0.1
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	10	0.1



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	10	0.1
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	10	0.1
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	10	0.1
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	10	0.1
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	10	0.1
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	10	0.1
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	3	0.1
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	3	0.1
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	3	0.1
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	3	0.1
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	3	0.1
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	3	0.1
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	3	0.1
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	3	0.1
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	3	0.1
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	9	0.1
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	9	0.1
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	9	0.1
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	9	0.1
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	9	0.1
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	9	0.1
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	9	0.1
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	9	0.1
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	9	0.1
(1,2901)	1:A:20:ASN:HD22	1:B:51:ILE:HG21	13	0.1
(1,2901)	1:A:20:ASN:HD22	1:B:51:ILE:HG22	13	0.1
(1,2901)	1:A:20:ASN:HD22	1:B:51:ILE:HG23	13	0.1
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	16	0.1
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	16	0.1
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	16	0.1
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	17	0.1
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	17	0.1
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	17	0.1
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	1	0.1
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	1	0.1
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	1	0.1
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	9	0.1
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	9	0.1
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	9	0.1
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	6	0.1
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	10	0.1
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	14	0.1



 $Continued\ from\ previous\ page...$

(1,2547) 1:A:40:ALA:HA 1:A:44:ILE:HG13 2 0.1 (1,2547) 1:A:40:ALA:HA 1:A:44:ILE:HG13 11 0.1 (1,2547) 1:A:40:ALA:HA 1:A:44:ILE:HG13 14 0.1 (1,2547) 1:A:40:ALA:HA 1:A:44:ILE:HG13 14 0.1 (1,2547) 1:A:40:ALA:HA 1:A:44:ILE:HG13 20 0.1 (1,2522) 1:B:14:ASP:HB2 1:B:43:GLY:HA3 8 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD11 6 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD12 6 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 6 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 14 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 14 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 14 0.1 (1,2304) 1:B:36:ILE:HG21 1:B:48:ASN:H 2 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 2 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 2 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 12 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 12 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 12 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 19 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 19 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 19 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 19 0.1 (1,2303) 1:A:36:ILE:HG21 1:B:48:ASN:H 19 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 19 0.1 (1,2305) 1:A:19:THR:H 1:A:38:LEU:HD11 9 0.1 (1,2306) 1:A:19:THR:H 1:A:38:LEU:HD11 9 0.1 (1,2307) 1:A:19:THR:H 1:A:38:LEU:HD11 9 0.1 (1,2308) 1:A:36:ILE:HG23 1:B:48:ASN:H 19 0.1 (1,2309) 1:A:19:THR:H 1:A:38:LEU:HD11 9 0.1 (1,2300) 1:A:19:THR:H 1:A:38:LEU:HD11 9 0.1 (1,2301) 1:A:19:THR:H 1:A:38:LEU:HD12 9 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG23 16 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG23 16 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG23 3 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG22 3 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG23 1	Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,2547) 1:A:40:ALA:HA 1:A:44:ILE:HG13 14 0.1 (1,2547) 1:A:40:ALA:HA 1:A:44:ILE:HG13 20 0.1 (1,2547) 1:A:40:ALA:HA 1:A:44:ILE:HG13 20 0.1 (1,2547) 1:B:14:ASP:HB2 1:B:33:LEU:HD11 6 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 6 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD11 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD11 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 14 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 14 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 14 0.1 (1,2304) 1:B:36:ILE:HG21 1:B:48:ASN:H 2 </td <td>(1,2547)</td> <td>1:A:40:ALA:HA</td> <td>1:A:44:ILE:HG13</td> <td>2</td> <td>0.1</td>	(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	2	0.1
(1,2547)	(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	11	0.1
(1,2522) 1:B:14:ASP:HB2 1:B:43:GLY:HA3 8 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD11 6 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD12 6 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 6 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 6 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD11 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD12 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD11 14 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD12 14 0.1 (1,230) 1:B:19:THR:H 1:B:38:LEU:HD12 14 0.1 (1,230) 1:B:19:THR:H 1:B:38:LEU:HD13 14 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 2 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 2 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 2 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 12 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 19 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 19 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 19 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 19 0.1 (1,2303) 1:A:36:ILE:HG22 1:A:48:ASN:H 9 0.1 (1,2303) 1:A:36:ILE:HG23 1:B:48:ASN:H 9 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 9 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 9 0.1 (1,2306) 1:A:19:THR:H 1:A:38:LEU:HD11 9 0.1 (1,2306) 1:A:19:THR:H 1:A:38:LEU:HD11 9 0.1 (1,2306) 1:A:19:THR:H 1:A:38:LEU:HD13 9 0.1 (1,2306) 1:A:19:THR:H 1:A:38:LEU:HD13 9 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG21 16 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG21 20 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG22 30 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG22 30 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG22 30 0.1 (1,2	(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	14	0.1
(1,231) 1:B:19:THR:H 1:B:38:LEU:HD11 6 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD12 6 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 6 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD11 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD12 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD12 14 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD12 14 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 14 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 14 0.1 (1,231) 1:B:36:ILE:HG21 1:B:48:ASN:H 2 0.1 (1,2304) 1:B:36:ILE:HG21 1:B:48:ASN:H 2 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 12 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 19	(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	20	0.1
(1,231) 1:B:19:THR:H 1:B:38:LEU:HD12 6 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 6 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD11 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD12 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD11 14 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD12 14 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 14 0.1 (1,2304) 1:B:36:ILE:HG21 1:B:48:ASN:H 2 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 2 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 2 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 12 0.1 (1,2304) 1:B:36:ILE:HG21 1:B:48:ASN:H 12 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 12 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 12 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 19 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 19 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 19 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 19 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 19 0.1 (1,2303) 1:A:36:ILE:HG22 1:B:48:ASN:H 19 0.1 (1,2303) 1:A:36:ILE:HG21 1:A:48:ASN:H 9 0.1 (1,2303) 1:A:36:ILE:HG23 1:B:48:ASN:H 9 0.1 (1,2303) 1:A:36:ILE:HG23 1:A:48:ASN:H 9 0.1 (1,2303) 1:A:36:ILE:HG23 1:A:48:ASN:H 9 0.1 (1,2303) 1:A:36:ILE:HG23 1:A:48:ASN:H 9 0.1 (1,2304) 1:B:36:ILE:HG23 1:A:48:ASN:H 9 0.1 (1,2305) 1:A:19:THR:H 1:A:38:LEU:HD11 9 0.1 (1,2306) 1:A:19:THR:H 1:A:38:LEU:HD11 9 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG21 16 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG22 16 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG23 16 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG23 16 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG23 20 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG23 30 0.1 (1,2285) 1:A:23:THR:HB 1:B:36:ILE:HG23 30 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG23 30 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG23 30 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG23 30 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG23 11 0.1	(1,2522)	1:B:14:ASP:HB2	1:B:43:GLY:HA3	8	0.1
(1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 6 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD11 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD12 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 12 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD11 14 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD12 14 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 14 0.1 (1,231) 1:B:19:THR:H 1:B:38:LEU:HD13 14 0.1 (1,2304) 1:B:36:ILE:HG21 1:B:48:ASN:H 2 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 2 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 2 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 12 0.1 (1,2304) 1:B:36:ILE:HG21 1:B:48:ASN:H 12 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 12 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 12 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 19 0.1 (1,2304) 1:B:36:ILE:HG21 1:B:48:ASN:H 19 0.1 (1,2304) 1:B:36:ILE:HG21 1:B:48:ASN:H 19 0.1 (1,2304) 1:B:36:ILE:HG22 1:B:48:ASN:H 19 0.1 (1,2303) 1:A:36:ILE:HG23 1:B:48:ASN:H 19 0.1 (1,2304) 1:B:36:ILE:HG23 1:B:48:ASN:H 19 0.1 (1,2305) 1:A:36:ILE:HG23 1:B:48:ASN:H 19 0.1 (1,2306) 1:A:19:THR:H 1:A:38:LEU:HD11 1 10 (1,2307) 1:A:19:THR:H 1:A:38:LEU:HD11 1 10 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG21 16 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG21 16 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG21 16 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG22 20 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG23 30 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG23 30 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG23 30 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG23 30 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG23 30 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG22 11 0.1	(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	6	0.1
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(1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG22 20 0.1 (1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG23 20 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG21 3 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG22 3 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG23 3 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG21 11 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG22 11 0.1	` '	1:B:23:THR:HB	1:B:36:ILE:HG21	20	0.1
(1,2286) 1:B:23:THR:HB 1:B:36:ILE:HG23 20 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG21 3 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG22 3 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG23 3 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG21 11 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG22 11 0.1		1:B:23:THR:HB	1:B:36:ILE:HG22	20	0.1
(1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG21 3 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG22 3 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG23 3 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG21 11 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG22 11 0.1		1:B:23:THR:HB	1:B:36:ILE:HG23	20	0.1
(1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG22 3 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG23 3 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG21 11 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG22 11 0.1		1:A:23:THR:HB	1:A:36:ILE:HG21	3	0.1
(1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG23 3 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG21 11 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG22 11 0.1		1:A:23:THR:HB	1:A:36:ILE:HG22	3	0.1
(1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG21 11 0.1 (1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG22 11 0.1		1:A:23:THR:HB	1:A:36:ILE:HG23	3	0.1
(1,2285) 1:A:23:THR:HB 1:A:36:ILE:HG22 11 0.1		1:A:23:THR:HB	1:A:36:ILE:HG21	11	0.1
	(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	11	0.1
	· · /	1:A:23:THR:HB	1:A:36:ILE:HG23	11	0.1
(1,2164) 1:B:27:SER:HG 1:B:28:LYS:HG2 13 0.1		1:B:27:SER:HG	1:B:28:LYS:HG2	13	



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	4	0.1
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	4	0.1
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	4	0.1
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	16	0.1
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	16	0.1
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	16	0.1
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	6	0.1
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	6	0.1
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	6	0.1
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	2	0.1
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	6	0.1
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	10	0.1
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	11	0.1
(1,1813)	1:B:25:VAL:HG21	1:B:65:LYS:HE2	6	0.1
(1,1813)	1:B:25:VAL:HG21	1:B:65:LYS:HE3	6	0.1
(1,1813)	1:B:25:VAL:HG22	1:B:65:LYS:HE2	6	0.1
(1,1813)	1:B:25:VAL:HG22	1:B:65:LYS:HE3	6	0.1
(1,1813)	1:B:25:VAL:HG23	1:B:65:LYS:HE2	6	0.1
(1,1813)	1:B:25:VAL:HG23	1:B:65:LYS:HE3	6	0.1
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG11	9	0.1
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG12	9	0.1
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG13	9	0.1
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG11	9	0.1
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG12	9	0.1
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG13	9	0.1
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG11	13	0.1
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG12	13	0.1
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG13	13	0.1
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG11	13	0.1
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG12	13	0.1
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG13	13	0.1
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	8	0.1
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	8	0.1
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	8	0.1
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	14	0.1
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	14	0.1
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	14	0.1
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	20	0.1
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	20	0.1
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	20	0.1
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	4	0.1
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	4	0.1



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	4	0.1
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	9	0.1
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	9	0.1
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	9	0.1
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	10	0.1
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	10	0.1
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	10	0.1
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	12	0.1
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	12	0.1
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	12	0.1
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	13	0.1
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	13	0.1
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	13	0.1
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	5	0.1
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	5	0.1
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	5	0.1
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	5	0.1
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	5	0.1
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG23	5	0.1
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	5	0.1
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	5	0.1
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	5	0.1
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG21	16	0.1
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG22	16	0.1
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG23	16	0.1
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG21	16	0.1
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG22	16	0.1
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG23	16	0.1
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG21	16	0.1
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG22	16	0.1
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG23	16	0.1
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	4	0.1
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	4	0.1
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	4	0.1
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	4	0.1
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	4	0.1
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	4	0.1
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	4	0.1
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	4	0.1
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	4	0.1
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	11	0.1
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	11	0.1



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	11	0.1
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	11	0.1
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	11	0.1
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	11	0.1
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	11	0.1
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	11	0.1
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	11	0.1
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	11	0.1
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	11	0.1
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	11	0.1
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	11	0.1
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	11	0.1
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	11	0.1
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	11	0.1
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	11	0.1
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	11	0.1
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	17	0.1
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	17	0.1
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	17	0.1
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	17	0.1
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	17	0.1
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	17	0.1
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	17	0.1
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	17	0.1
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	17	0.1
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	20	0.1
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	20	0.1
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	20	0.1
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	20	0.1
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	20	0.1
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	20	0.1
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	20	0.1
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	20	0.1
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	20	0.1
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	15	0.1
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	15	0.1
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	15	0.1
(1,1330)	1:B:78:LEU:HD21	1:B:79:SER:H	3	0.1
(1,1330)	1:B:78:LEU:HD22	1:B:79:SER:H	3	0.1
(1,1330)	1:B:78:LEU:HD23	1:B:79:SER:H	3	0.1
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	8	0.1
(1,1156)	1:B:67:ARG:HE	1:B:75:VAL:H	6	0.1



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1094)	1:B:65:LYS:H	1:B:68:LYS:HE2	16	0.1
(1,1094)	1:B:65:LYS:H	1:B:68:LYS:HE3	16	0.1
(1,1020)	1:A:58:LYS:HZ1	1:A:61:THR:H	4	0.1
(1,1020)	1:A:58:LYS:HZ2	1:A:61:THR:H	4	0.1
(1,1020)	1:A:58:LYS:HZ3	1:A:61:THR:H	4	0.1
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	13	0.09
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	9	0.09
(1,697)	1:B:41:LYS:H	1:B:41:LYS:HG2	13	0.09
(1,697)	1:B:41:LYS:H	1:B:41:LYS:HG3	13	0.09
(1,563)	1:A:32:ASN:HD21	1:A:33:ILE:HB	14	0.09
(1,4976)	1:B:63:MET:HE1	1:B:77:ARG:HB2	16	0.09
(1,4976)	1:B:63:MET:HE1	1:B:77:ARG:HB3	16	0.09
(1,4976)	1:B:63:MET:HE2	1:B:77:ARG:HB2	16	0.09
(1,4976)	1:B:63:MET:HE2	1:B:77:ARG:HB3	16	0.09
(1,4976)	1:B:63:MET:HE3	1:B:77:ARG:HB2	16	0.09
(1,4976)	1:B:63:MET:HE3	1:B:77:ARG:HB3	16	0.09
(1,4899)	1:B:39:ASN:HD21	1:B:46:THR:HB	6	0.09
(1,4899)	1:B:39:ASN:HD22	1:B:46:THR:HB	6	0.09
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB2	11	0.09
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB3	11	0.09
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB2	11	0.09
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB3	11	0.09
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD21	8	0.09
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD22	8	0.09
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD21	8	0.09
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD22	8	0.09
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD21	8	0.09
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD22	8	0.09
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD21	15	0.09
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD22	15	0.09
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD21	15	0.09
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD22	15	0.09
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD21	15	0.09
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD22	15	0.09
(1,4879)	1:B:36:ILE:HG12	1:B:37:VAL:HA	3	0.09
(1,4879)	1:B:36:ILE:HG13	1:B:37:VAL:HA	3	0.09
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG2	20	0.09
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	20	0.09
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	20	0.09
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG3	20	0.09
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	20	0.09
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	20	0.09



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(1,4765) 1:B:15:LYS:HB2 1:B:18:MET:HG2 14 0.09 (1,4765) 1:B:15:LYS:HB2 1:B:18:MET:HG3 14 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE1 9 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 9 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 9 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 9 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 9 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 9 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:48:ASN:HD22	
(1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE1 9 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 9 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 9 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 9 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 9 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 9 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB2 5 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 5 0.09	
(1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 9 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 9 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 9 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 9 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 9 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:39:ASN:HD21 1:A:41:LYS:HB2 5 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 5 0.09	
(1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 9 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 9 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 9 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 9 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:39:ASN:HD21 1:A:41:LYS:HB2 5 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 5 0.09	
(1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 9 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 9 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 9 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 5 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 5 0.09	
(1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 9 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 9 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB2 5 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 5 0.09	
(1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 9 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB2 5 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 5 0.09	
(1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB2 5 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 5 0.09	
(1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB2 5 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 5 0.09	
(1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB2 5 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 5 0.09	
(1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB2 5 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 5 0.09	
(1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 10 0.09 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB2 5 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 5 0.09	
(1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 10 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB2 5 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 5 0.09	
(1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB2 5 0.09 (1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 5 0.09	
(1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 5 0.09	
(1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 5 0.09	
(1.4602) 1:A:39:ASN:HD22 1:A·41·LYS·HB2 5 0.09	
(2,200=) 1:11:00:120:1101:1110= 0:00	
(1,4602) 1:A:39:ASN:HD22 1:A:41:LYS:HB3 5 0.09	
(1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB2 8 0.09	
(1,4602) 1:A:39:ASN:HD21 1:A:41:LYS:HB3 8 0.09	
(1,4602) 1:A:39:ASN:HD22 1:A:41:LYS:HB2 8 0.09	
(1,4602) 1:A:39:ASN:HD22 1:A:41:LYS:HB3 8 0.09	
(1,4591) 1:A:37:VAL:HG11 1:A:39:ASN:HD21 6 0.09	
(1,4591) 1:A:37:VAL:HG11 1:A:39:ASN:HD22 6 0.09	
(1,4591) 1:A:37:VAL:HG12 1:A:39:ASN:HD21 6 0.09	
(1,4591) 1:A:37:VAL:HG12 1:A:39:ASN:HD22 6 0.09	
(1,4591) 1:A:37:VAL:HG13 1:A:39:ASN:HD21 6 0.09	
(1,4591) 1:A:37:VAL:HG13 1:A:39:ASN:HD22 6 0.09	
(1,4585) 1:A:36:ILE:HG12 1:A:37:VAL:HA 10 0.09	
(1,4585) 1:A:36:ILE:HG13 1:A:37:VAL:HA 10 0.09	
(1,4560) 1:A:31:THR:HG21 1:A:58:LYS:HE2 10 0.09	
(1,4560) 1:A:31:THR:HG21 1:A:58:LYS:HE3 10 0.09	
(1,4560) 1:A:31:THR:HG22 1:A:58:LYS:HE2 10 0.09	
(1,4560) 1:A:31:THR:HG22 1:A:58:LYS:HE3 10 0.09	
(1,4560) 1:A:31:THR:HG23 1:A:58:LYS:HE2 10 0.09	
(1,4560) 1:A:31:THR:HG23 1:A:58:LYS:HE3 10 0.09	
(1,4538) 1:A:27:SER:HG 1:A:28:LYS:HD2 17 0.09	
(1,4538) 1:A:27:SER:HG 1:A:28:LYS:HD3 17 0.09	
(1,4524) 1:A:25:VAL:HG21 1:A:28:LYS:HG2 6 0.09	
(1,4524) 1:A:25:VAL:HG21 1:A:28:LYS:HG3 6 0.09	
(1,4524) 1:A:25:VAL:HG22 1:A:28:LYS:HG2 6 0.09	
(1,4524) 1:A:25:VAL:HG22 1:A:28:LYS:HG3 6 0.09	



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	:A:25:VAL:HG23	4		
(1.4594) 1		1:A:28:LYS:HG2	6	0.09
(1,4044) 1	:A:25:VAL:HG23	1:A:28:LYS:HG3	6	0.09
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	11	0.09
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	11	0.09
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	11	0.09
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	11	0.09
(1,4457)	1:A:15:LYS:HB2	1:A:18:MET:HB2	2	0.09
(1,4457)	1:A:15:LYS:HB2	1:A:18:MET:HB3	2	0.09
(1,4457)	1:A:15:LYS:HB3	1:A:18:MET:HB2	2	0.09
(1,4457)	1:A:15:LYS:HB3	1:A:18:MET:HB3	2	0.09
(1,4407)	1:A:3:ASP:HB2	1:A:52:PHE:HD1	1	0.09
(1,4407)	1:A:3:ASP:HB2	1:A:52:PHE:HD2	1	0.09
(1,4407)	1:A:3:ASP:HB3	1:A:52:PHE:HD1	1	0.09
	1:A:3:ASP:HB3	1:A:52:PHE:HD2	1	0.09
(1,4401) 1	:B:81:LEU:HD11	1:B:83:HIS:HE1	20	0.09
(1,4401) 1	:B:81:LEU:HD12	1:B:83:HIS:HE1	20	0.09
(1,4401) 1	:B:81:LEU:HD13	1:B:83:HIS:HE1	20	0.09
	1:A:4:PHE:HE1	1:A:53:VAL:HG11	5	0.09
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	5	0.09
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	5	0.09
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	5	0.09
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	5	0.09
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	5	0.09
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	15	0.09
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	15	0.09
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	15	0.09
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	15	0.09
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	15	0.09
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	15	0.09
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	19	0.09
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	19	0.09
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	19	0.09
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	19	0.09
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	19	0.09
	1:A:4:PHE:HE2	1:A:53:VAL:HG13	19	0.09
(1,4352) 1	:A:44:ILE:HG13	1:A:73:PHE:HE1	15	0.09
	:A:44:ILE:HG13	1:A:73:PHE:HE2	15	0.09
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE1	20	0.09
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE2	20	0.09
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE1	20	0.09
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE2	20	0.09
(1,4205) 1	l:B:29:PHE:HD1	1:B:65:LYS:HD2	1	0.09



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4205)	1:B:29:PHE:HD2	1:B:65:LYS:HD2	1	0.09
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	2	0.09
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	2	0.09
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	2	0.09
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	5	0.09
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	5	0.09
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	5	0.09
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	6	0.09
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	6	0.09
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	6	0.09
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	8	0.09
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	8	0.09
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	8	0.09
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	16	0.09
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	16	0.09
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	16	0.09
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	3	0.09
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	3	0.09
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	3	0.09
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	6	0.09
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	6	0.09
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	6	0.09
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	10	0.09
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	10	0.09
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	10	0.09
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	13	0.09
(1,3994)	1:A:82:GLU:H	1:A:83:HIS:HB3	6	0.09
(1,3890)	1:B:82:GLU:HA	1:B:83:HIS:HB2	7	0.09
(1,3798)	1:B:9:ARG:HD2	1:B:78:LEU:HD11	19	0.09
(1,3798)	1:B:9:ARG:HD2	1:B:78:LEU:HD12	19	0.09
(1,3798)	1:B:9:ARG:HD2	1:B:78:LEU:HD13	19	0.09
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD11	19	0.09
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD12	19	0.09
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD13	19	0.09
(1,3734)	1:B:74:THR:HA	1:B:76:GLU:HG2	17	0.09
(1,3734)	1:B:74:THR:HA	1:B:76:GLU:HG3	17	0.09
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	9	0.09
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	9	0.09
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	9	0.09
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	13	0.09
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	13	0.09
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	13	0.09



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	15	0.09
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	15	0.09
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	15	0.09
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	1	0.09
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	1	0.09
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	1	0.09
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	4	0.09
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	4	0.09
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	4	0.09
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	11	0.09
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	11	0.09
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	11	0.09
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	4	0.09
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	4	0.09
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	4	0.09
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	6	0.09
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	6	0.09
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	6	0.09
(1,3592)	1:B:20:ASN:HA	1:B:22:ILE:HB	8	0.09
(1,3592)	1:B:20:ASN:HA	1:B:22:ILE:HB	9	0.09
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG11	15	0.09
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG12	15	0.09
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG13	15	0.09
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG11	15	0.09
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG12	15	0.09
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG13	15	0.09
(1,3559)	1:A:15:LYS:HE2	1:A:16:ASN:HD21	1	0.09
(1,3559)	1:A:15:LYS:HE3	1:A:16:ASN:HD21	1	0.09
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	5	0.09
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	5	0.09
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	5	0.09
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	9	0.09
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	9	0.09
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	9	0.09
(1,3176)	1:B:30:ASP:HB2	1:B:58:LYS:HD2	16	0.09
(1,3176)	1:B:30:ASP:HB2	1:B:58:LYS:HD3	16	0.09
(1,3176)	1:B:30:ASP:HB3	1:B:58:LYS:HD2	16	0.09
(1,3176)	1:B:30:ASP:HB3	1:B:58:LYS:HD3	16	0.09
(1,3104)	1:B:54:LYS:HE2	1:B:55:ASN:HD21	12	0.09
(1,3104)	1:B:54:LYS:HE3	1:B:55:ASN:HD21	12	0.09
(1,3098)	1:B:15:LYS:HD2	1:B:16:ASN:HD21	20	0.09
(1,3098)	1:B:15:LYS:HD3	1:B:16:ASN:HD21	20	0.09



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3093)	1:A:15:LYS:HD2	1:A:16:ASN:HD22	8	0.09
(1,3093)	1:A:15:LYS:HD3	1:A:16:ASN:HD22	8	0.09
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	13	0.09
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	13	0.09
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	13	0.09
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	13	0.09
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	13	0.09
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	13	0.09
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	16	0.09
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	16	0.09
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	16	0.09
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	16	0.09
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	16	0.09
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	16	0.09
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	20	0.09
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	20	0.09
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	20	0.09
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	20	0.09
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	20	0.09
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	20	0.09
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	14	0.09
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	14	0.09
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	14	0.09
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	14	0.09
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	14	0.09
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	14	0.09
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	5	0.09
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	5	0.09
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	5	0.09
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	5	0.09
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	5	0.09
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	5	0.09
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	5	0.09
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	5	0.09
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	5	0.09
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	6	0.09
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	6	0.09
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	6	0.09
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	6	0.09
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	6	0.09
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	6	0.09
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	6	0.09



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	6	0.09
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	6	0.09
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	15	0.09
(1,278)	1:B:20:ASN:H	1:B:20:ASN:HD22	15	0.09
(1,2680)	1:B:9:ARG:HG2	1:B:48:ASN:HA	8	0.09
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	8	0.09
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	12	0.09
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	13	0.09
(1,2521)	1:A:14:ASP:HB2	1:A:43:GLY:HA3	7	0.09
(1,234)	1:A:15:LYS:HG2	1:A:19:THR:H	18	0.09
(1,234)	1:A:15:LYS:HG3	1:A:19:THR:H	18	0.09
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	17	0.09
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	17	0.09
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	17	0.09
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	11	0.09
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	11	0.09
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	11	0.09
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	13	0.09
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	13	0.09
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	13	0.09
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	16	0.09
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	16	0.09
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	16	0.09
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	1	0.09
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	1	0.09
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	1	0.09
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	2	0.09
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	2	0.09
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	2	0.09
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	1	0.09
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	1	0.09
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	1	0.09
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	4	0.09
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	4	0.09
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	4	0.09
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	9	0.09
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	9	0.09
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	9	0.09
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	11	0.09
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	11	0.09
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	11	0.09
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	10	0.09



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	10	0.09
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	10	0.09
(1,2181)	1:A:29:PHE:HD1	1:A:31:THR:HB	14	0.09
(1,2181)	1:A:29:PHE:HD2	1:A:31:THR:HB	14	0.09
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	3	0.09
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	3	0.09
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	3	0.09
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	5	0.09
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	5	0.09
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	5	0.09
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	8	0.09
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	8	0.09
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	8	0.09
(1,2089)	1:A:25:VAL:HG21	1:A:28:LYS:HE2	13	0.09
(1,2089)	1:A:25:VAL:HG21	1:A:28:LYS:HE3	13	0.09
(1,2089)	1:A:25:VAL:HG22	1:A:28:LYS:HE2	13	0.09
(1,2089)	1:A:25:VAL:HG22	1:A:28:LYS:HE3	13	0.09
(1,2089)	1:A:25:VAL:HG23	1:A:28:LYS:HE2	13	0.09
(1,2089)	1:A:25:VAL:HG23	1:A:28:LYS:HE3	13	0.09
(1,2052)	1:B:67:ARG:HE	1:B:75:VAL:HG11	19	0.09
(1,2052)	1:B:67:ARG:HE	1:B:75:VAL:HG12	19	0.09
(1,2052)	1:B:67:ARG:HE	1:B:75:VAL:HG13	19	0.09
(1,2051)	1:A:67:ARG:HE	1:A:75:VAL:HG11	1	0.09
(1,2051)	1:A:67:ARG:HE	1:A:75:VAL:HG12	1	0.09
(1,2051)	1:A:67:ARG:HE	1:A:75:VAL:HG13	1	0.09
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	15	0.09
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	15	0.09
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	15	0.09
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	18	0.09
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	18	0.09
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	18	0.09
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	9	0.09
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	9	0.09
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	9	0.09
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	3	0.09
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	3	0.09
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	3	0.09
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	20	0.09
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	3	0.09
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	16	0.09
(1,1832)	1:B:16:ASN:HB3	1:B:17:GLY:H	18	0.09
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG11	4	0.09



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(1,1761) 1:B:13:0 (1,1761) 1:B:13:0 (1,1761) 1:B:13:0		1:B:69:VAL:HG12	4	0.09
	GLU:HG2		_	0.09
(1,1761) 1:B:13:0		1:B:69:VAL:HG13	4	0.09
	GLU:HG3	1:B:69:VAL:HG11	4	0.09
(1,1761) 1:B:13:0	GLU:HG3	1:B:69:VAL:HG12	4	0.09
(1,1761) 1:B:13:0	GLU:HG3	1:B:69:VAL:HG13	4	0.09
(1,1695) 1:B:11:V	/AL:HG21	1:B:40:ALA:HA	1	0.09
(1,1695) 1:B:11:V	VAL:HG22	1:B:40:ALA:HA	1	0.09
(1,1695) 1:B:11:V	VAL:HG23	1:B:40:ALA:HA	1	0.09
(1,1695) 1:B:11:V	VAL:HG21	1:B:40:ALA:HA	3	0.09
(1,1695) 1:B:11:V	VAL:HG22	1:B:40:ALA:HA	3	0.09
(1,1695) 1:B:11:V	VAL:HG23	1:B:40:ALA:HA	3	0.09
(1,1695) 1:B:11:V	VAL:HG21	1:B:40:ALA:HA	11	0.09
(1,1695) 1:B:11:V	VAL:HG22	1:B:40:ALA:HA	11	0.09
(1,1695) 1:B:11:V	VAL:HG23	1:B:40:ALA:HA	11	0.09
(1,1695) 1:B:11:V	/AL:HG21	1:B:40:ALA:HA	13	0.09
(1,1695) 1:B:11:V	/AL:HG22	1:B:40:ALA:HA	13	0.09
(1,1695) 1:B:11:V	VAL:HG23	1:B:40:ALA:HA	13	0.09
(1,1695) 1:B:11:V	VAL:HG21	1:B:40:ALA:HA	17	0.09
(1,1695) 1:B:11:V	/AL:HG22	1:B:40:ALA:HA	17	0.09
(1,1695) 1:B:11:V	VAL:HG23	1:B:40:ALA:HA	17	0.09
(1,1695) 1:B:11:V	VAL:HG21	1:B:40:ALA:HA	18	0.09
(1,1695) 1:B:11:V	VAL:HG22	1:B:40:ALA:HA	18	0.09
(1,1695) 1:B:11:V	VAL:HG23	1:B:40:ALA:HA	18	0.09
(1,1694) 1:A:11:V	VAL:HG21	1:A:40:ALA:HA	6	0.09
(1,1694) 1:A:11:V	VAL:HG22	1:A:40:ALA:HA	6	0.09
(1,1694) 1:A:11:V	VAL:HG23	1:A:40:ALA:HA	6	0.09
(1,1694) 1:A:11:V	VAL:HG21	1:A:40:ALA:HA	7	0.09
(1,1694) 1:A:11:V	VAL:HG22	1:A:40:ALA:HA	7	0.09
(1,1694) 1:A:11:V	VAL:HG23	1:A:40:ALA:HA	7	0.09
(1,1686) 1:A:11:V	VAL:HG21	1:A:46:THR:HG21	2	0.09
(1,1686) 1:A:11:V	VAL:HG21	1:A:46:THR:HG22	2	0.09
(1,1686) 1:A:11:V	VAL:HG21	1:A:46:THR:HG23	2	0.09
(1,1686) 1:A:11:V	VAL:HG22	1:A:46:THR:HG21	2	0.09
(1,1686) 1:A:11:V	VAL:HG22	1:A:46:THR:HG22	2	0.09
(1,1686) 1:A:11:V	VAL:HG22	1:A:46:THR:HG23	2	0.09
(1,1686) 1:A:11:V	VAL:HG23	1:A:46:THR:HG21	2	0.09
(1,1686) 1:A:11:V	VAL:HG23	1:A:46:THR:HG22	2	0.09
	VAL:HG23	1:A:46:THR:HG23	2	0.09
(1,1538) 1:B:8:I	LE:HD11	1:B:62:LEU:HD21	9	0.09
(1,1538) 1:B:8:I	LE:HD11	1:B:62:LEU:HD22	9	0.09
(1,1538) 1:B:8:I	LE:HD11	1:B:62:LEU:HD23	9	0.09
(1,1538) 1:B:8:I	LE:HD12	1:B:62:LEU:HD21	9	0.09



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Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	9	0.09
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	9	0.09
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	9	0.09
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	9	0.09
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	9	0.09
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	12	0.09
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	12	0.09
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	12	0.09
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	12	0.09
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	12	0.09
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	12	0.09
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	12	0.09
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	12	0.09
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	12	0.09
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	20	0.09
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	20	0.09
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	20	0.09
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	20	0.09
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	20	0.09
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	20	0.09
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	20	0.09
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	20	0.09
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	20	0.09
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	7	0.09
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	7	0.09
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	7	0.09
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	7	0.09
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	7	0.09
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	7	0.09
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	7	0.09
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	7	0.09
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	7	0.09
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	16	0.09
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	16	0.09
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	16	0.09
(1,1413)	1:A:3:ASP:HB2	1:A:53:VAL:H	13	0.09
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	10	0.09
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	3	0.09
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	3	0.09
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	3	0.09
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	11	0.09
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	11	0.09



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(4 4 5 5 .)	Atom-1	$\mathbf{Atom-2}$	Model	Violation (Å)
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	11	0.09
(1,928)	1:A:55:ASN:H	1:A:56:THR:HG21	2	0.08
(1,928)	1:A:55:ASN:H	1:A:56:THR:HG22	2	0.08
(1,928)	1:A:55:ASN:H	1:A:56:THR:HG23	2	0.08
(1,83)	1:B:9:ARG:HE	1:B:11:VAL:HG21	18	0.08
(1,83)	1:B:9:ARG:HE	1:B:11:VAL:HG22	18	0.08
(1,83)	1:B:9:ARG:HE	1:B:11:VAL:HG23	18	0.08
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	20	0.08
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	10	0.08
(1,735)	1:B:40:ALA:HB1	1:B:43:GLY:H	4	0.08
(1,735)	1:B:40:ALA:HB2	1:B:43:GLY:H	4	0.08
(1,735)	1:B:40:ALA:HB3	1:B:43:GLY:H	4	0.08
(1,719)	1:B:41:LYS:H	1:B:46:THR:H	3	0.08
(1,719)	1:B:41:LYS:H	1:B:46:THR:H	13	0.08
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD1	6	0.08
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD2	6	0.08
(1,4959)	1:B:59:LEU:HD11	1:B:77:ARG:HG2	8	0.08
(1,4959)	1:B:59:LEU:HD11	1:B:77:ARG:HG3	8	0.08
(1,4959)	1:B:59:LEU:HD12	1:B:77:ARG:HG2	8	0.08
(1,4959)	1:B:59:LEU:HD12	1:B:77:ARG:HG3	8	0.08
(1,4959)	1:B:59:LEU:HD13	1:B:77:ARG:HG2	8	0.08
(1,4959)	1:B:59:LEU:HD13	1:B:77:ARG:HG3	8	0.08
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE1	3	0.08
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE2	3	0.08
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE3	3	0.08
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE1	3	0.08
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE2	3	0.08
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE3	3	0.08
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE1	15	0.08
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE2	15	0.08
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE3	15	0.08
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE1	15	0.08
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE2	15	0.08
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE3	15	0.08
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB2	12	0.08
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB3	12	0.08
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB2	12	0.08
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB3	12	0.08
(1,4851)	1:B:31:THR:HG21	1:B:58:LYS:HE2	14	0.08
(1,4851)	1:B:31:THR:HG21	1:B:58:LYS:HE3	14	0.08
(1,4851)	1:B:31:THR:HG22	1:B:58:LYS:HE2	14	0.08
(1,4851)	1:B:31:THR:HG22	1:B:58:LYS:HE3	14	0.08



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4851)	1:B:31:THR:HG23	1:B:58:LYS:HE2	14	0.08
(1,4851)	1:B:31:THR:HG23	1:B:58:LYS:HE3	14	0.08
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG2	2	0.08
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	2	0.08
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	2	0.08
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG3	2	0.08
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	2	0.08
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	2	0.08
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG2	15	0.08
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	15	0.08
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	15	0.08
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG3	15	0.08
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	15	0.08
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	15	0.08
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG2	18	0.08
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	18	0.08
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	18	0.08
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG3	18	0.08
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	18	0.08
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	18	0.08
(1,4768)	1:B:15:LYS:HG2	1:B:16:ASN:HD21	17	0.08
(1,4768)	1:B:15:LYS:HG2	1:B:16:ASN:HD22	17	0.08
(1,4768)	1:B:15:LYS:HG3	1:B:16:ASN:HD21	17	0.08
(1,4768)	1:B:15:LYS:HG3	1:B:16:ASN:HD22	17	0.08
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	10	0.08
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	10	0.08
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	10	0.08
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	10	0.08
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	12	0.08
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	12	0.08
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	12	0.08
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	12	0.08
(1,4640)	1:A:54:LYS:HG2	1:A:55:ASN:HD21	2	0.08
(1,4640)	1:A:54:LYS:HG2	1:A:55:ASN:HD22	2	0.08
(1,4640)	1:A:54:LYS:HG3	1:A:55:ASN:HD21	2	0.08
(1,4640)	1:A:54:LYS:HG3	1:A:55:ASN:HD22	2	0.08
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB2	17	0.08
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB3	17	0.08
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB2	17	0.08
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB3	17	0.08
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD21	12	0.08
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD22	12	0.08



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD21	12	0.08
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD22	12	0.08
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD21	12	0.08
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD22	12	0.08
(1,4577)	1:A:34:ARG:HG2	1:A:52:PHE:HD1	19	0.08
(1,4577)	1:A:34:ARG:HG2	1:A:52:PHE:HD2	19	0.08
(1,4577)	1:A:34:ARG:HG3	1:A:52:PHE:HD1	19	0.08
(1,4577)	1:A:34:ARG:HG3	1:A:52:PHE:HD2	19	0.08
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	3	0.08
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	3	0.08
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	3	0.08
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	3	0.08
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	3	0.08
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	3	0.08
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	8	0.08
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	8	0.08
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	8	0.08
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	8	0.08
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	8	0.08
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	8	0.08
(1,4463)	1:A:15:LYS:HD2	1:A:16:ASN:HD21	20	0.08
(1,4463)	1:A:15:LYS:HD2	1:A:16:ASN:HD22	20	0.08
(1,4463)	1:A:15:LYS:HD3	1:A:16:ASN:HD21	20	0.08
(1,4463)	1:A:15:LYS:HD3	1:A:16:ASN:HD22	20	0.08
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	3	0.08
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	3	0.08
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	3	0.08
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	3	0.08
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	1	0.08
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	1	0.08
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	1	0.08
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	2	0.08
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	2	0.08
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	2	0.08
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	4	0.08
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	4	0.08
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	4	0.08
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	10	0.08
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	10	0.08
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	10	0.08
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	1	0.08
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	1	0.08



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	1	0.08
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	7	0.08
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	7	0.08
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	7	0.08
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	8	0.08
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	8	0.08
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	8	0.08
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	12	0.08
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	12	0.08
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	12	0.08
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	13	0.08
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	13	0.08
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	13	0.08
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	18	0.08
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	18	0.08
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	18	0.08
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	19	0.08
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	19	0.08
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	19	0.08
(1,4388)	1:A:81:LEU:HB2	1:A:83:HIS:HD2	5	0.08
(1,4388)	1:A:81:LEU:HB3	1:A:83:HIS:HD2	5	0.08
(1,4388)	1:A:81:LEU:HB2	1:A:83:HIS:HD2	14	0.08
(1,4388)	1:A:81:LEU:HB3	1:A:83:HIS:HD2	14	0.08
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	11	0.08
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	11	0.08
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	11	0.08
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	11	0.08
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	11	0.08
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	11	0.08
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	16	0.08
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	16	0.08
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	16	0.08
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	16	0.08
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	16	0.08
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	16	0.08
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG21	6	0.08
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG22	6	0.08
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG23	6	0.08
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE1	1	0.08
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE2	1	0.08
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE1	1	0.08
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE2	1	0.08



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE1	13	0.08
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE2	13	0.08
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE1	13	0.08
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE2	13	0.08
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE1	15	0.08
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE2	15	0.08
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE1	15	0.08
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE2	15	0.08
(1,4209)	1:B:29:PHE:HA	1:B:29:PHE:HD1	6	0.08
(1,4209)	1:B:29:PHE:HA	1:B:29:PHE:HD2	6	0.08
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	14	0.08
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	14	0.08
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	14	0.08
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	18	0.08
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	18	0.08
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	18	0.08
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	20	0.08
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	20	0.08
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	20	0.08
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	5	0.08
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	5	0.08
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	5	0.08
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	14	0.08
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	14	0.08
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	14	0.08
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	18	0.08
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	18	0.08
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	18	0.08
(1,4053)	1:B:41:LYS:HG2	1:B:42:ASP:HA	8	0.08
(1,4053)	1:B:41:LYS:HG3	1:B:42:ASP:HA	8	0.08
(1,4053)	1:B:41:LYS:HG2	1:B:42:ASP:HA	10	0.08
(1,4053)	1:B:41:LYS:HG3	1:B:42:ASP:HA	10	0.08
(1,4053)	1:B:41:LYS:HG2	1:B:42:ASP:HA	12	0.08
(1,4053)	1:B:41:LYS:HG3	1:B:42:ASP:HA	12	0.08
(1,4052)	1:A:41:LYS:HG2	1:A:42:ASP:HA	6	0.08
(1,4052)	1:A:41:LYS:HG3	1:A:42:ASP:HA	6	0.08
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	3	0.08
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	16	0.08
(1,3994)	1:A:82:GLU:H	1:A:83:HIS:HB3	7	0.08
(1,3994)	1:A:82:GLU:H	1:A:83:HIS:HB3	18	0.08
(1,3994)	1:A:82:GLU:H	1:A:83:HIS:HB3	20	0.08
(1,3987)	1:B:81:LEU:HD11	1:B:83:HIS:HB3	5	0.08



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3987)	1:B:81:LEU:HD12	1:B:83:HIS:HB3	5	0.08
(1,3987)	1:B:81:LEU:HD13	1:B:83:HIS:HB3	5	0.08
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD11	14	0.08
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD12	14	0.08
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD13	14	0.08
(1,3846)	1:B:80:ASN:HB3	1:B:81:LEU:HD21	8	0.08
(1,3846)	1:B:80:ASN:HB3	1:B:81:LEU:HD22	8	0.08
(1,3846)	1:B:80:ASN:HB3	1:B:81:LEU:HD23	8	0.08
(1,3839)	1:A:78:LEU:H	1:A:79:SER:HB2	11	0.08
(1,3839)	1:A:78:LEU:H	1:A:79:SER:HB3	11	0.08
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD11	10	0.08
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD12	10	0.08
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD13	10	0.08
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	2	0.08
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	2	0.08
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	2	0.08
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	18	0.08
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	18	0.08
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	18	0.08
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	1	0.08
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	1	0.08
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	1	0.08
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	6	0.08
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	6	0.08
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	6	0.08
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	7	0.08
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	7	0.08
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	7	0.08
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	10	0.08
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	10	0.08
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	10	0.08
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	5	0.08
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	5	0.08
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	5	0.08
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	6	0.08
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	6	0.08
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	6	0.08
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	15	0.08
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	15	0.08
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	15	0.08
(1,3592)	1:B:20:ASN:HA	1:B:22:ILE:HB	4	0.08
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG11	18	0.08



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG12	18	0.08
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG13	18	0.08
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG11	18	0.08
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG12	18	0.08
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG13	18	0.08
(1,3561)	1:A:15:LYS:HE2	1:A:18:MET:H	11	0.08
(1,3561)	1:A:15:LYS:HE3	1:A:18:MET:H	11	0.08
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	5	0.08
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	5	0.08
(1,3423)	1:B:9:ARG:H	1:B:63:MET:HE1	4	0.08
(1,3423)	1:B:9:ARG:H	1:B:63:MET:HE2	4	0.08
(1,3423)	1:B:9:ARG:H	1:B:63:MET:HE3	4	0.08
(1,3413)	1:B:63:MET:HE1	1:B:76:GLU:HA	18	0.08
(1,3413)	1:B:63:MET:HE2	1:B:76:GLU:HA	18	0.08
(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	18	0.08
(1,3413)	1:B:63:MET:HE1	1:B:76:GLU:HA	19	0.08
(1,3413)	1:B:63:MET:HE2	1:B:76:GLU:HA	19	0.08
(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	19	0.08
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE1	6	0.08
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE2	6	0.08
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE3	6	0.08
(1,3360)	1:A:30:ASP:H	1:A:62:LEU:HD11	17	0.08
(1,3360)	1:A:30:ASP:H	1:A:62:LEU:HD12	17	0.08
(1,3360)	1:A:30:ASP:H	1:A:62:LEU:HD13	17	0.08
(1,3176)	1:B:30:ASP:HB2	1:B:58:LYS:HD2	15	0.08
(1,3176)	1:B:30:ASP:HB2	1:B:58:LYS:HD3	15	0.08
(1,3176)	1:B:30:ASP:HB3	1:B:58:LYS:HD2	15	0.08
(1,3176)	1:B:30:ASP:HB3	1:B:58:LYS:HD3	15	0.08
(1,3175)	1:A:30:ASP:HB2	1:A:58:LYS:HD2	8	0.08
(1,3175)	1:A:30:ASP:HB2	1:A:58:LYS:HD3	8	0.08
(1,3175)	1:A:30:ASP:HB3	1:A:58:LYS:HD2	8	0.08
(1,3175)	1:A:30:ASP:HB3	1:A:58:LYS:HD3	8	0.08
(1,3104)	1:B:54:LYS:HE2	1:B:55:ASN:HD21	8	0.08
(1,3104)	1:B:54:LYS:HE3	1:B:55:ASN:HD21	8	0.08
(1,3102)	1:B:54:LYS:HA	1:B:54:LYS:HE2	17	0.08
(1,3102)	1:B:54:LYS:HA	1:B:54:LYS:HE3	17	0.08
(1,3)	1:A:2:THR:HG21	1:A:4:PHE:H	16	0.08
(1,3)	1:A:2:THR:HG22	1:A:4:PHE:H	16	0.08
(1,3)	1:A:2:THR:HG23	1:A:4:PHE:H	16	0.08
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	5	0.08
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	5	0.08
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	5	0.08



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Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	5	0.08
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	5	0.08
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	5	0.08
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	6	0.08
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	6	0.08
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	6	0.08
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	6	0.08
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	6	0.08
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	6	0.08
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	10	0.08
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	10	0.08
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	10	0.08
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	10	0.08
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	10	0.08
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	10	0.08
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	2	0.08
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	2	0.08
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	2	0.08
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	2	0.08
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	2	0.08
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	2	0.08
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	8	0.08
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	8	0.08
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	8	0.08
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	8	0.08
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	8	0.08
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	8	0.08
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	18	0.08
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	18	0.08
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	18	0.08
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	18	0.08
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	18	0.08
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	18	0.08
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	19	0.08
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	19	0.08
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	19	0.08
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	19	0.08
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	19	0.08
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	19	0.08
(1,289)	1:A:33:ILE:HG13	1:B:20:ASN:HD21	6	0.08
(1,2871)	1:A:15:LYS:HG2	1:A:16:ASN:H	20	0.08
(1,2871)	1:A:15:LYS:HG3	1:A:16:ASN:H	20	0.08



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	10	0.08
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	10	0.08
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	10	0.08
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	3	0.08
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	11	0.08
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	11	0.08
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	11	0.08
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	15	0.08
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	15	0.08
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	15	0.08
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	1	0.08
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	16	0.08
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	1	0.08
(1,2522)	1:B:14:ASP:HB2	1:B:43:GLY:HA3	6	0.08
(1,2485)	1:A:40:ALA:HA	1:A:45:PHE:HA	10	0.08
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	7	0.08
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	7	0.08
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	7	0.08
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	1	0.08
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	1	0.08
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	1	0.08
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	3	0.08
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	3	0.08
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	3	0.08
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	11	0.08
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	11	0.08
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	11	0.08
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	8	0.08
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	8	0.08
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	8	0.08
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	14	0.08
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	14	0.08
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	14	0.08
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	2	0.08
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	2	0.08
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	2	0.08
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	17	0.08
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	17	0.08
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	17	0.08
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	19	0.08
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	19	0.08
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	19	0.08



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2284)	1:A:36:ILE:HG21	1:B:39:ASN:HB2	4	0.08
(1,2284)	1:A:36:ILE:HG21	1:B:39:ASN:HB3	4	0.08
(1,2284)	1:A:36:ILE:HG22	1:B:39:ASN:HB2	4	0.08
(1,2284)	1:A:36:ILE:HG22	1:B:39:ASN:HB3	4	0.08
(1,2284)	1:A:36:ILE:HG23	1:B:39:ASN:HB2	4	0.08
(1,2284)	1:A:36:ILE:HG23	1:B:39:ASN:HB3	4	0.08
(1,2182)	1:B:29:PHE:HD1	1:B:31:THR:HB	1	0.08
(1,2182)	1:B:29:PHE:HD2	1:B:31:THR:HB	1	0.08
(1,2182)	1:B:29:PHE:HD1	1:B:31:THR:HB	14	0.08
(1,2182)	1:B:29:PHE:HD2	1:B:31:THR:HB	14	0.08
(1,2181)	1:A:29:PHE:HD1	1:A:31:THR:HB	6	0.08
(1,2181)	1:A:29:PHE:HD2	1:A:31:THR:HB	6	0.08
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	19	0.08
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	19	0.08
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	19	0.08
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	2	0.08
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	2	0.08
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	2	0.08
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	12	0.08
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	12	0.08
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	12	0.08
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	1	0.08
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	1	0.08
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	1	0.08
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	2	0.08
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	2	0.08
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	2	0.08
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	4	0.08
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	4	0.08
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	4	0.08
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	5	0.08
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	5	0.08
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	5	0.08
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	12	0.08
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	12	0.08
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	12	0.08
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	18	0.08
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	18	0.08
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	18	0.08
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	2	0.08
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	2	0.08
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	2	0.08



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	20	0.08
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	20	0.08
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	20	0.08
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	11	0.08
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	11	0.08
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	11	0.08
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	14	0.08
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	14	0.08
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	14	0.08
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	4	0.08
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	7	0.08
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	18	0.08
(1,1832)	1:B:16:ASN:HB3	1:B:17:GLY:H	2	0.08
(1,1831)	1:A:16:ASN:HB3	1:A:17:GLY:H	5	0.08
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG11	1	0.08
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG12	1	0.08
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG13	1	0.08
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG11	1	0.08
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG12	1	0.08
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG13	1	0.08
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG11	16	0.08
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG12	16	0.08
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG13	16	0.08
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG11	16	0.08
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG12	16	0.08
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG13	16	0.08
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	9	0.08
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	9	0.08
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	9	0.08
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	14	0.08
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	14	0.08
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	14	0.08
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	16	0.08
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	16	0.08
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	16	0.08
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	17	0.08
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	17	0.08
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	17	0.08
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	4	0.08
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	4	0.08
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	4	0.08
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	4	0.08



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	4	0.08
	1:B:11:VAL:HG22	1:B:46:THR:HG23	4	0.08
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	4	0.08
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	4	0.08
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	4	0.08
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	10	0.08
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	10	0.08
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	10	0.08
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	10	0.08
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	10	0.08
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG23	10	0.08
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	10	0.08
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	10	0.08
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	10	0.08
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	19	0.08
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	19	0.08
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	19	0.08
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	19	0.08
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	19	0.08
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	19	0.08
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	19	0.08
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	19	0.08
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	19	0.08
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	2	0.08
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	2	0.08
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	2	0.08
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	2	0.08
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	2	0.08
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	2	0.08
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	2	0.08
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	2	0.08
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	2	0.08
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	6	0.08
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	6	0.08
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	6	0.08
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	6	0.08
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	6	0.08
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	6	0.08
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	6	0.08
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	6	0.08
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	6	0.08
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	8	0.08



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	8	0.08
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	8	0.08
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	8	0.08
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	8	0.08
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	8	0.08
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	8	0.08
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	8	0.08
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	8	0.08
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	9	0.08
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	9	0.08
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	9	0.08
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	9	0.08
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	9	0.08
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	9	0.08
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	4	0.08
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	4	0.08
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	4	0.08
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	4	0.08
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	4	0.08
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	4	0.08
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	15	0.08
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	15	0.08
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	15	0.08
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	15	0.08
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	15	0.08
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	15	0.08
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	2	0.08
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	2	0.08
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	2	0.08
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	10	0.08
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	10	0.08
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	10	0.08
(1,1414)	1:B:3:ASP:HB2	1:B:53:VAL:H	12	0.08
(1,1302)	1:B:77:ARG:H	1:B:77:ARG:HB2	16	0.08
(1,1212)	1:B:69:VAL:HG11	1:B:71:GLY:H	15	0.08
(1,1212)	1:B:69:VAL:HG12	1:B:71:GLY:H	15	0.08
(1,1212)	1:B:69:VAL:HG13	1:B:71:GLY:H	15	0.08
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	14	0.08
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	19	0.08
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	3	0.08
(1,1134)	1:B:67:ARG:H	1:B:67:ARG:HD2	6	0.08
(1,1134)	1:B:67:ARG:H	1:B:67:ARG:HD3	6	0.08



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	14	0.08
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	14	0.08
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	14	0.08
(1,1020)	1:A:58:LYS:HZ1	1:A:61:THR:H	10	0.08
(1,1020)	1:A:58:LYS:HZ2	1:A:61:THR:H	10	0.08
(1,1020)	1:A:58:LYS:HZ3	1:A:61:THR:H	10	0.08
(1,1020)	1:A:58:LYS:HZ1	1:A:61:THR:H	17	0.08
(1,1020)	1:A:58:LYS:HZ2	1:A:61:THR:H	17	0.08
(1,1020)	1:A:58:LYS:HZ3	1:A:61:THR:H	17	0.08
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	9	0.07
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	10	0.07
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	4	0.07
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	13	0.07
(1,736)	1:A:41:LYS:HG2	1:A:43:GLY:H	1	0.07
(1,736)	1:A:41:LYS:HG3	1:A:43:GLY:H	1	0.07
(1,719)	1:B:41:LYS:H	1:B:46:THR:H	19	0.07
(1,718)	1:A:41:LYS:H	1:A:46:THR:H	1	0.07
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD1	9	0.07
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD2	9	0.07
(1,696)	1:A:41:LYS:H	1:A:41:LYS:HG2	1	0.07
(1,696)	1:A:41:LYS:H	1:A:41:LYS:HG3	1	0.07
(1,668)	1:A:39:ASN:H	1:A:48:ASN:H	9	0.07
(1,568)	1:A:20:ASN:H	1:B:32:ASN:HD21	2	0.07
(1,568)	1:A:20:ASN:H	1:B:32:ASN:HD21	15	0.07
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD11	20	0.07
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD12	20	0.07
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD13	20	0.07
(1,546)	1:B:29:PHE:HD1	1:B:31:THR:H	4	0.07
(1,546)	1:B:29:PHE:HD2	1:B:31:THR:H	4	0.07
(1,4936)	1:B:54:LYS:HE2	1:B:55:ASN:HD21	17	0.07
(1,4936)	1:B:54:LYS:HE2	1:B:55:ASN:HD22	17	0.07
(1,4936)	1:B:54:LYS:HE3	1:B:55:ASN:HD21	17	0.07
(1,4936)	1:B:54:LYS:HE3	1:B:55:ASN:HD22	17	0.07
(1,4906)	1:B:42:ASP:HB2	1:B:44:ILE:HG12	14	0.07
(1,4906)	1:B:42:ASP:HB3	1:B:44:ILE:HG12	14	0.07
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB2	4	0.07
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB3	4	0.07
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB2	4	0.07
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB3	4	0.07
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB2	14	0.07
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB3	14	0.07
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB2	14	0.07



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB3	14	0.07
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB2	18	0.07
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB3	18	0.07
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB2	18	0.07
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB3	18	0.07
(1,4887)	1:B:37:VAL:HG11	1:B:48:ASN:HD21	20	0.07
(1,4887)	1:B:37:VAL:HG11	1:B:48:ASN:HD22	20	0.07
(1,4887)	1:B:37:VAL:HG12	1:B:48:ASN:HD21	20	0.07
(1,4887)	1:B:37:VAL:HG12	1:B:48:ASN:HD22	20	0.07
(1,4887)	1:B:37:VAL:HG13	1:B:48:ASN:HD21	20	0.07
(1,4887)	1:B:37:VAL:HG13	1:B:48:ASN:HD22	20	0.07
(1,4861)	1:B:32:ASN:HD21	1:B:33:ILE:HB	14	0.07
(1,4861)	1:B:32:ASN:HD22	1:B:33:ILE:HB	14	0.07
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG2	9	0.07
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	9	0.07
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	9	0.07
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG3	9	0.07
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	9	0.07
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	9	0.07
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG2	14	0.07
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	14	0.07
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	14	0.07
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG3	14	0.07
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	14	0.07
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	14	0.07
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG2	17	0.07
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	17	0.07
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	17	0.07
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG3	17	0.07
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	17	0.07
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	17	0.07
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	6	0.07
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	6	0.07
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	6	0.07
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	6	0.07
(1,4613)	1:A:42:ASP:HB2	1:A:44:ILE:HG12	7	0.07
(1,4613)	1:A:42:ASP:HB3	1:A:44:ILE:HG12	7	0.07
(1,4613)	1:A:42:ASP:HB2	1:A:44:ILE:HG12	15	0.07
(1,4613)	1:A:42:ASP:HB3	1:A:44:ILE:HG12	15	0.07
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB2	16	0.07
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB3	16	0.07
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB2	16	0.07



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB3	16	0.07
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB2	19	0.07
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB3	19	0.07
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB2	19	0.07
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB3	19	0.07
(1,4593)	1:A:37:VAL:HG11	1:A:48:ASN:HD21	12	0.07
(1,4593)	1:A:37:VAL:HG11	1:A:48:ASN:HD22	12	0.07
(1,4593)	1:A:37:VAL:HG12	1:A:48:ASN:HD21	12	0.07
(1,4593)	1:A:37:VAL:HG12	1:A:48:ASN:HD22	12	0.07
(1,4593)	1:A:37:VAL:HG13	1:A:48:ASN:HD21	12	0.07
(1,4593)	1:A:37:VAL:HG13	1:A:48:ASN:HD22	12	0.07
(1,4560)	1:A:31:THR:HG21	1:A:58:LYS:HE2	12	0.07
(1,4560)	1:A:31:THR:HG21	1:A:58:LYS:HE3	12	0.07
(1,4560)	1:A:31:THR:HG22	1:A:58:LYS:HE2	12	0.07
(1,4560)	1:A:31:THR:HG22	1:A:58:LYS:HE3	12	0.07
(1,4560)	1:A:31:THR:HG23	1:A:58:LYS:HE2	12	0.07
(1,4560)	1:A:31:THR:HG23	1:A:58:LYS:HE3	12	0.07
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	1	0.07
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	1	0.07
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	1	0.07
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	1	0.07
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	1	0.07
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	1	0.07
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	13	0.07
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	13	0.07
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	13	0.07
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	4	0.07
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	4	0.07
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	4	0.07
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	5	0.07
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	5	0.07
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	5	0.07
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	11	0.07
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	11	0.07
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	11	0.07
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	17	0.07
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	17	0.07
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	17	0.07
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	17	0.07
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	17	0.07
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	17	0.07
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	20	0.07



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Key	$egin{aligned} Atom-1 \end{aligned}$	Atom-2	Model	Violation (Å)
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	20	0.07
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	20	0.07
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	20	0.07
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	20	0.07
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	20	0.07
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	2	0.07
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	2	0.07
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	2	0.07
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	2	0.07
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	2	0.07
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	2	0.07
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	3	0.07
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	3	0.07
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	3	0.07
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	3	0.07
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	3	0.07
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	3	0.07
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	12	0.07
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	12	0.07
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	12	0.07
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	12	0.07
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	12	0.07
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	12	0.07
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	17	0.07
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	17	0.07
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	17	0.07
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	17	0.07
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	17	0.07
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	17	0.07
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG21	8	0.07
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG22	8	0.07
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG23	8	0.07
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG21	14	0.07
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG22	14	0.07
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG23	14	0.07
(1,4353)	1:B:44:ILE:HG13	1:B:73:PHE:HE1	1	0.07
(1,4353)	1:B:44:ILE:HG13	1:B:73:PHE:HE2	1	0.07
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE1	4	0.07
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE2	4	0.07
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE1	4	0.07
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE2	4	0.07
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE1	6	0.07



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Key	$egin{aligned} Atom-1 \end{aligned}$	Atom-2	Model	Violation (Å)
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE2	6	0.07
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE1	6	0.07
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE2	6	0.07
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE1	2	0.07
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE2	2	0.07
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE1	2	0.07
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE2	2	0.07
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE1	3	0.07
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE2	3	0.07
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE1	3	0.07
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE2	3	0.07
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE1	17	0.07
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE2	17	0.07
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE1	17	0.07
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE2	17	0.07
(1,4323)	1:B:52:PHE:HD1	1:B:53:VAL:H	15	0.07
(1,4323)	1:B:52:PHE:HD2	1:B:53:VAL:H	15	0.07
(1,4323)	1:B:52:PHE:HD1	1:B:53:VAL:H	19	0.07
(1,4323)	1:B:52:PHE:HD2	1:B:53:VAL:H	19	0.07
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	13	0.07
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	3	0.07
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	3	0.07
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	3	0.07
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	17	0.07
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	17	0.07
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	17	0.07
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	8	0.07
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	8	0.07
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	8	0.07
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	20	0.07
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	20	0.07
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	20	0.07
(1,4164)	1:A:4:PHE:HE1	1:A:55:ASN:HA	15	0.07
(1,4164)	1:A:4:PHE:HE2	1:A:55:ASN:HA	15	0.07
(1,4162)	1:A:4:PHE:HE1	1:A:56:THR:HA	6	0.07
(1,4162)	1:A:4:PHE:HE2	1:A:56:THR:HA	6	0.07
(1,4119)	1:B:80:ASN:HA	1:B:81:LEU:HG	5	0.07
(1,4050)	1:A:41:LYS:HA	1:A:42:ASP:H	15	0.07
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	12	0.07
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	12	0.07
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	9	0.07
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	20	0.07



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	4	0.07
(1,3994)	1:A:82:GLU:H	1:A:83:HIS:HB3	19	0.07
(1,3987)	1:B:81:LEU:HD11	1:B:83:HIS:HB3	6	0.07
(1,3987)	1:B:81:LEU:HD12	1:B:83:HIS:HB3	6	0.07
(1,3987)	1:B:81:LEU:HD13	1:B:83:HIS:HB3	6	0.07
(1,3984)	1:A:5:LEU:HD11	1:A:81:LEU:HD11	17	0.07
(1,3984)	1:A:5:LEU:HD11	1:A:81:LEU:HD12	17	0.07
(1,3984)	1:A:5:LEU:HD11	1:A:81:LEU:HD13	17	0.07
(1,3984)	1:A:5:LEU:HD12	1:A:81:LEU:HD11	17	0.07
(1,3984)	1:A:5:LEU:HD12	1:A:81:LEU:HD12	17	0.07
(1,3984)	1:A:5:LEU:HD12	1:A:81:LEU:HD13	17	0.07
(1,3984)	1:A:5:LEU:HD13	1:A:81:LEU:HD11	17	0.07
(1,3984)	1:A:5:LEU:HD13	1:A:81:LEU:HD12	17	0.07
(1,3984)	1:A:5:LEU:HD13	1:A:81:LEU:HD13	17	0.07
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD11	5	0.07
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD12	5	0.07
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD13	5	0.07
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD11	6	0.07
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD12	6	0.07
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD13	6	0.07
(1,3917)	1:A:18:MET:HE1	1:A:21:GLN:HE21	17	0.07
(1,3917)	1:A:18:MET:HE2	1:A:21:GLN:HE21	17	0.07
(1,3917)	1:A:18:MET:HE3	1:A:21:GLN:HE21	17	0.07
(1,3890)	1:B:82:GLU:HA	1:B:83:HIS:HB2	4	0.07
(1,3798)	1:B:9:ARG:HD2	1:B:78:LEU:HD11	15	0.07
(1,3798)	1:B:9:ARG:HD2	1:B:78:LEU:HD12	15	0.07
(1,3798)	1:B:9:ARG:HD2	1:B:78:LEU:HD13	15	0.07
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD11	15	0.07
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD12	15	0.07
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD13	15	0.07
(1,3758)	1:B:6:ALA:HB1	1:B:77:ARG:HD2	16	0.07
(1,3758)	1:B:6:ALA:HB1	1:B:77:ARG:HD3	16	0.07
(1,3758)	1:B:6:ALA:HB2	1:B:77:ARG:HD2	16	0.07
(1,3758)	1:B:6:ALA:HB2	1:B:77:ARG:HD3	16	0.07
(1,3758)	1:B:6:ALA:HB3	1:B:77:ARG:HD2	16	0.07
(1,3758)	1:B:6:ALA:HB3	1:B:77:ARG:HD3	16	0.07
(1,3733)	1:A:74:THR:HA	1:A:76:GLU:HG2	15	0.07
(1,3733)	1:A:74:THR:HA	1:A:76:GLU:HG3	15	0.07
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	15	0.07
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	15	0.07
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	15	0.07
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	16	0.07



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	16	0.07
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	16	0.07
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	11	0.07
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	11	0.07
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	11	0.07
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	18	0.07
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	18	0.07
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	18	0.07
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	8	0.07
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	8	0.07
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	8	0.07
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	12	0.07
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	12	0.07
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	12	0.07
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	14	0.07
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	14	0.07
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	14	0.07
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG11	17	0.07
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG12	17	0.07
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG13	17	0.07
(1,3614)	1:B:69:VAL:H	1:B:70:GLN:HB2	5	0.07
(1,3614)	1:B:69:VAL:H	1:B:70:GLN:HB3	5	0.07
(1,3614)	1:B:69:VAL:H	1:B:70:GLN:HB2	15	0.07
(1,3614)	1:B:69:VAL:H	1:B:70:GLN:HB3	15	0.07
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB2	17	0.07
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB3	17	0.07
(1,3593)	1:A:66:LEU:HA	1:A:69:VAL:HB	18	0.07
(1,3592)	1:B:20:ASN:HA	1:B:22:ILE:HB	1	0.07
(1,3592)	1:B:20:ASN:HA	1:B:22:ILE:HB	5	0.07
(1,3591)	1:A:20:ASN:HA	1:A:22:ILE:HB	3	0.07
(1,3591)	1:A:20:ASN:HA	1:A:22:ILE:HB	4	0.07
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG11	11	0.07
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG12	11	0.07
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG13	11	0.07
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG11	11	0.07
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG12	11	0.07
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG13	11	0.07
(1,3560)	1:B:15:LYS:HE2	1:B:16:ASN:HD21	1	0.07
(1,3560)	1:B:15:LYS:HE3	1:B:16:ASN:HD21	1	0.07
(1,3560)	1:B:15:LYS:HE2	1:B:16:ASN:HD21	19	0.07
(1,3560)	1:B:15:LYS:HE3	1:B:16:ASN:HD21	19	0.07
(1,3559)	1:A:15:LYS:HE2	1:A:16:ASN:HD21	11	0.07



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3559)	1:A:15:LYS:HE3	1:A:16:ASN:HD21	11	0.07
(1,3422)	1:A:9:ARG:H	1:A:63:MET:HE1	15	0.07
(1,3422)	1:A:9:ARG:H	1:A:63:MET:HE2	15	0.07
(1,3422)	1:A:9:ARG:H	1:A:63:MET:HE3	15	0.07
(1,3413)	1:B:63:MET:HE1	1:B:76:GLU:HA	2	0.07
(1,3413)	1:B:63:MET:HE2	1:B:76:GLU:HA	2	0.07
(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	2	0.07
(1,3413)	1:B:63:MET:HE1	1:B:76:GLU:HA	3	0.07
(1,3413)	1:B:63:MET:HE2	1:B:76:GLU:HA	3	0.07
(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	3	0.07
(1,3412)	1:A:63:MET:HE1	1:A:76:GLU:HA	5	0.07
(1,3412)	1:A:63:MET:HE2	1:A:76:GLU:HA	5	0.07
(1,3412)	1:A:63:MET:HE3	1:A:76:GLU:HA	5	0.07
(1,3412)	1:A:63:MET:HE1	1:A:76:GLU:HA	6	0.07
(1,3412)	1:A:63:MET:HE2	1:A:76:GLU:HA	6	0.07
(1,3412)	1:A:63:MET:HE3	1:A:76:GLU:HA	6	0.07
(1,3412)	1:A:63:MET:HE1	1:A:76:GLU:HA	12	0.07
(1,3412)	1:A:63:MET:HE2	1:A:76:GLU:HA	12	0.07
(1,3412)	1:A:63:MET:HE3	1:A:76:GLU:HA	12	0.07
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	6	0.07
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	6	0.07
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	6	0.07
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	7	0.07
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	7	0.07
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	7	0.07
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	11	0.07
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	11	0.07
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	11	0.07
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	14	0.07
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	14	0.07
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	14	0.07
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE1	3	0.07
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE2	3	0.07
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE3	3	0.07
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE1	17	0.07
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE2	17	0.07
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE3	17	0.07
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE1	7	0.07
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE2	7	0.07
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE3	7	0.07
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE1	7	0.07
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE2	7	0.07



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Key	$rac{Atom-1}{Atom-1}$	Atom-2	Model	Violation (Å)
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE3	7	0.07
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE1	7	0.07
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE2	7	0.07
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE3	7	0.07
(1,3360)	1:A:30:ASP:H	1:A:62:LEU:HD11	4	0.07
(1,3360)	1:A:30:ASP:H	1:A:62:LEU:HD12	4	0.07
(1,3360)	1:A:30:ASP:H	1:A:62:LEU:HD13	4	0.07
(1,3104)	1:B:54:LYS:HE2	1:B:55:ASN:HD21	14	0.07
(1,3104)	1:B:54:LYS:HE3	1:B:55:ASN:HD21	14	0.07
(1,3094)	1:B:15:LYS:HD2	1:B:16:ASN:HD22	10	0.07
(1,3094)	1:B:15:LYS:HD3	1:B:16:ASN:HD22	10	0.07
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD2	5	0.07
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD3	5	0.07
(1,3091)	1:A:54:LYS:HA	1:A:54:LYS:HD2	14	0.07
(1,3091)	1:A:54:LYS:HA	1:A:54:LYS:HD3	14	0.07
(1,3)	1:A:2:THR:HG21	1:A:4:PHE:H	20	0.07
(1,3)	1:A:2:THR:HG22	1:A:4:PHE:H	20	0.07
(1,3)	1:A:2:THR:HG23	1:A:4:PHE:H	20	0.07
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	15	0.07
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	15	0.07
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	15	0.07
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	15	0.07
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	15	0.07
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	15	0.07
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	1	0.07
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	1	0.07
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	1	0.07
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	1	0.07
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	1	0.07
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	1	0.07
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	20	0.07
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	20	0.07
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	20	0.07
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	20	0.07
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	20	0.07
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	20	0.07
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD11	4	0.07
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD12	4	0.07
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD13	4	0.07
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	11	0.07
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	11	0.07
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	11	0.07



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	11	0.07
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	11	0.07
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	11	0.07
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	11	0.07
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	11	0.07
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	11	0.07
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD11	12	0.07
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD12	12	0.07
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD13	12	0.07
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD11	12	0.07
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD12	12	0.07
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD13	12	0.07
(1,2816)	1:B:50:MET:HE1	1:B:51:ILE:HG13	3	0.07
(1,2816)	1:B:50:MET:HE2	1:B:51:ILE:HG13	3	0.07
(1,2816)	1:B:50:MET:HE3	1:B:51:ILE:HG13	3	0.07
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	1	0.07
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	1	0.07
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	1	0.07
(1,2791)	1:A:8:ILE:H	1:A:50:MET:HG3	6	0.07
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	10	0.07
(1,278)	1:B:20:ASN:H	1:B:20:ASN:HD22	13	0.07
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD21	4	0.07
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD22	4	0.07
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD23	4	0.07
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD21	4	0.07
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD22	4	0.07
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD23	4	0.07
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD21	4	0.07
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD22	4	0.07
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD23	4	0.07
(1,2618)	1:B:9:ARG:HD2	1:B:46:THR:HG21	20	0.07
(1,2618)	1:B:9:ARG:HD2	1:B:46:THR:HG22	20	0.07
(1,2618)	1:B:9:ARG:HD2	1:B:46:THR:HG23	20	0.07
(1,2618)	1:B:9:ARG:HD3	1:B:46:THR:HG21	20	0.07
(1,2618)	1:B:9:ARG:HD3	1:B:46:THR:HG22	20	0.07
(1,2618)	1:B:9:ARG:HD3	1:B:46:THR:HG23	20	0.07
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	2	0.07
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	2	0.07
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	2	0.07
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	5	0.07
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	5	0.07
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	5	0.07



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	6	0.07
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	6	0.07
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	6	0.07
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	19	0.07
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	19	0.07
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	19	0.07
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	8	0.07
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	7	0.07
(1,2502)	1:B:15:LYS:H	1:B:40:ALA:HB1	19	0.07
(1,2502)	1:B:15:LYS:H	1:B:40:ALA:HB2	19	0.07
(1,2502)	1:B:15:LYS:H	1:B:40:ALA:HB3	19	0.07
(1,2424)	1:B:38:LEU:HD11	1:B:39:ASN:H	19	0.07
(1,2424)	1:B:38:LEU:HD12	1:B:39:ASN:H	19	0.07
(1,2424)	1:B:38:LEU:HD13	1:B:39:ASN:H	19	0.07
(1,2330)	1:B:36:ILE:HD11	1:B:38:LEU:H	10	0.07
(1,2330)	1:B:36:ILE:HD12	1:B:38:LEU:H	10	0.07
(1,2330)	1:B:36:ILE:HD13	1:B:38:LEU:H	10	0.07
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	1	0.07
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	1	0.07
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	1	0.07
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	6	0.07
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	6	0.07
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	6	0.07
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	19	0.07
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	19	0.07
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	19	0.07
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	10	0.07
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	10	0.07
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	10	0.07
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	17	0.07
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	17	0.07
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	17	0.07
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	15	0.07
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	15	0.07
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	15	0.07
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	18	0.07
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	18	0.07
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	18	0.07
(1,2181)	1:A:29:PHE:HD1	1:A:31:THR:HB	10	0.07
(1,2181)	1:A:29:PHE:HD2	1:A:31:THR:HB	10	0.07
(1,2173)	1:A:68:LYS:HA	1:A:68:LYS:HD2	11	0.07
(1,2163)	1:A:27:SER:HG	1:A:28:LYS:HG2	7	0.07



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	5	0.07
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	5	0.07
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	5	0.07
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	11	0.07
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	11	0.07
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	11	0.07
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	16	0.07
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	16	0.07
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	16	0.07
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	17	0.07
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	17	0.07
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	17	0.07
(1,208)	1:B:16:ASN:HA	1:B:17:GLY:H	17	0.07
(1,207)	1:A:16:ASN:HA	1:A:17:GLY:H	8	0.07
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	6	0.07
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	6	0.07
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	6	0.07
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	7	0.07
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	7	0.07
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	7	0.07
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	8	0.07
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	8	0.07
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	8	0.07
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	13	0.07
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	13	0.07
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	13	0.07
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	14	0.07
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	14	0.07
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	14	0.07
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	16	0.07
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	16	0.07
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	16	0.07
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	4	0.07
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	4	0.07
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	4	0.07
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	14	0.07
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	14	0.07
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	14	0.07
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	2	0.07
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	2	0.07
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	2	0.07
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	6	0.07



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	6	0.07
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	6	0.07
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	15	0.07
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	15	0.07
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	15	0.07
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	17	0.07
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	17	0.07
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	17	0.07
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	1	0.07
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	1	0.07
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	1	0.07
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	9	0.07
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	9	0.07
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	9	0.07
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	12	0.07
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	12	0.07
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	12	0.07
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	13	0.07
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	13	0.07
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	13	0.07
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	11	0.07
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	6	0.07
(1,1832)	1:B:16:ASN:HB3	1:B:17:GLY:H	13	0.07
(1,1832)	1:B:16:ASN:HB3	1:B:17:GLY:H	16	0.07
(1,1831)	1:A:16:ASN:HB3	1:A:17:GLY:H	6	0.07
(1,1831)	1:A:16:ASN:HB3	1:A:17:GLY:H	12	0.07
(1,1812)	1:A:25:VAL:HG21	1:A:65:LYS:HE2	5	0.07
(1,1812)	1:A:25:VAL:HG21	1:A:65:LYS:HE3	5	0.07
(1,1812)	1:A:25:VAL:HG22	1:A:65:LYS:HE2	5	0.07
(1,1812)	1:A:25:VAL:HG22	1:A:65:LYS:HE3	5	0.07
(1,1812)	1:A:25:VAL:HG23	1:A:65:LYS:HE2	5	0.07
(1,1812)	1:A:25:VAL:HG23	1:A:65:LYS:HE3	5	0.07
(1,1810)	1:A:41:LYS:HE2	1:A:44:ILE:HD11	12	0.07
(1,1810)	1:A:41:LYS:HE2	1:A:44:ILE:HD12	12	0.07
(1,1810)	1:A:41:LYS:HE2	1:A:44:ILE:HD13	12	0.07
(1,1810)	1:A:41:LYS:HE3	1:A:44:ILE:HD11	12	0.07
(1,1810)	1:A:41:LYS:HE3	1:A:44:ILE:HD12	12	0.07
(1,1810)	1:A:41:LYS:HE3	1:A:44:ILE:HD13	12	0.07
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG11	20	0.07
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG12	20	0.07
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG13	20	0.07
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG11	20	0.07



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG12	20	0.07
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG13	20	0.07
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG11	20	0.07
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG12	20	0.07
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG13	20	0.07
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG11	20	0.07
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG12	20	0.07
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG13	20	0.07
(1,175)	1:A:15:LYS:H	1:A:18:MET:HG2	4	0.07
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	16	0.07
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	16	0.07
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	16	0.07
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	20	0.07
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	20	0.07
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	20	0.07
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	12	0.07
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	12	0.07
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	12	0.07
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	12	0.07
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	12	0.07
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG23	12	0.07
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	12	0.07
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	12	0.07
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	12	0.07
(1,168)	1:B:15:LYS:H	1:B:18:MET:HE1	20	0.07
(1,168)	1:B:15:LYS:H	1:B:18:MET:HE2	20	0.07
(1,168)	1:B:15:LYS:H	1:B:18:MET:HE3	20	0.07
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	7	0.07
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	7	0.07
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	7	0.07
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	7	0.07
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	7	0.07
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	7	0.07
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	7	0.07
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	7	0.07
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	7	0.07
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	8	0.07
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	8	0.07
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	8	0.07
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	8	0.07
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	8	0.07
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	8	0.07



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Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	8	0.07
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	8	0.07
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	8	0.07
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	14	0.07
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	14	0.07
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	14	0.07
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	14	0.07
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	14	0.07
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	14	0.07
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	14	0.07
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	14	0.07
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	14	0.07
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	12	0.07
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	12	0.07
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	12	0.07
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	12	0.07
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	12	0.07
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	12	0.07
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	12	0.07
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	12	0.07
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	12	0.07
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	13	0.07
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	13	0.07
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	13	0.07
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	13	0.07
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	13	0.07
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	13	0.07
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	13	0.07
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	13	0.07
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	13	0.07
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	4	0.07
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	4	0.07
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	4	0.07
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	4	0.07
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	4	0.07
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	4	0.07
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	14	0.07
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	14	0.07
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	14	0.07
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	14	0.07
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	14	0.07
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	14	0.07



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	5	0.07
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	5	0.07
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	5	0.07
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	1	0.07
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	1	0.07
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	1	0.07
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	4	0.07
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	4	0.07
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	4	0.07
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	9	0.07
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	9	0.07
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	9	0.07
(1,1414)	1:B:3:ASP:HB2	1:B:53:VAL:H	4	0.07
(1,1413)	1:A:3:ASP:HB2	1:A:53:VAL:H	17	0.07
(1,1318)	1:B:77:ARG:HG2	1:B:78:LEU:H	16	0.07
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	8	0.07
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	12	0.07
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	15	0.07
(1,1150)	1:B:67:ARG:HE	1:B:75:VAL:HB	14	0.07
(1,1105)	1:A:62:LEU:HD11	1:A:66:LEU:H	4	0.07
(1,1105)	1:A:62:LEU:HD12	1:A:66:LEU:H	4	0.07
(1,1105)	1:A:62:LEU:HD13	1:A:66:LEU:H	4	0.07
(1,1104)	1:B:62:LEU:HD11	1:B:65:LYS:H	16	0.07
(1,1104)	1:B:62:LEU:HD12	1:B:65:LYS:H	16	0.07
(1,1104)	1:B:62:LEU:HD13	1:B:65:LYS:H	16	0.07
(1,909)	1:B:3:ASP:HB3	1:B:53:VAL:H	12	0.06
(1,908)	1:A:3:ASP:HB3	1:A:53:VAL:H	1	0.06
(1,908)	1:A:3:ASP:HB3	1:A:53:VAL:H	17	0.06
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	1	0.06
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	16	0.06
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	17	0.06
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	19	0.06
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	2	0.06
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	3	0.06
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	5	0.06
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	8	0.06
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	17	0.06
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	18	0.06
(1,761)	1:B:43:GLY:H	1:B:44:ILE:H	4	0.06
(1,726)	1:A:41:LYS:HB2	1:A:42:ASP:H	1	0.06
(1,726)	1:A:41:LYS:HB3	1:A:42:ASP:H	1	0.06
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD1	8	0.06



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD2	8	0.06
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD1	13	0.06
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD2	13	0.06
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD1	17	0.06
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD2	17	0.06
(1,614)	1:A:35:THR:H	1:A:83:HIS:HE1	3	0.06
(1,563)	1:A:32:ASN:HD21	1:A:33:ILE:HB	4	0.06
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD11	15	0.06
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD12	15	0.06
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD13	15	0.06
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD11	19	0.06
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD12	19	0.06
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD13	19	0.06
(1,545)	1:A:29:PHE:HD1	1:A:31:THR:H	16	0.06
(1,545)	1:A:29:PHE:HD2	1:A:31:THR:H	16	0.06
(1,4934)	1:B:54:LYS:HD2	1:B:55:ASN:HB2	10	0.06
(1,4934)	1:B:54:LYS:HD2	1:B:55:ASN:HB3	10	0.06
(1,4934)	1:B:54:LYS:HD3	1:B:55:ASN:HB2	10	0.06
(1,4934)	1:B:54:LYS:HD3	1:B:55:ASN:HB3	10	0.06
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD21	20	0.06
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD22	20	0.06
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD21	20	0.06
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD22	20	0.06
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE1	18	0.06
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE2	18	0.06
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE3	18	0.06
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE1	18	0.06
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE2	18	0.06
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE3	18	0.06
(1,4906)	1:B:42:ASP:HB2	1:B:44:ILE:HG12	1	0.06
(1,4906)	1:B:42:ASP:HB3	1:B:44:ILE:HG12	1	0.06
(1,4898)	1:B:39:ASN:HD21	1:B:41:LYS:HE2	2	0.06
(1,4898)	1:B:39:ASN:HD21	1:B:41:LYS:HE3	2	0.06
(1,4898)	1:B:39:ASN:HD22	1:B:41:LYS:HE2	2	0.06
(1,4898)	1:B:39:ASN:HD22	1:B:41:LYS:HE3	2	0.06
(1,4887)	1:B:37:VAL:HG11	1:B:48:ASN:HD21	10	0.06
(1,4887)	1:B:37:VAL:HG11	1:B:48:ASN:HD22	10	0.06
(1,4887)	1:B:37:VAL:HG12	1:B:48:ASN:HD21	10	0.06
(1,4887)	1:B:37:VAL:HG12	1:B:48:ASN:HD22	10	0.06
(1,4887)	1:B:37:VAL:HG13	1:B:48:ASN:HD21	10	0.06
(1,4887)	1:B:37:VAL:HG13	1:B:48:ASN:HD22	10	0.06
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD21	6	0.06



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD22	6	0.06
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD21	6	0.06
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD22	6	0.06
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD21	6	0.06
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD22	6	0.06
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB2	1	0.06
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB3	1	0.06
(1,4872)	1:B:34:ARG:HG2	1:B:52:PHE:HD1	10	0.06
(1,4872)	1:B:34:ARG:HG2	1:B:52:PHE:HD2	10	0.06
(1,4872)	1:B:34:ARG:HG3	1:B:52:PHE:HD1	10	0.06
(1,4872)	1:B:34:ARG:HG3	1:B:52:PHE:HD2	10	0.06
(1,4872)	1:B:34:ARG:HG2	1:B:52:PHE:HD1	15	0.06
(1,4872)	1:B:34:ARG:HG2	1:B:52:PHE:HD2	15	0.06
(1,4872)	1:B:34:ARG:HG3	1:B:52:PHE:HD1	15	0.06
(1,4872)	1:B:34:ARG:HG3	1:B:52:PHE:HD2	15	0.06
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD11	12	0.06
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD12	12	0.06
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD13	12	0.06
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD11	12	0.06
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD12	12	0.06
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD13	12	0.06
(1,4851)	1:B:31:THR:HG21	1:B:58:LYS:HE2	6	0.06
(1,4851)	1:B:31:THR:HG21	1:B:58:LYS:HE3	6	0.06
(1,4851)	1:B:31:THR:HG22	1:B:58:LYS:HE2	6	0.06
(1,4851)	1:B:31:THR:HG22	1:B:58:LYS:HE3	6	0.06
(1,4851)	1:B:31:THR:HG23	1:B:58:LYS:HE2	6	0.06
(1,4851)	1:B:31:THR:HG23	1:B:58:LYS:HE3	6	0.06
(1,4851)	1:B:31:THR:HG21	1:B:58:LYS:HE2	18	0.06
(1,4851)	1:B:31:THR:HG21	1:B:58:LYS:HE3	18	0.06
(1,4851)	1:B:31:THR:HG22	1:B:58:LYS:HE2	18	0.06
(1,4851)	1:B:31:THR:HG22	1:B:58:LYS:HE3	18	0.06
(1,4851)	1:B:31:THR:HG23	1:B:58:LYS:HE2	18	0.06
(1,4851)	1:B:31:THR:HG23	1:B:58:LYS:HE3	18	0.06
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG2	10	0.06
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	10	0.06
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	10	0.06
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG3	10	0.06
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	10	0.06
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	10	0.06
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD11	7	0.06
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD12	7	0.06
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD13	7	0.06



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD11	7	0.06
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD12	7	0.06
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD13	7	0.06
(1,4560)	1:A:31:THR:HG21	1:A:58:LYS:HE2	1	0.06
(1,4560)	1:A:31:THR:HG21	1:A:58:LYS:HE3	1	0.06
(1,4560)	1:A:31:THR:HG22	1:A:58:LYS:HE2	1	0.06
(1,4560)	1:A:31:THR:HG22	1:A:58:LYS:HE3	1	0.06
(1,4560)	1:A:31:THR:HG23	1:A:58:LYS:HE2	1	0.06
(1,4560)	1:A:31:THR:HG23	1:A:58:LYS:HE3	1	0.06
(1,4538)	1:A:27:SER:HG	1:A:28:LYS:HD2	9	0.06
(1,4538)	1:A:27:SER:HG	1:A:28:LYS:HD3	9	0.06
(1,4514)	1:A:24:GLY:HA2	1:A:28:LYS:HE2	19	0.06
(1,4514)	1:A:24:GLY:HA2	1:A:28:LYS:HE3	19	0.06
(1,4514)	1:A:24:GLY:HA3	1:A:28:LYS:HE2	19	0.06
(1,4514)	1:A:24:GLY:HA3	1:A:28:LYS:HE3	19	0.06
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	7	0.06
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	7	0.06
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	7	0.06
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	3	0.06
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	3	0.06
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	3	0.06
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	9	0.06
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	9	0.06
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	9	0.06
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	14	0.06
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	14	0.06
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	14	0.06
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	15	0.06
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	15	0.06
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	15	0.06
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	16	0.06
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	16	0.06
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	16	0.06
(1,4389)	1:B:81:LEU:HB2	1:B:83:HIS:HD2	11	0.06
(1,4389)	1:B:81:LEU:HB3	1:B:83:HIS:HD2	11	0.06
(1,4388)	1:A:81:LEU:HB2	1:A:83:HIS:HD2	3	0.06
(1,4388)	1:A:81:LEU:HB3	1:A:83:HIS:HD2	3	0.06
(1,4386)	1:A:5:LEU:HG	1:A:83:HIS:HD2	2	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	2	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	2	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	2	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	2	0.06



 $Continued\ from\ previous\ page...$

Key	$\frac{t \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	2	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	2	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	3	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	3	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	3	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	3	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	3	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	3	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	8	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	8	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	8	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	8	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	8	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	8	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	9	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	9	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	9	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	9	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	9	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	9	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	10	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	10	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	10	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	10	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	10	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	10	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	12	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	12	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	12	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	12	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	12	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	12	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	15	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	15	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	15	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	15	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	15	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	15	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	18	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	18	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	18	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	18	0.06



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	18	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	18	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	19	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	19	0.06
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	19	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	19	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	19	0.06
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	19	0.06
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	11	0.06
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	11	0.06
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	11	0.06
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	11	0.06
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	11	0.06
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	11	0.06
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	20	0.06
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	20	0.06
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	20	0.06
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	20	0.06
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	20	0.06
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	20	0.06
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG21	3	0.06
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG22	3	0.06
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG23	3	0.06
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE1	2	0.06
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE2	2	0.06
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE1	2	0.06
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE2	2	0.06
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE1	8	0.06
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE2	8	0.06
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE1	8	0.06
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE2	8	0.06
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE1	9	0.06
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE2	9	0.06
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE1	9	0.06
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE2	9	0.06
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE1	10	0.06
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE2	10	0.06
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE1	10	0.06
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE2	10	0.06
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE1	14	0.06
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE2	14	0.06
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE1	14	0.06



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(1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 14 0.06 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE1 17 0.06 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE2 17 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE1 17 0.06 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE2 17 0.06 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE1 18 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 18 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 18 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 20 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 20 0.06 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE2 20 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 20 0.06 (1,4333) 1:A:4:PHE:HB3 1:B:52:PHE:HE1 4 0.06 (1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE2 <th>Key</th> <th>Atom-1</th> <th>Atom-2</th> <th>Model</th> <th>Violation (Å)</th>	Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE2 17 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE1 17 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 17 0.06 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE1 18 0.06 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE2 18 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 18 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 18 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 20 0.06 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE2 20 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 20 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 20 0.06 (1,4333) 1:A:4:PHE:HB3 1:A:52:PHE:HE2 4 0.06 (1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE2 4 0.06 (1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE2 <td>(1,4333)</td> <td>1:B:4:PHE:HB3</td> <td>1:B:52:PHE:HE2</td> <td>14</td> <td>0.06</td>	(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE2	14	0.06
(1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 17 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 17 0.06 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE1 18 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE1 18 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE1 18 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 18 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 20 0.06 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE2 20 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 20 0.06 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 20 0.06 (1,4333) 1:A:4:PHE:HB3 1:B:52:PHE:HE2 20 0.06 (1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE2 4 0.06 (1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE2 4 0.06 (1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE1 <td>(1,4333)</td> <td>1:B:4:PHE:HB2</td> <td>1:B:52:PHE:HE1</td> <td>17</td> <td>0.06</td>	(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE1	17	0.06
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(1,4332) 1:A:4:PHE:HB2 1:A:52:PHE:HE2 19 0.06 (1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE1 19 0.06 (1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE2 19 0.06 (1,4323) 1:B:52:PHE:HD1 1:B:53:VAL:H 5 0.06 (1,4323) 1:B:52:PHE:HD2 1:B:53:VAL:H 5 0.06	(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE2	16	0.06
(1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE1 19 0.06 (1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE2 19 0.06 (1,4323) 1:B:52:PHE:HD1 1:B:53:VAL:H 5 0.06 (1,4323) 1:B:52:PHE:HD2 1:B:53:VAL:H 5 0.06	(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE1	19	0.06
(1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE2 19 0.06 (1,4323) 1:B:52:PHE:HD1 1:B:53:VAL:H 5 0.06 (1,4323) 1:B:52:PHE:HD2 1:B:53:VAL:H 5 0.06	(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE2	19	0.06
(1,4323) 1:B:52:PHE:HD1 1:B:53:VAL:H 5 0.06 (1,4323) 1:B:52:PHE:HD2 1:B:53:VAL:H 5 0.06	(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE1	19	0.06
(1,4323) 1:B:52:PHE:HD1 1:B:53:VAL:H 5 0.06 (1,4323) 1:B:52:PHE:HD2 1:B:53:VAL:H 5 0.06	(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE2	19	0.06
		1:B:52:PHE:HD1	1:B:53:VAL:H	5	0.06
(1.4299) 1.4.59.DUE.UD1 1.4.59.VAL.II 19 0.06	(1,4323)	1:B:52:PHE:HD2	1:B:53:VAL:H	5	0.06
$\lfloor (1,4522) \rfloor$ 1:A: 02 :PDE:DD1 1:A: 03 :VAL:D 12 0.00	(1,4322)	1:A:52:PHE:HD1	1:A:53:VAL:H	12	0.06
(1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 12 0.06	(1,4322)	1:A:52:PHE:HD2	1:A:53:VAL:H	12	0.06
(1,4234) 1:A:45:PHE:HD1 1:A:47:CYS:HG 15 0.06	(1,4234)	1:A:45:PHE:HD1	1:A:47:CYS:HG	15	0.06
(1,4234) 1:A:45:PHE:HD2 1:A:47:CYS:HG 15 0.06	(1,4234)	1:A:45:PHE:HD2	1:A:47:CYS:HG	15	0.06
(1,4211) 1:B:29:PHE:H 1:B:29:PHE:HD1 4 0.06	(1,4211)	1:B:29:PHE:H	1:B:29:PHE:HD1	4	0.06
(1,4211) 1:B:29:PHE:H 1:B:29:PHE:HD2 4 0.06	(1,4211)	1:B:29:PHE:H	1:B:29:PHE:HD2	4	0.06
(1,4205) 1:B:29:PHE:HD1 1:B:65:LYS:HD2 12 0.06	. ,	1:B:29:PHE:HD1	1:B:65:LYS:HD2	12	0.06



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4205)	1:B:29:PHE:HD2	1:B:65:LYS:HD2	12	0.06
(1,4205)	1:B:29:PHE:HD1	1:B:65:LYS:HD2	14	0.06
(1,4205)	1:B:29:PHE:HD2	1:B:65:LYS:HD2	14	0.06
(1,4204)	1:A:29:PHE:HD1	1:A:65:LYS:HD2	8	0.06
(1,4204)	1:A:29:PHE:HD2	1:A:65:LYS:HD2	8	0.06
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	9	0.06
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	9	0.06
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	9	0.06
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	13	0.06
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	13	0.06
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	13	0.06
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	2	0.06
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	2	0.06
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	2	0.06
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	9	0.06
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	9	0.06
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	9	0.06
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	12	0.06
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	12	0.06
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	12	0.06
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	13	0.06
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	13	0.06
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	13	0.06
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	16	0.06
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	16	0.06
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	16	0.06
(1,4164)	1:A:4:PHE:HE1	1:A:55:ASN:HA	19	0.06
(1,4164)	1:A:4:PHE:HE2	1:A:55:ASN:HA	19	0.06
(1,4128)	1:A:83:HIS:HA	1:A:83:HIS:HD2	2	0.06
(1,4119)	1:B:80:ASN:HA	1:B:81:LEU:HG	13	0.06
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	5	0.06
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	5	0.06
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	10	0.06
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	10	0.06
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	15	0.06
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	15	0.06
(1,4036)	1:A:15:LYS:HA	1:A:17:GLY:H	5	0.06
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	10	0.06
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	12	0.06
(1,3987)	1:B:81:LEU:HD11	1:B:83:HIS:HB3	16	0.06
(1,3987)	1:B:81:LEU:HD12	1:B:83:HIS:HB3	16	0.06
(1,3987)	1:B:81:LEU:HD13	1:B:83:HIS:HB3	16	0.06



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3984)	1:A:5:LEU:HD11	1:A:81:LEU:HD11	12	0.06
(1,3984)	1:A:5:LEU:HD11	1:A:81:LEU:HD12	12	0.06
(1,3984)	1:A:5:LEU:HD11	1:A:81:LEU:HD13	12	0.06
(1,3984)	1:A:5:LEU:HD12	1:A:81:LEU:HD11	12	0.06
(1,3984)	1:A:5:LEU:HD12	1:A:81:LEU:HD12	12	0.06
(1,3984)	1:A:5:LEU:HD12	1:A:81:LEU:HD13	12	0.06
(1,3984)	1:A:5:LEU:HD13	1:A:81:LEU:HD11	12	0.06
(1,3984)	1:A:5:LEU:HD13	1:A:81:LEU:HD12	12	0.06
(1,3984)	1:A:5:LEU:HD13	1:A:81:LEU:HD13	12	0.06
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD11	1	0.06
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD12	1	0.06
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD13	1	0.06
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD11	8	0.06
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD12	8	0.06
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD13	8	0.06
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD11	10	0.06
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD12	10	0.06
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD13	10	0.06
(1,3890)	1:B:82:GLU:HA	1:B:83:HIS:HB2	15	0.06
(1,3889)	1:A:82:GLU:HA	1:A:83:HIS:HB2	1	0.06
(1,3889)	1:A:82:GLU:HA	1:A:83:HIS:HB2	11	0.06
(1,3758)	1:B:6:ALA:HB1	1:B:77:ARG:HD2	17	0.06
(1,3758)	1:B:6:ALA:HB1	1:B:77:ARG:HD3	17	0.06
(1,3758)	1:B:6:ALA:HB2	1:B:77:ARG:HD2	17	0.06
(1,3758)	1:B:6:ALA:HB2	1:B:77:ARG:HD3	17	0.06
(1,3758)	1:B:6:ALA:HB3	1:B:77:ARG:HD2	17	0.06
(1,3758)	1:B:6:ALA:HB3	1:B:77:ARG:HD3	17	0.06
(1,3758)	1:B:6:ALA:HB1	1:B:77:ARG:HD2	18	0.06
(1,3758)	1:B:6:ALA:HB1	1:B:77:ARG:HD3	18	0.06
(1,3758)	1:B:6:ALA:HB2	1:B:77:ARG:HD2	18	0.06
(1,3758)	1:B:6:ALA:HB2	1:B:77:ARG:HD3	18	0.06
(1,3758)	1:B:6:ALA:HB3	1:B:77:ARG:HD2	18	0.06
(1,3758)	1:B:6:ALA:HB3	1:B:77:ARG:HD3	18	0.06
(1,3754)	1:B:59:LEU:HD11	1:B:77:ARG:HD2	4	0.06
(1,3754)	1:B:59:LEU:HD11	1:B:77:ARG:HD3	4	0.06
(1,3754)	1:B:59:LEU:HD12	1:B:77:ARG:HD2	4	0.06
(1,3754)	1:B:59:LEU:HD12	1:B:77:ARG:HD3	4	0.06
(1,3754)	1:B:59:LEU:HD13	1:B:77:ARG:HD2	4	0.06
(1,3754)	1:B:59:LEU:HD13	1:B:77:ARG:HD3	4	0.06
(1,3754)	1:B:59:LEU:HD11	1:B:77:ARG:HD2	6	0.06
(1,3754)	1:B:59:LEU:HD11	1:B:77:ARG:HD3	6	0.06
(1,3754)	1:B:59:LEU:HD12	1:B:77:ARG:HD2	6	0.06



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3754)	1:B:59:LEU:HD12	1:B:77:ARG:HD3	6	0.06
(1,3754)	1:B:59:LEU:HD13	1:B:77:ARG:HD2	6	0.06
(1,3754)	1:B:59:LEU:HD13	1:B:77:ARG:HD3	6	0.06
(1,3734)	1:B:74:THR:HA	1:B:76:GLU:HG2	12	0.06
(1,3734)	1:B:74:THR:HA	1:B:76:GLU:HG3	12	0.06
(1,3733)	1:A:74:THR:HA	1:A:76:GLU:HG2	14	0.06
(1,3733)	1:A:74:THR:HA	1:A:76:GLU:HG3	14	0.06
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	10	0.06
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	10	0.06
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	10	0.06
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	14	0.06
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	14	0.06
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	14	0.06
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	16	0.06
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	16	0.06
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	16	0.06
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	20	0.06
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	20	0.06
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	20	0.06
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	3	0.06
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	3	0.06
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	3	0.06
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	13	0.06
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	13	0.06
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	13	0.06
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	7	0.06
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	7	0.06
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	7	0.06
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	8	0.06
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	8	0.06
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	8	0.06
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	9	0.06
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	9	0.06
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	9	0.06
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	16	0.06
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	16	0.06
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	16	0.06
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	17	0.06
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	17	0.06
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	17	0.06
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	18	0.06
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	18	0.06



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	18	0.06
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG11	4	0.06
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG12	4	0.06
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG13	4	0.06
(1,3592)	1:B:20:ASN:HA	1:B:22:ILE:HB	13	0.06
(1,3591)	1:A:20:ASN:HA	1:A:22:ILE:HB	2	0.06
(1,3591)	1:A:20:ASN:HA	1:A:22:ILE:HB	10	0.06
(1,3591)	1:A:20:ASN:HA	1:A:22:ILE:HB	19	0.06
(1,3562)	1:B:15:LYS:HE2	1:B:18:MET:H	5	0.06
(1,3562)	1:B:15:LYS:HE3	1:B:18:MET:H	5	0.06
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	3	0.06
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	3	0.06
(1,3551)	1:A:68:LYS:HA	1:A:68:LYS:HE2	6	0.06
(1,3551)	1:A:68:LYS:HA	1:A:68:LYS:HE3	6	0.06
(1,3421)	1:B:63:MET:HE1	1:B:77:ARG:H	2	0.06
(1,3421)	1:B:63:MET:HE2	1:B:77:ARG:H	2	0.06
(1,3421)	1:B:63:MET:HE3	1:B:77:ARG:H	2	0.06
(1,3413)	1:B:63:MET:HE1	1:B:76:GLU:HA	1	0.06
(1,3413)	1:B:63:MET:HE2	1:B:76:GLU:HA	1	0.06
(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	1	0.06
(1,3413)	1:B:63:MET:HE1	1:B:76:GLU:HA	9	0.06
(1,3413)	1:B:63:MET:HE2	1:B:76:GLU:HA	9	0.06
(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	9	0.06
(1,3413)	1:B:63:MET:HE1	1:B:76:GLU:HA	13	0.06
(1,3413)	1:B:63:MET:HE2	1:B:76:GLU:HA	13	0.06
(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	13	0.06
(1,3412)	1:A:63:MET:HE1	1:A:76:GLU:HA	1	0.06
(1,3412)	1:A:63:MET:HE2	1:A:76:GLU:HA	1	0.06
(1,3412)	1:A:63:MET:HE3	1:A:76:GLU:HA	1	0.06
(1,3412)	1:A:63:MET:HE1	1:A:76:GLU:HA	3	0.06
(1,3412)	1:A:63:MET:HE2	1:A:76:GLU:HA	3	0.06
(1,3412)	1:A:63:MET:HE3	1:A:76:GLU:HA	3	0.06
(1,3412)	1:A:63:MET:HE1	1:A:76:GLU:HA	14	0.06
(1,3412)	1:A:63:MET:HE2	1:A:76:GLU:HA	14	0.06
(1,3412)	1:A:63:MET:HE3	1:A:76:GLU:HA	14	0.06
(1,3411)	1:B:63:MET:HE1	1:B:77:ARG:HA	20	0.06
(1,3411)	1:B:63:MET:HE2	1:B:77:ARG:HA	20	0.06
(1,3411)	1:B:63:MET:HE3	1:B:77:ARG:HA	20	0.06
(1,3410)	1:A:63:MET:HE1	1:A:77:ARG:HA	7	0.06
(1,3410)	1:A:63:MET:HE2	1:A:77:ARG:HA	7	0.06
(1,3410)	1:A:63:MET:HE3	1:A:77:ARG:HA	7	0.06
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	12	0.06



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	12	0.06
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	12	0.06
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE1	10	0.06
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE2	10	0.06
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE3	10	0.06
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE1	10	0.06
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE2	10	0.06
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE3	10	0.06
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE1	10	0.06
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE2	10	0.06
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE3	10	0.06
(1,3287)	1:A:61:THR:HG21	1:A:65:LYS:HE2	19	0.06
(1,3287)	1:A:61:THR:HG21	1:A:65:LYS:HE3	19	0.06
(1,3287)	1:A:61:THR:HG22	1:A:65:LYS:HE2	19	0.06
(1,3287)	1:A:61:THR:HG22	1:A:65:LYS:HE3	19	0.06
(1,3287)	1:A:61:THR:HG23	1:A:65:LYS:HE2	19	0.06
(1,3287)	1:A:61:THR:HG23	1:A:65:LYS:HE3	19	0.06
(1,3186)	1:B:58:LYS:H	1:B:58:LYS:HD2	3	0.06
(1,3186)	1:B:58:LYS:H	1:B:58:LYS:HD3	3	0.06
(1,3186)	1:B:58:LYS:H	1:B:58:LYS:HD2	18	0.06
(1,3186)	1:B:58:LYS:H	1:B:58:LYS:HD3	18	0.06
(1,3175)	1:A:30:ASP:HB2	1:A:58:LYS:HD2	15	0.06
(1,3175)	1:A:30:ASP:HB2	1:A:58:LYS:HD3	15	0.06
(1,3175)	1:A:30:ASP:HB3	1:A:58:LYS:HD2	15	0.06
(1,3175)	1:A:30:ASP:HB3	1:A:58:LYS:HD3	15	0.06
(1,3130)	1:B:4:PHE:HD1	1:B:56:THR:HG21	3	0.06
(1,3130)	1:B:4:PHE:HD1	1:B:56:THR:HG22	3	0.06
(1,3130)	1:B:4:PHE:HD1	1:B:56:THR:HG23	3	0.06
(1,3130)	1:B:4:PHE:HD2	1:B:56:THR:HG21	3	0.06
(1,3130)	1:B:4:PHE:HD2	1:B:56:THR:HG22	3	0.06
(1,3130)	1:B:4:PHE:HD2	1:B:56:THR:HG23	3	0.06
(1,3130)	1:B:4:PHE:HD1	1:B:56:THR:HG21	15	0.06
(1,3130)	1:B:4:PHE:HD1	1:B:56:THR:HG22	15	0.06
(1,3130)	1:B:4:PHE:HD1	1:B:56:THR:HG23	15	0.06
(1,3130)	1:B:4:PHE:HD2	1:B:56:THR:HG21	15	0.06
(1,3130)	1:B:4:PHE:HD2	1:B:56:THR:HG22	15	0.06
(1,3130)	1:B:4:PHE:HD2	1:B:56:THR:HG23	15	0.06
(1,3100)	1:B:54:LYS:H	1:B:54:LYS:HD2	14	0.06
(1,3100)	1:B:54:LYS:H	1:B:54:LYS:HD3	14	0.06
(1,3094)	1:B:15:LYS:HD2	1:B:16:ASN:HD22	8	0.06
(1,3094)	1:B:15:LYS:HD3	1:B:16:ASN:HD22	8	0.06
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD2	15	0.06



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD3	15	0.06
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD2	19	0.06
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD3	19	0.06
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD2	20	0.06
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD3	20	0.06
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	7	0.06
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	7	0.06
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	7	0.06
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	7	0.06
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	7	0.06
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	7	0.06
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	8	0.06
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	8	0.06
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	8	0.06
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	8	0.06
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	8	0.06
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	8	0.06
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	9	0.06
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	9	0.06
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	9	0.06
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	9	0.06
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	9	0.06
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	9	0.06
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	11	0.06
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	11	0.06
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	11	0.06
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	11	0.06
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	11	0.06
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	11	0.06
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	17	0.06
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	17	0.06
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	17	0.06
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	17	0.06
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	17	0.06
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	17	0.06
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	11	0.06
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	11	0.06
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	11	0.06
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	11	0.06
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	11	0.06
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	11	0.06
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	12	0.06



 $Continued\ from\ previous\ page...$

Key	$egin{aligned} Atom-1 \end{aligned}$	Atom-2	Model	Violation (Å)
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	12	0.06
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	12	0.06
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	12	0.06
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	12	0.06
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	12	0.06
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	16	0.06
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	16	0.06
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	16	0.06
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	16	0.06
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	16	0.06
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	16	0.06
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	17	0.06
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	17	0.06
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	17	0.06
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	17	0.06
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	17	0.06
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	17	0.06
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD11	11	0.06
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD12	11	0.06
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD13	11	0.06
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	1	0.06
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	1	0.06
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	1	0.06
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	1	0.06
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	1	0.06
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	1	0.06
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	1	0.06
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	1	0.06
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	1	0.06
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	15	0.06
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	15	0.06
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	15	0.06
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	15	0.06
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	15	0.06
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	15	0.06
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	15	0.06
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	15	0.06
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	15	0.06
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	4	0.06
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	4	0.06
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	4	0.06
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	4	0.06



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	4	0.06
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	4	0.06
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	4	0.06
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	4	0.06
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	4	0.06
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	13	0.06
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	13	0.06
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	13	0.06
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	13	0.06
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	13	0.06
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	13	0.06
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	13	0.06
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	13	0.06
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	13	0.06
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	20	0.06
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	20	0.06
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	20	0.06
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	20	0.06
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	20	0.06
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	20	0.06
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	20	0.06
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	20	0.06
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	20	0.06
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD11	4	0.06
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD12	4	0.06
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD13	4	0.06
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD11	4	0.06
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD12	4	0.06
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD13	4	0.06
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD11	9	0.06
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD12	9	0.06
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD13	9	0.06
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD11	9	0.06
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD12	9	0.06
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD13	9	0.06
(1,2902)	1:A:51:ILE:HG21	1:B:20:ASN:HD22	11	0.06
(1,2902)	1:A:51:ILE:HG22	1:B:20:ASN:HD22	11	0.06
(1,2902)	1:A:51:ILE:HG23	1:B:20:ASN:HD22	11	0.06
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG21	5	0.06
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG22	5	0.06
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG23	5	0.06
(1,2882)	1:B:8:ILE:HG21	1:B:62:LEU:HD11	17	0.06



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2882)	1:B:8:ILE:HG21	1:B:62:LEU:HD12	17	0.06
(1,2882)	1:B:8:ILE:HG21	1:B:62:LEU:HD13	17	0.06
(1,2882)	1:B:8:ILE:HG22	1:B:62:LEU:HD11	17	0.06
(1,2882)	1:B:8:ILE:HG22	1:B:62:LEU:HD12	17	0.06
(1,2882)	1:B:8:ILE:HG22	1:B:62:LEU:HD13	17	0.06
(1,2882)	1:B:8:ILE:HG23	1:B:62:LEU:HD11	17	0.06
(1,2882)	1:B:8:ILE:HG23	1:B:62:LEU:HD12	17	0.06
(1,2882)	1:B:8:ILE:HG23	1:B:62:LEU:HD13	17	0.06
(1,2816)	1:B:50:MET:HE1	1:B:51:ILE:HG13	8	0.06
(1,2816)	1:B:50:MET:HE2	1:B:51:ILE:HG13	8	0.06
(1,2816)	1:B:50:MET:HE3	1:B:51:ILE:HG13	8	0.06
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	14	0.06
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	14	0.06
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	14	0.06
(1,2792)	1:B:8:ILE:H	1:B:50:MET:HG3	5	0.06
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	5	0.06
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	1	0.06
(1,2668)	1:B:23:THR:HG1	1:B:47:CYS:HB3	20	0.06
(1,2667)	1:A:23:THR:HG1	1:A:47:CYS:HB3	4	0.06
(1,2583)	1:A:44:ILE:HD11	1:A:46:THR:HB	11	0.06
(1,2583)	1:A:44:ILE:HD12	1:A:46:THR:HB	11	0.06
(1,2583)	1:A:44:ILE:HD13	1:A:46:THR:HB	11	0.06
(1,2575)	1:A:44:ILE:HG21	1:A:45:PHE:H	20	0.06
(1,2575)	1:A:44:ILE:HG22	1:A:45:PHE:H	20	0.06
(1,2575)	1:A:44:ILE:HG23	1:A:45:PHE:H	20	0.06
(1,2572)	1:B:14:ASP:H	1:B:44:ILE:HG21	8	0.06
(1,2572)	1:B:14:ASP:H	1:B:44:ILE:HG22	8	0.06
(1,2572)	1:B:14:ASP:H	1:B:44:ILE:HG23	8	0.06
(1,2551)	1:A:44:ILE:HG13	1:A:45:PHE:H	7	0.06
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD21	13	0.06
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD22	13	0.06
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD23	13	0.06
(1,2423)	1:A:38:LEU:HD11	1:A:39:ASN:H	12	0.06
(1,2423)	1:A:38:LEU:HD12	1:A:39:ASN:H	12	0.06
(1,2423)	1:A:38:LEU:HD13	1:A:39:ASN:H	12	0.06
(1,2316)	1:B:23:THR:HG1	1:B:36:ILE:HD11	9	0.06
(1,2316)	1:B:23:THR:HG1	1:B:36:ILE:HD12	9	0.06
(1,2316)	1:B:23:THR:HG1	1:B:36:ILE:HD13	9	0.06
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	2	0.06
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	2	0.06
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	2	0.06
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	13	0.06



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Key	Atom-1	$\mathbf{Atom-2}$	Model	Violation (Å)
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	13	0.06
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	13	0.06
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	5	0.06
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	5	0.06
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	5	0.06
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	17	0.06
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	17	0.06
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	17	0.06
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	12	0.06
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	12	0.06
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	12	0.06
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	3	0.06
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	3	0.06
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	3	0.06
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	6	0.06
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	6	0.06
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	6	0.06
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	17	0.06
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	17	0.06
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	17	0.06
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	1	0.06
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	1	0.06
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	1	0.06
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	6	0.06
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	6	0.06
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	6	0.06
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	20	0.06
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	20	0.06
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	20	0.06
(1,2181)	1:A:29:PHE:HD1	1:A:31:THR:HB	12	0.06
(1,2181)	1:A:29:PHE:HD2	1:A:31:THR:HB	12	0.06
(1,2163)	1:A:27:SER:HG	1:A:28:LYS:HG2	9	0.06
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	1	0.06
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	1	0.06
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	1	0.06
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	2	0.06
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	2	0.06
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	2	0.06
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	6	0.06
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	6	0.06
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	6	0.06
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	20	0.06



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	20	0.06
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	20	0.06
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	9	0.06
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	9	0.06
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	9	0.06
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	19	0.06
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	19	0.06
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	19	0.06
(1,208)	1:B:16:ASN:HA	1:B:17:GLY:H	4	0.06
(1,208)	1:B:16:ASN:HA	1:B:17:GLY:H	7	0.06
(1,208)	1:B:16:ASN:HA	1:B:17:GLY:H	11	0.06
(1,208)	1:B:16:ASN:HA	1:B:17:GLY:H	14	0.06
(1,208)	1:B:16:ASN:HA	1:B:17:GLY:H	20	0.06
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	3	0.06
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	3	0.06
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	3	0.06
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	10	0.06
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	10	0.06
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	10	0.06
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	11	0.06
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	11	0.06
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	11	0.06
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	15	0.06
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	15	0.06
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	15	0.06
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	1	0.06
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	1	0.06
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	1	0.06
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	10	0.06
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	10	0.06
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	10	0.06
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	12	0.06
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	12	0.06
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	12	0.06
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	19	0.06
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	19	0.06
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	19	0.06
(1,200)	1:B:15:LYS:HE2	1:B:16:ASN:HD22	4	0.06
(1,200)	1:B:15:LYS:HE3	1:B:16:ASN:HD22	4	0.06
(1,200)	1:B:15:LYS:HE2	1:B:16:ASN:HD22	7	0.06
(1,200)	1:B:15:LYS:HE3	1:B:16:ASN:HD22	7	0.06
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	1	0.06



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	1	0.06
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	1	0.06
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	7	0.06
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	7	0.06
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	7	0.06
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	8	0.06
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	8	0.06
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	8	0.06
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	19	0.06
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	19	0.06
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	19	0.06
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	8	0.06
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	8	0.06
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	8	0.06
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	10	0.06
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	10	0.06
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	10	0.06
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	14	0.06
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	14	0.06
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	14	0.06
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	16	0.06
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	16	0.06
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	16	0.06
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	18	0.06
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	18	0.06
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	18	0.06
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	3	0.06
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	17	0.06
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	10	0.06
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	19	0.06
(1,1832)	1:B:16:ASN:HB3	1:B:17:GLY:H	6	0.06
(1,1809)	1:B:11:VAL:HG21	1:B:41:LYS:HE2	1	0.06
(1,1809)	1:B:11:VAL:HG21	1:B:41:LYS:HE3	1	0.06
(1,1809)	1:B:11:VAL:HG22	1:B:41:LYS:HE2	1	0.06
(1,1809)	1:B:11:VAL:HG22	1:B:41:LYS:HE3	1	0.06
(1,1809)	1:B:11:VAL:HG23	1:B:41:LYS:HE2	1	0.06
(1,1809)	1:B:11:VAL:HG23	1:B:41:LYS:HE3	1	0.06
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG11	18	0.06
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG12	18	0.06
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG13	18	0.06
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG11	18	0.06
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG12	18	0.06



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG13	18	0.06
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG11	8	0.06
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG12	8	0.06
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG13	8	0.06
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG11	8	0.06
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG12	8	0.06
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG13	8	0.06
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	4	0.06
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	4	0.06
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	4	0.06
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	12	0.06
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	12	0.06
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	12	0.06
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	8	0.06
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	8	0.06
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	8	0.06
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	8	0.06
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	8	0.06
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG23	8	0.06
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	8	0.06
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	8	0.06
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	8	0.06
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG21	17	0.06
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG22	17	0.06
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG23	17	0.06
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG21	17	0.06
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG22	17	0.06
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG23	17	0.06
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG21	17	0.06
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG22	17	0.06
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG23	17	0.06
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD11	4	0.06
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD12	4	0.06
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD13	4	0.06
(1,1558)	1:B:24:GLY:H	1:B:26:ILE:HD11	4	0.06
(1,1558)	1:B:24:GLY:H	1:B:26:ILE:HD12	4	0.06
(1,1558)	1:B:24:GLY:H	1:B:26:ILE:HD13	4	0.06
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	2	0.06
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	2	0.06
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	2	0.06
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	2	0.06
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	2	0.06



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Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	2	0.06
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	2	0.06
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	2	0.06
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	2	0.06
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	3	0.06
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	3	0.06
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	3	0.06
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	3	0.06
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	3	0.06
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	3	0.06
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	3	0.06
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	3	0.06
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	3	0.06
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	13	0.06
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	13	0.06
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	13	0.06
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	13	0.06
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	13	0.06
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	13	0.06
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	13	0.06
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	13	0.06
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	13	0.06
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	7	0.06
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	7	0.06
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	7	0.06
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	7	0.06
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	7	0.06
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	7	0.06
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	19	0.06
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	19	0.06
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	19	0.06
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	16	0.06
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	16	0.06
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	16	0.06
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	17	0.06
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	17	0.06
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	17	0.06
(1,1377)	1:A:40:ALA:H	1:A:41:LYS:HD2	9	0.06
(1,1377)	1:A:40:ALA:H	1:A:41:LYS:HD3	9	0.06
(1,1302)	1:B:77:ARG:H	1:B:77:ARG:HB2	8	0.06
(1,1195)	1:A:69:VAL:H	1:A:70:GLN:H	11	0.06
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	1	0.06



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	6	0.06
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	13	0.06
(1,1105)	1:A:62:LEU:HD11	1:A:66:LEU:H	19	0.06
(1,1105)	1:A:62:LEU:HD12	1:A:66:LEU:H	19	0.06
(1,1105)	1:A:62:LEU:HD13	1:A:66:LEU:H	19	0.06
(1,1067)	1:B:64:ASP:H	1:B:75:VAL:HG11	14	0.06
(1,1067)	1:B:64:ASP:H	1:B:75:VAL:HG12	14	0.06
(1,1067)	1:B:64:ASP:H	1:B:75:VAL:HG13	14	0.06
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	13	0.06
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	13	0.06
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	13	0.06
(1,1020)	1:A:58:LYS:HZ1	1:A:61:THR:H	13	0.06
(1,1020)	1:A:58:LYS:HZ2	1:A:61:THR:H	13	0.06
(1,1020)	1:A:58:LYS:HZ3	1:A:61:THR:H	13	0.06
(1,899)	1:B:51:ILE:HG12	1:B:52:PHE:H	14	0.05
(1,898)	1:A:51:ILE:HG12	1:A:52:PHE:H	13	0.05
(1,898)	1:A:51:ILE:HG12	1:A:52:PHE:H	19	0.05
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	2	0.05
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	3	0.05
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	4	0.05
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	5	0.05
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	8	0.05
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	12	0.05
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	18	0.05
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	12	0.05
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	16	0.05
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	19	0.05
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	20	0.05
(1,82)	1:A:9:ARG:HE	1:A:11:VAL:HG21	14	0.05
(1,82)	1:A:9:ARG:HE	1:A:11:VAL:HG22	14	0.05
(1,82)	1:A:9:ARG:HE	1:A:11:VAL:HG23	14	0.05
(1,719)	1:B:41:LYS:H	1:B:46:THR:H	17	0.05
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD1	11	0.05
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD2	11	0.05
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD1	4	0.05
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD2	4	0.05
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD1	7	0.05
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD2	7	0.05
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD1	8	0.05
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD2	8	0.05
(1,615)	1:B:35:THR:H	1:B:83:HIS:HE1	9	0.05
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD11	6	0.05



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD12	6	0.05
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD13	6	0.05
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD11	15	0.05
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD12	15	0.05
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD13	15	0.05
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD11	17	0.05
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD12	17	0.05
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD13	17	0.05
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD11	18	0.05
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD12	18	0.05
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD13	18	0.05
(1,548)	1:A:31:THR:H	1:B:20:ASN:HD21	13	0.05
(1,5002)	1:B:69:VAL:HG11	1:B:70:GLN:HE21	2	0.05
(1,5002)	1:B:69:VAL:HG11	1:B:70:GLN:HE22	2	0.05
(1,5002)	1:B:69:VAL:HG12	1:B:70:GLN:HE21	2	0.05
(1,5002)	1:B:69:VAL:HG12	1:B:70:GLN:HE22	2	0.05
(1,5002)	1:B:69:VAL:HG13	1:B:70:GLN:HE21	2	0.05
(1,5002)	1:B:69:VAL:HG13	1:B:70:GLN:HE22	2	0.05
(1,4976)	1:B:63:MET:HE1	1:B:77:ARG:HB2	18	0.05
(1,4976)	1:B:63:MET:HE1	1:B:77:ARG:HB3	18	0.05
(1,4976)	1:B:63:MET:HE2	1:B:77:ARG:HB2	18	0.05
(1,4976)	1:B:63:MET:HE2	1:B:77:ARG:HB3	18	0.05
(1,4976)	1:B:63:MET:HE3	1:B:77:ARG:HB2	18	0.05
(1,4976)	1:B:63:MET:HE3	1:B:77:ARG:HB3	18	0.05
(1,4936)	1:B:54:LYS:HE2	1:B:55:ASN:HD21	12	0.05
(1,4936)	1:B:54:LYS:HE2	1:B:55:ASN:HD22	12	0.05
(1,4936)	1:B:54:LYS:HE3	1:B:55:ASN:HD21	12	0.05
(1,4936)	1:B:54:LYS:HE3	1:B:55:ASN:HD22	12	0.05
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD21	10	0.05
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD22	10	0.05
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD21	10	0.05
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD22	10	0.05
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD21	11	0.05
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD22	11	0.05
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD21	11	0.05
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD22	11	0.05
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE1	7	0.05
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE2	7	0.05
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE3	7	0.05
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE1	7	0.05
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE2	7	0.05
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE3	7	0.05



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(1,4916) 1:B:48:ASN:HD21 1:B:50:MET:HE2 14 0 (1,4916) 1:B:48:ASN:HD21 1:B:50:MET:HE3 14 0 (1,4916) 1:B:48:ASN:HD22 1:B:50:MET:HE1 14 0 (1,4916) 1:B:48:ASN:HD22 1:B:50:MET:HE2 14 0 (1,4916) 1:B:48:ASN:HD22 1:B:50:MET:HE3 14 0 (1,4916) 1:B:48:ASN:HD22 1:B:50:MET:HE3 14 0 (1,4906) 1:B:42:ASP:HB2 1:B:44:ILE:HG12 18 0 (1,4906) 1:B:42:ASP:HB3 1:B:44:ILE:HG12 18 0 (1,4899) 1:B:39:ASN:HD21 1:B:46:THR:HB 10 0	0.05 0.05 0.05 0.05 0.05
(1,4916) 1:B:48:ASN:HD21 1:B:50:MET:HE3 14 0 (1,4916) 1:B:48:ASN:HD22 1:B:50:MET:HE1 14 0 (1,4916) 1:B:48:ASN:HD22 1:B:50:MET:HE2 14 0 (1,4916) 1:B:48:ASN:HD22 1:B:50:MET:HE3 14 0 (1,4906) 1:B:42:ASP:HB2 1:B:44:ILE:HG12 18 0 (1,4906) 1:B:42:ASP:HB3 1:B:44:ILE:HG12 18 0 (1,4899) 1:B:39:ASN:HD21 1:B:46:THR:HB 10 0	0.05
(1,4916) 1:B:48:ASN:HD22 1:B:50:MET:HE1 14 0 (1,4916) 1:B:48:ASN:HD22 1:B:50:MET:HE2 14 0 (1,4916) 1:B:48:ASN:HD22 1:B:50:MET:HE3 14 0 (1,4906) 1:B:42:ASP:HB2 1:B:44:ILE:HG12 18 0 (1,4906) 1:B:42:ASP:HB3 1:B:44:ILE:HG12 18 0 (1,4899) 1:B:39:ASN:HD21 1:B:46:THR:HB 10 0	0.05
(1,4916) 1:B:48:ASN:HD22 1:B:50:MET:HE2 14 0 (1,4916) 1:B:48:ASN:HD22 1:B:50:MET:HE3 14 0 (1,4906) 1:B:42:ASP:HB2 1:B:44:ILE:HG12 18 0 (1,4906) 1:B:42:ASP:HB3 1:B:44:ILE:HG12 18 0 (1,4899) 1:B:39:ASN:HD21 1:B:46:THR:HB 10 0	
(1,4916) 1:B:48:ASN:HD22 1:B:50:MET:HE3 14 0 (1,4906) 1:B:42:ASP:HB2 1:B:44:ILE:HG12 18 0 (1,4906) 1:B:42:ASP:HB3 1:B:44:ILE:HG12 18 0 (1,4899) 1:B:39:ASN:HD21 1:B:46:THR:HB 10 0	0.05
(1,4906) 1:B:42:ASP:HB2 1:B:44:ILE:HG12 18 (1,4906) 1:B:42:ASP:HB3 1:B:44:ILE:HG12 18 (1,4899) 1:B:39:ASN:HD21 1:B:46:THR:HB 10	
(1,4906) 1:B:42:ASP:HB3 1:B:44:ILE:HG12 18 (1,4899) 1:B:39:ASN:HD21 1:B:46:THR:HB 10	0.05
(1,4899) 1:B:39:ASN:HD21 1:B:46:THR:HB 10 (0.05
	0.05
(1,4899) 1:B:39:ASN:HD22 1:B:46:THR:HB 10	0.05
	0.05
(1,4897) 1:B:39:ASN:HD21 1:B:41:LYS:HD2 13 (0.05
(1,4897) 1:B:39:ASN:HD21 1:B:41:LYS:HD3 13 (0.05
(1,4897) 1:B:39:ASN:HD22 1:B:41:LYS:HD2 13	0.05
(1,4897) 1:B:39:ASN:HD22 1:B:41:LYS:HD3 13 (0.05
(1,4896) 1:B:39:ASN:HD21 1:B:41:LYS:HB2 1	0.05
(1,4896) 1:B:39:ASN:HD21 1:B:41:LYS:HB3 1	0.05
(1,4896) 1:B:39:ASN:HD22 1:B:41:LYS:HB2 1	0.05
(1,4896) 1:B:39:ASN:HD22 1:B:41:LYS:HB3 1	0.05
(1,4896) 1:B:39:ASN:HD21 1:B:41:LYS:HB2 10 (0.05
(1,4896) 1:B:39:ASN:HD21 1:B:41:LYS:HB3 10 (0.05
(1,4896) 1:B:39:ASN:HD22 1:B:41:LYS:HB2 10 (0.05
(1,4896) 1:B:39:ASN:HD22 1:B:41:LYS:HB3 10 (0.05
(1,4885) 1:B:37:VAL:HG11 1:B:39:ASN:HD21 19 (0.05
(1,4885) 1:B:37:VAL:HG11 1:B:39:ASN:HD22 19 (0.05
(1,4885) 1:B:37:VAL:HG12 1:B:39:ASN:HD21 19 (0.05
(1,4885) 1:B:37:VAL:HG12 1:B:39:ASN:HD22 19 (0.05
(1,4885) 1:B:37:VAL:HG13 1:B:39:ASN:HD21 19 (0.05
(1,4885) 1:B:37:VAL:HG13 1:B:39:ASN:HD22 19 (0.05
(1,4875) 1:B:35:THR:HB 1:B:50:MET:HB2 11 (0.05
(1,4875) 1:B:35:THR:HB 1:B:50:MET:HB3 11 (0.05
(1,4869) 1:B:34:ARG:HB2 1:B:51:ILE:H 1	0.05
(1,4869) 1:B:34:ARG:HB3 1:B:51:ILE:H 1	0.05
(1,4815) 1:B:25:VAL:HG21 1:B:28:LYS:HG2 3	0.05
	0.05
(1,4815) 1:B:25:VAL:HG22 1:B:28:LYS:HG2 3	0.05
(1,4815) 1:B:25:VAL:HG22 1:B:28:LYS:HG3 3	0.05
(1,4815) 1:B:25:VAL:HG23 1:B:28:LYS:HG2 3	0.05
(1,4815) 1:B:25:VAL:HG23 1:B:28:LYS:HG3 3	0.05
(1,4775) 1:B:16:ASN:HB2 1:B:17:GLY:H 2	0.05
(1,4775) 1:B:16:ASN:HB3 1:B:17:GLY:H 2	0.05
(1,4775) 1:B:16:ASN:HB2 1:B:17:GLY:H 18 (0.05
(1,4775) 1:B:16:ASN:HB3 1:B:17:GLY:H 18 (0.05



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4770)	1:B:15:LYS:HD2	1:B:16:ASN:HB2	18	0.05
(1,4770)	1:B:15:LYS:HD2	1:B:16:ASN:HB3	18	0.05
(1,4770)	1:B:15:LYS:HD3	1:B:16:ASN:HB2	18	0.05
(1,4770)	1:B:15:LYS:HD3	1:B:16:ASN:HB3	18	0.05
(1,4768)	1:B:15:LYS:HG2	1:B:16:ASN:HD21	14	0.05
(1,4768)	1:B:15:LYS:HG2	1:B:16:ASN:HD22	14	0.05
(1,4768)	1:B:15:LYS:HG3	1:B:16:ASN:HD21	14	0.05
(1,4768)	1:B:15:LYS:HG3	1:B:16:ASN:HD22	14	0.05
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	9	0.05
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	9	0.05
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	9	0.05
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	9	0.05
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	19	0.05
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	19	0.05
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	19	0.05
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	19	0.05
(1,4765)	1:B:15:LYS:HB2	1:B:18:MET:HG2	15	0.05
(1,4765)	1:B:15:LYS:HB2	1:B:18:MET:HG3	15	0.05
(1,4642)	1:A:54:LYS:HD2	1:A:55:ASN:HD21	6	0.05
(1,4642)	1:A:54:LYS:HD2	1:A:55:ASN:HD22	6	0.05
(1,4642)	1:A:54:LYS:HD3	1:A:55:ASN:HD21	6	0.05
(1,4642)	1:A:54:LYS:HD3	1:A:55:ASN:HD22	6	0.05
(1,4642)	1:A:54:LYS:HD2	1:A:55:ASN:HD21	9	0.05
(1,4642)	1:A:54:LYS:HD2	1:A:55:ASN:HD22	9	0.05
(1,4642)	1:A:54:LYS:HD3	1:A:55:ASN:HD21	9	0.05
(1,4642)	1:A:54:LYS:HD3	1:A:55:ASN:HD22	9	0.05
(1,4640)	1:A:54:LYS:HG2	1:A:55:ASN:HD21	10	0.05
(1,4640)	1:A:54:LYS:HG2	1:A:55:ASN:HD22	10	0.05
(1,4640)	1:A:54:LYS:HG3	1:A:55:ASN:HD21	10	0.05
(1,4640)	1:A:54:LYS:HG3	1:A:55:ASN:HD22	10	0.05
(1,4638)	1:A:54:LYS:HB2	1:A:55:ASN:HD21	18	0.05
(1,4638)	1:A:54:LYS:HB2	1:A:55:ASN:HD22	18	0.05
(1,4638)	1:A:54:LYS:HB3	1:A:55:ASN:HD21	18	0.05
(1,4638)	1:A:54:LYS:HB3	1:A:55:ASN:HD22	18	0.05
(1,4613)	1:A:42:ASP:HB2	1:A:44:ILE:HG12	1	0.05
(1,4613)	1:A:42:ASP:HB3	1:A:44:ILE:HG12	1	0.05
(1,4613)	1:A:42:ASP:HB2	1:A:44:ILE:HG12	10	0.05
(1,4613)	1:A:42:ASP:HB3	1:A:44:ILE:HG12	10	0.05
(1,4606)	1:A:39:ASN:HD21	1:A:46:THR:HG21	1	0.05
(1,4606)	1:A:39:ASN:HD21	1:A:46:THR:HG22	1	0.05
(1,4606)	1:A:39:ASN:HD21	1:A:46:THR:HG23	1	0.05
(1,4606)	1:A:39:ASN:HD22	1:A:46:THR:HG21	1	0.05



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Key	$\frac{\text{4 from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
	1:A:39:ASN:HD22	1:A:46:THR:HG22	1	0.05
(1,4606)	1:A:39:ASN:HD22	1:A:46:THR:HG23	1	0.05
(1,4606)	1:A:39:ASN:HD21	1:A:46:THR:HG21	15	0.05
(1,4606)	1:A:39:ASN:HD21	1:A:46:THR:HG22	15	0.05
(1,4606)	1:A:39:ASN:HD21	1:A:46:THR:HG23	15	0.05
(1,4606)	1:A:39:ASN:HD22	1:A:46:THR:HG21	15	0.05
(1,4606)	1:A:39:ASN:HD22	1:A:46:THR:HG22	15	0.05
(1,4606)	1:A:39:ASN:HD22	1:A:46:THR:HG23	15	0.05
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB2	9	0.05
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB3	9	0.05
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB2	9	0.05
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB3	9	0.05
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB2	18	0.05
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB3	18	0.05
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB2	18	0.05
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB3	18	0.05
(1,4538)	1:A:27:SER:HG	1:A:28:LYS:HD2	7	0.05
(1,4538)	1:A:27:SER:HG	1:A:28:LYS:HD3	7	0.05
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	5	0.05
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	5	0.05
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	5	0.05
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	5	0.05
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	5	0.05
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	5	0.05
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	15	0.05
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	15	0.05
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	15	0.05
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	15	0.05
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	15	0.05
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	15	0.05
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	19	0.05
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	19	0.05
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	19	0.05
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	19	0.05
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	19	0.05
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	19	0.05
(1,4407)	1:A:3:ASP:HB2	1:A:52:PHE:HD1	17	0.05
(1,4407)	1:A:3:ASP:HB2	1:A:52:PHE:HD2	17	0.05
(1,4407)	1:A:3:ASP:HB3	1:A:52:PHE:HD1	17	0.05
(1,4407)	1:A:3:ASP:HB3	1:A:52:PHE:HD2	17	0.05
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	8	0.05
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	8	0.05



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	8	0.05
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	9	0.05
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	9	0.05
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	9	0.05
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	12	0.05
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	12	0.05
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	12	0.05
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	6	0.05
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	6	0.05
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	6	0.05
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	10	0.05
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	10	0.05
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	10	0.05
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	17	0.05
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	17	0.05
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	17	0.05
(1,4397)	1:B:82:GLU:HA	1:B:83:HIS:HD2	7	0.05
(1,4387)	1:B:5:LEU:HG	1:B:83:HIS:HD2	15	0.05
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	4	0.05
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	4	0.05
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	4	0.05
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	4	0.05
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	4	0.05
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	4	0.05
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	5	0.05
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	5	0.05
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	5	0.05
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	5	0.05
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	5	0.05
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	5	0.05
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	6	0.05
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	6	0.05
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	6	0.05
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	6	0.05
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	6	0.05
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	6	0.05
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	7	0.05
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	7	0.05
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	7	0.05
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	7	0.05
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	7	0.05
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	7	0.05
(, - , - ,	1	== 3:=3		ord on mort mage



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	1	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	1	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	1	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	1	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	1	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	1	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	8	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	8	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	8	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	8	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	8	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	8	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	9	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	9	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	9	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	9	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	9	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	9	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	13	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	13	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	13	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	13	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	13	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	13	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	14	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	14	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	14	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	14	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	14	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	14	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	18	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	18	0.05
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	18	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	18	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	18	0.05
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	18	0.05
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG21	14	0.05
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG22	14	0.05
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG23	14	0.05
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE1	3	0.05
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE2	3	0.05
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE1	3	0.05



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(1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 3 0.05 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE1 5 0.05 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE2 5 0.05 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE1 5 0.05 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 5 0.05 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE1 7 0.05 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE2 7 0.05 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 7 0.05 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE1 13 0.05 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE2 13 0.05 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE1 13 0.05 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE:HE2 13 0.05 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE1 16 0.05 (1,4333) 1:B:4:PHE:HB2 1:B:52:PHE:HE2 16 0.05 (1,4333) 1:B:4:PHE:HB3 1:B:52:PHE	
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(1,4332) 1:A:4:PHE:HB2 1:A:52:PHE:HE2 10 0.05	
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(1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE1 10 0.05	
(1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE2 10 0.05	
(1,4332) 1:A:4:PHE:HB2 1:A:52:PHE:HE1 14 0.05	
(1,4332) 1:A:4:PHE:HB2 1:A:52:PHE:HE2 14 0.05	
(1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE1 14 0.05	
(1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE2 14 0.05	
(1,4322) 1:A:52:PHE:HD1 1:A:53:VAL:H 5 0.05	
(1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 5 0.05	
(1,4322) 1:A:52:PHE:HD1 1:A:53:VAL:H 11 0.05	
(1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 11 0.05	
(1,4310) 1:A:5:LEU:HA 1:A:52:PHE:HD1 17 0.05	
(1,4310) 1:A:5:LEU:HA 1:A:52:PHE:HD2 17 0.05	
(1,4295) 1:B:22:ILE:HG13 1:B:45:PHE:HZ 2 0.05	
(1,4295) 1:B:22:ILE:HG13 1:B:45:PHE:HZ 9 0.05	
(1,4295) 1:B:22:ILE:HG13 1:B:45:PHE:HZ 10 0.05	
(1,4294) 1:A:22:ILE:HG13 1:A:45:PHE:HZ 1 0.05	
(1,4265) 1:B:22:ILE:HD11 1:B:45:PHE:HE1 18 0.05	
(1,4265) 1:B:22:ILE:HD11 1:B:45:PHE:HE2 18 0.05	
(1,4265) 1:B:22:ILE:HD12 1:B:45:PHE:HE1 18 0.05	
(1,4265) 1:B:22:ILE:HD12 1:B:45:PHE:HE2 18 0.05	
(1,4265) 1:B:22:ILE:HD13 1:B:45:PHE:HE1 18 0.05	
(1,4265) 1:B:22:ILE:HD13 1:B:45:PHE:HE2 18 0.05	
(1,4208) 1:A:29:PHE:HA 1:A:29:PHE:HD1 20 0.05	



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4208)	1:A:29:PHE:HA	1:A:29:PHE:HD2	20	0.05
(1,4205)	1:B:29:PHE:HD1	1:B:65:LYS:HD2	5	0.05
(1,4205)	1:B:29:PHE:HD2	1:B:65:LYS:HD2	5	0.05
(1,4205)	1:B:29:PHE:HD1	1:B:65:LYS:HD2	10	0.05
(1,4205)	1:B:29:PHE:HD2	1:B:65:LYS:HD2	10	0.05
(1,4204)	1:A:29:PHE:HD1	1:A:65:LYS:HD2	2	0.05
(1,4204)	1:A:29:PHE:HD2	1:A:65:LYS:HD2	2	0.05
(1,4204)	1:A:29:PHE:HD1	1:A:65:LYS:HD2	7	0.05
(1,4204)	1:A:29:PHE:HD2	1:A:65:LYS:HD2	7	0.05
(1,4204)	1:A:29:PHE:HD1	1:A:65:LYS:HD2	14	0.05
(1,4204)	1:A:29:PHE:HD2	1:A:65:LYS:HD2	14	0.05
(1,4187)	1:B:4:PHE:HZ	1:B:6:ALA:HA	2	0.05
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	7	0.05
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	7	0.05
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	7	0.05
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	7	0.05
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	7	0.05
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	7	0.05
(1,4129)	1:B:83:HIS:HA	1:B:83:HIS:HD2	15	0.05
(1,4129)	1:B:83:HIS:HA	1:B:83:HIS:HD2	17	0.05
(1,4119)	1:B:80:ASN:HA	1:B:81:LEU:HG	18	0.05
(1,4087)	1:B:73:PHE:HA	1:B:75:VAL:HG21	14	0.05
(1,4087)	1:B:73:PHE:HA	1:B:75:VAL:HG22	14	0.05
(1,4087)	1:B:73:PHE:HA	1:B:75:VAL:HG23	14	0.05
(1,4053)	1:B:41:LYS:HG2	1:B:42:ASP:HA	19	0.05
(1,4053)	1:B:41:LYS:HG3	1:B:42:ASP:HA	19	0.05
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG2	7	0.05
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG3	7	0.05
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG2	16	0.05
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG3	16	0.05
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG2	19	0.05
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG3	19	0.05
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	2	0.05
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	2	0.05
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	8	0.05
(1,3994)	1:A:82:GLU:H	1:A:83:HIS:HB3	10	0.05
(1,3994)	1:A:82:GLU:H	1:A:83:HIS:HB3	11	0.05
(1,3984)	1:A:5:LEU:HD11	1:A:81:LEU:HD11	5	0.05
(1,3984)	1:A:5:LEU:HD11	1:A:81:LEU:HD12	5	0.05
(1,3984)	1:A:5:LEU:HD11	1:A:81:LEU:HD13	5	0.05
(1,3984)	1:A:5:LEU:HD12	1:A:81:LEU:HD11	5	0.05
(1,3984)	1:A:5:LEU:HD12	1:A:81:LEU:HD12	5	0.05



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Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,3984)	1:A:5:LEU:HD12	1:A:81:LEU:HD13	5	0.05
(1,3984)	1:A:5:LEU:HD13	1:A:81:LEU:HD11	5	0.05
(1,3984)	1:A:5:LEU:HD13	1:A:81:LEU:HD12	5	0.05
(1,3984)	1:A:5:LEU:HD13	1:A:81:LEU:HD13	5	0.05
(1,3984)	1:A:5:LEU:HD11	1:A:81:LEU:HD11	8	0.05
(1,3984)	1:A:5:LEU:HD11	1:A:81:LEU:HD12	8	0.05
(1,3984)	1:A:5:LEU:HD11	1:A:81:LEU:HD13	8	0.05
(1,3984)	1:A:5:LEU:HD12	1:A:81:LEU:HD11	8	0.05
(1,3984)	1:A:5:LEU:HD12	1:A:81:LEU:HD12	8	0.05
(1,3984)	1:A:5:LEU:HD12	1:A:81:LEU:HD13	8	0.05
(1,3984)	1:A:5:LEU:HD13	1:A:81:LEU:HD11	8	0.05
(1,3984)	1:A:5:LEU:HD13	1:A:81:LEU:HD12	8	0.05
(1,3984)	1:A:5:LEU:HD13	1:A:81:LEU:HD13	8	0.05
(1,3954)	1:A:41:LYS:HE2	1:A:44:ILE:HB	15	0.05
(1,3954)	1:A:41:LYS:HE3	1:A:44:ILE:HB	15	0.05
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD11	3	0.05
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD12	3	0.05
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD13	3	0.05
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD11	18	0.05
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD12	18	0.05
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD13	18	0.05
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD11	9	0.05
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD12	9	0.05
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD13	9	0.05
(1,3889)	1:A:82:GLU:HA	1:A:83:HIS:HB2	7	0.05
(1,3873)	1:A:6:ALA:H	1:A:81:LEU:HD11	4	0.05
(1,3873)	1:A:6:ALA:H	1:A:81:LEU:HD12	4	0.05
(1,3873)	1:A:6:ALA:H	1:A:81:LEU:HD13	4	0.05
(1,3824)	1:B:9:ARG:HD2	1:B:78:LEU:HD21	8	0.05
(1,3824)	1:B:9:ARG:HD2	1:B:78:LEU:HD22	8	0.05
(1,3824)	1:B:9:ARG:HD2	1:B:78:LEU:HD23	8	0.05
(1,3824)	1:B:9:ARG:HD3	1:B:78:LEU:HD21	8	0.05
(1,3824)	1:B:9:ARG:HD3	1:B:78:LEU:HD22	8	0.05
(1,3824)	1:B:9:ARG:HD3	1:B:78:LEU:HD23	8	0.05
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD11	2	0.05
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD12	2	0.05
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD13	2	0.05
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD11	16	0.05
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD12	16	0.05
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD13	16	0.05
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD11	7	0.05
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD12	7	0.05



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(1,3817)				Violation (Å)
	1:A:76:GLU:H	1:A:78:LEU:HD13	7	0.05
(1,3798)	1:B:9:ARG:HD2	1:B:78:LEU:HD11	6	0.05
(1,3798)	1:B:9:ARG:HD2	1:B:78:LEU:HD12	6	0.05
(1,3798)	1:B:9:ARG:HD2	1:B:78:LEU:HD13	6	0.05
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD11	6	0.05
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD12	6	0.05
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD13	6	0.05
(1,3733)	1:A:74:THR:HA	1:A:76:GLU:HG2	5	0.05
(1,3733)	1:A:74:THR:HA	1:A:76:GLU:HG3	5	0.05
(1,3733)	1:A:74:THR:HA	1:A:76:GLU:HG2	20	0.05
(1,3733)	1:A:74:THR:HA	1:A:76:GLU:HG3	20	0.05
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	1	0.05
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	1	0.05
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	1	0.05
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	4	0.05
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	4	0.05
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	4	0.05
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	12	0.05
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	12	0.05
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	12	0.05
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	2	0.05
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	2	0.05
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	2	0.05
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	5	0.05
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	5	0.05
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	5	0.05
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	8	0.05
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	8	0.05
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	8	0.05
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	12	0.05
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	12	0.05
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	12	0.05
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG21	10	0.05
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG22	10	0.05
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG23	10	0.05
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG21	10	0.05
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG22	10	0.05
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG23	10	0.05
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG21	19	0.05
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG22	19	0.05
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG23	19	0.05
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	19	0.05



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	19	0.05
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	19	0.05
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG11	3	0.05
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG12	3	0.05
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG13	3	0.05
(1,3627)	1:A:70:GLN:HG2	1:A:72:VAL:H	19	0.05
(1,3627)	1:A:70:GLN:HG3	1:A:72:VAL:H	19	0.05
(1,3614)	1:B:69:VAL:H	1:B:70:GLN:HB2	10	0.05
(1,3614)	1:B:69:VAL:H	1:B:70:GLN:HB3	10	0.05
(1,3593)	1:A:66:LEU:HA	1:A:69:VAL:HB	15	0.05
(1,3593)	1:A:66:LEU:HA	1:A:69:VAL:HB	19	0.05
(1,3592)	1:B:20:ASN:HA	1:B:22:ILE:HB	2	0.05
(1,3592)	1:B:20:ASN:HA	1:B:22:ILE:HB	12	0.05
(1,3592)	1:B:20:ASN:HA	1:B:22:ILE:HB	20	0.05
(1,3591)	1:A:20:ASN:HA	1:A:22:ILE:HB	11	0.05
(1,3591)	1:A:20:ASN:HA	1:A:22:ILE:HB	12	0.05
(1,3591)	1:A:20:ASN:HA	1:A:22:ILE:HB	17	0.05
(1,3591)	1:A:20:ASN:HA	1:A:22:ILE:HB	20	0.05
(1,3561)	1:A:15:LYS:HE2	1:A:18:MET:H	5	0.05
(1,3561)	1:A:15:LYS:HE3	1:A:18:MET:H	5	0.05
(1,3561)	1:A:15:LYS:HE2	1:A:18:MET:H	12	0.05
(1,3561)	1:A:15:LYS:HE3	1:A:18:MET:H	12	0.05
(1,3559)	1:A:15:LYS:HE2	1:A:16:ASN:HD21	12	0.05
(1,3559)	1:A:15:LYS:HE3	1:A:16:ASN:HD21	12	0.05
(1,3483)	1:A:41:LYS:HE2	1:A:44:ILE:H	14	0.05
(1,3483)	1:A:41:LYS:HE3	1:A:44:ILE:H	14	0.05
(1,3483)	1:A:41:LYS:HE2	1:A:44:ILE:H	20	0.05
(1,3483)	1:A:41:LYS:HE3	1:A:44:ILE:H	20	0.05
(1,3423)	1:B:9:ARG:H	1:B:63:MET:HE1	17	0.05
(1,3423)	1:B:9:ARG:H	1:B:63:MET:HE2	17	0.05
(1,3423)	1:B:9:ARG:H	1:B:63:MET:HE3	17	0.05
(1,3422)	1:A:9:ARG:H	1:A:63:MET:HE1	19	0.05
(1,3422)	1:A:9:ARG:H	1:A:63:MET:HE2	19	0.05
(1,3422)	1:A:9:ARG:H	1:A:63:MET:HE3	19	0.05
(1,3421)	1:B:63:MET:HE1	1:B:77:ARG:H	5	0.05
(1,3421)	1:B:63:MET:HE2	1:B:77:ARG:H	5	0.05
(1,3421)	1:B:63:MET:HE3	1:B:77:ARG:H	5	0.05
(1,3421)	1:B:63:MET:HE1	1:B:77:ARG:H	6	0.05
(1,3421)	1:B:63:MET:HE2	1:B:77:ARG:H	6	0.05
(1,3421)	1:B:63:MET:HE3	1:B:77:ARG:H	6	0.05
(1,3420)	1:A:63:MET:HE1	1:A:77:ARG:H	14	0.05
(1,3420)	1:A:63:MET:HE2	1:A:77:ARG:H	14	0.05



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3420)	1:A:63:MET:HE3	1:A:77:ARG:H	14	0.05
(1,3413)	1:B:63:MET:HE1	1:B:76:GLU:HA	10	0.05
(1,3413)	1:B:63:MET:HE2	1:B:76:GLU:HA	10	0.05
(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	10	0.05
(1,3413)	1:B:63:MET:HE1	1:B:76:GLU:HA	14	0.05
(1,3413)	1:B:63:MET:HE2	1:B:76:GLU:HA	14	0.05
(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	14	0.05
(1,3412)	1:A:63:MET:HE1	1:A:76:GLU:HA	9	0.05
(1,3412)	1:A:63:MET:HE2	1:A:76:GLU:HA	9	0.05
(1,3412)	1:A:63:MET:HE3	1:A:76:GLU:HA	9	0.05
(1,3411)	1:B:63:MET:HE1	1:B:77:ARG:HA	4	0.05
(1,3411)	1:B:63:MET:HE2	1:B:77:ARG:HA	4	0.05
(1,3411)	1:B:63:MET:HE3	1:B:77:ARG:HA	4	0.05
(1,3410)	1:A:63:MET:HE1	1:A:77:ARG:HA	19	0.05
(1,3410)	1:A:63:MET:HE2	1:A:77:ARG:HA	19	0.05
(1,3410)	1:A:63:MET:HE3	1:A:77:ARG:HA	19	0.05
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	1	0.05
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	1	0.05
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	1	0.05
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE1	9	0.05
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE2	9	0.05
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE3	9	0.05
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE1	11	0.05
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE2	11	0.05
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE3	11	0.05
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE1	11	0.05
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE2	11	0.05
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE3	11	0.05
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE1	11	0.05
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE2	11	0.05
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE3	11	0.05
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE1	13	0.05
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE2	13	0.05
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE3	13	0.05
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE1	13	0.05
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE2	13	0.05
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE3	13	0.05
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE1	13	0.05
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE2	13	0.05
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE3	13	0.05
(1,3335)	1:B:58:LYS:HE2	1:B:62:LEU:HD11	20	0.05
(1,3335)	1:B:58:LYS:HE2	1:B:62:LEU:HD12	20	0.05



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Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,3335)	1:B:58:LYS:HE2	1:B:62:LEU:HD13	20	0.05
(1,3258)	1:B:60:THR:HA	1:B:60:THR:HG21	3	0.05
(1,3258)	1:B:60:THR:HA	1:B:60:THR:HG22	3	0.05
(1,3258)	1:B:60:THR:HA	1:B:60:THR:HG23	3	0.05
(1,3257)	1:A:60:THR:HA	1:A:60:THR:HG21	2	0.05
(1,3257)	1:A:60:THR:HA	1:A:60:THR:HG22	2	0.05
(1,3257)	1:A:60:THR:HA	1:A:60:THR:HG23	2	0.05
(1,3257)	1:A:60:THR:HA	1:A:60:THR:HG21	14	0.05
(1,3257)	1:A:60:THR:HA	1:A:60:THR:HG22	14	0.05
(1,3257)	1:A:60:THR:HA	1:A:60:THR:HG23	14	0.05
(1,3175)	1:A:30:ASP:HB2	1:A:58:LYS:HD2	11	0.05
(1,3175)	1:A:30:ASP:HB2	1:A:58:LYS:HD3	11	0.05
(1,3175)	1:A:30:ASP:HB3	1:A:58:LYS:HD2	11	0.05
(1,3175)	1:A:30:ASP:HB3	1:A:58:LYS:HD3	11	0.05
(1,3099)	1:A:54:LYS:H	1:A:54:LYS:HD2	8	0.05
(1,3099)	1:A:54:LYS:H	1:A:54:LYS:HD3	8	0.05
(1,3093)	1:A:15:LYS:HD2	1:A:16:ASN:HD22	14	0.05
(1,3093)	1:A:15:LYS:HD3	1:A:16:ASN:HD22	14	0.05
(1,3093)	1:A:15:LYS:HD2	1:A:16:ASN:HD22	19	0.05
(1,3093)	1:A:15:LYS:HD3	1:A:16:ASN:HD22	19	0.05
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG11	2	0.05
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG12	2	0.05
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG13	2	0.05
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	1	0.05
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	1	0.05
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	1	0.05
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	1	0.05
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	1	0.05
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	1	0.05
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	4	0.05
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	4	0.05
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	4	0.05
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	4	0.05
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	4	0.05
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	4	0.05
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	14	0.05
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	14	0.05
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	14	0.05
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	14	0.05
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	14	0.05
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	14	0.05
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	7	0.05



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	7	0.05
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	7	0.05
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	7	0.05
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	7	0.05
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	7	0.05
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD11	12	0.05
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD12	12	0.05
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD13	12	0.05
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD11	16	0.05
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD12	16	0.05
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD13	16	0.05
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD11	20	0.05
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD12	20	0.05
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD13	20	0.05
(1,2924)	1:B:51:ILE:HD11	1:B:62:LEU:HD21	16	0.05
(1,2924)	1:B:51:ILE:HD11	1:B:62:LEU:HD22	16	0.05
(1,2924)	1:B:51:ILE:HD11	1:B:62:LEU:HD23	16	0.05
(1,2924)	1:B:51:ILE:HD12	1:B:62:LEU:HD21	16	0.05
(1,2924)	1:B:51:ILE:HD12	1:B:62:LEU:HD22	16	0.05
(1,2924)	1:B:51:ILE:HD12	1:B:62:LEU:HD23	16	0.05
(1,2924)	1:B:51:ILE:HD13	1:B:62:LEU:HD21	16	0.05
(1,2924)	1:B:51:ILE:HD13	1:B:62:LEU:HD22	16	0.05
(1,2924)	1:B:51:ILE:HD13	1:B:62:LEU:HD23	16	0.05
(1,2924)	1:B:51:ILE:HD11	1:B:62:LEU:HD21	20	0.05
(1,2924)	1:B:51:ILE:HD11	1:B:62:LEU:HD22	20	0.05
(1,2924)	1:B:51:ILE:HD11	1:B:62:LEU:HD23	20	0.05
(1,2924)	1:B:51:ILE:HD12	1:B:62:LEU:HD21	20	0.05
(1,2924)	1:B:51:ILE:HD12	1:B:62:LEU:HD22	20	0.05
(1,2924)	1:B:51:ILE:HD12	1:B:62:LEU:HD23	20	0.05
(1,2924)	1:B:51:ILE:HD13	1:B:62:LEU:HD21	20	0.05
(1,2924)	1:B:51:ILE:HD13	1:B:62:LEU:HD22	20	0.05
(1,2924)	1:B:51:ILE:HD13	1:B:62:LEU:HD23	20	0.05
(1,2902)	1:A:51:ILE:HG21	1:B:20:ASN:HD22	12	0.05
(1,2902)	1:A:51:ILE:HG22	1:B:20:ASN:HD22	12	0.05
(1,2902)	1:A:51:ILE:HG23	1:B:20:ASN:HD22	12	0.05
(1,2901)	1:A:20:ASN:HD22	1:B:51:ILE:HG21	7	0.05
(1,2901)	1:A:20:ASN:HD22	1:B:51:ILE:HG22	7	0.05
(1,2901)	1:A:20:ASN:HD22	1:B:51:ILE:HG23	7	0.05
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG21	3	0.05
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG22	3	0.05
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG23	3	0.05
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG21	19	0.05



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG22	19	0.05
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG23	19	0.05
(1,2882)	1:B:8:ILE:HG21	1:B:62:LEU:HD11	12	0.05
(1,2882)	1:B:8:ILE:HG21	1:B:62:LEU:HD12	12	0.05
(1,2882)	1:B:8:ILE:HG21	1:B:62:LEU:HD13	12	0.05
(1,2882)	1:B:8:ILE:HG22	1:B:62:LEU:HD11	12	0.05
(1,2882)	1:B:8:ILE:HG22	1:B:62:LEU:HD12	12	0.05
(1,2882)	1:B:8:ILE:HG22	1:B:62:LEU:HD13	12	0.05
(1,2882)	1:B:8:ILE:HG23	1:B:62:LEU:HD11	12	0.05
(1,2882)	1:B:8:ILE:HG23	1:B:62:LEU:HD12	12	0.05
(1,2882)	1:B:8:ILE:HG23	1:B:62:LEU:HD13	12	0.05
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD11	10	0.05
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD12	10	0.05
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD13	10	0.05
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD11	10	0.05
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD12	10	0.05
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD13	10	0.05
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD11	10	0.05
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD12	10	0.05
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD13	10	0.05
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD11	11	0.05
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD12	11	0.05
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD13	11	0.05
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD11	11	0.05
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD12	11	0.05
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD13	11	0.05
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD11	11	0.05
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD12	11	0.05
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD13	11	0.05
(1,2816)	1:B:50:MET:HE1	1:B:51:ILE:HG13	10	0.05
(1,2816)	1:B:50:MET:HE2	1:B:51:ILE:HG13	10	0.05
(1,2816)	1:B:50:MET:HE3	1:B:51:ILE:HG13	10	0.05
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	5	0.05
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	5	0.05
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	5	0.05
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	9	0.05
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	9	0.05
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	9	0.05
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	11	0.05
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	11	0.05
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	11	0.05
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	19	0.05



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	19	0.05
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	19	0.05
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	8	0.05
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	14	0.05
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	19	0.05
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	5	0.05
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	6	0.05
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	7	0.05
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	9	0.05
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	14	0.05
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	16	0.05
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	17	0.05
(1,2668)	1:B:23:THR:HG1	1:B:47:CYS:HB3	1	0.05
(1,2668)	1:B:23:THR:HG1	1:B:47:CYS:HB3	18	0.05
(1,2667)	1:A:23:THR:HG1	1:A:47:CYS:HB3	19	0.05
(1,2618)	1:B:9:ARG:HD2	1:B:46:THR:HG21	2	0.05
(1,2618)	1:B:9:ARG:HD2	1:B:46:THR:HG22	2	0.05
(1,2618)	1:B:9:ARG:HD2	1:B:46:THR:HG23	2	0.05
(1,2618)	1:B:9:ARG:HD3	1:B:46:THR:HG21	2	0.05
(1,2618)	1:B:9:ARG:HD3	1:B:46:THR:HG22	2	0.05
(1,2618)	1:B:9:ARG:HD3	1:B:46:THR:HG23	2	0.05
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG21	6	0.05
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG22	6	0.05
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG23	6	0.05
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	5	0.05
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	5	0.05
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	5	0.05
(1,2580)	1:B:42:ASP:HB2	1:B:44:ILE:HD11	1	0.05
(1,2580)	1:B:42:ASP:HB2	1:B:44:ILE:HD12	1	0.05
(1,2580)	1:B:42:ASP:HB2	1:B:44:ILE:HD13	1	0.05
(1,2576)	1:B:44:ILE:HG21	1:B:45:PHE:H	12	0.05
(1,2576)	1:B:44:ILE:HG22	1:B:45:PHE:H	12	0.05
(1,2576)	1:B:44:ILE:HG23	1:B:45:PHE:H	12	0.05
(1,2552)	1:B:44:ILE:HG13	1:B:45:PHE:H	3	0.05
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD21	16	0.05
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD22	16	0.05
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD23	16	0.05
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD21	17	0.05
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD22	17	0.05
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD23	17	0.05
(1,2448)	1:B:23:THR:HG1	1:B:38:LEU:HD21	2	0.05
(1,2448)	1:B:23:THR:HG1	1:B:38:LEU:HD22	2	0.05



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(4 0 1 1 - 1	Atom-1	Atom-2	Model	Violation (Å)
(1,2448)	1:B:23:THR:HG1	1:B:38:LEU:HD23	2	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	3	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	3	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	3	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	5	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	5	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	5	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	9	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	9	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	9	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	10	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	10	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	10	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	11	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	11	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	11	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	13	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	13	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	13	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	18	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	18	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	18	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	20	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	20	0.05
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	20	0.05
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	5	0.05
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	5	0.05
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	5	0.05
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	6	0.05
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	6	0.05
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	6	0.05
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	8	0.05
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	8	0.05
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	8	0.05
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	16	0.05
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	16	0.05
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	16	0.05
(1,2258)	1:B:35:THR:HB	1:B:50:MET:HB2	11	0.05
(1,2248)	1:B:33:ILE:HD11	1:B:34:ARG:H	14	0.05
(1,2248)	1:B:33:ILE:HD12	1:B:34:ARG:H	14	0.05
(1,2248)	1:B:33:ILE:HD13	1:B:34:ARG:H	14	0.05
(1,2182)	1:B:29:PHE:HD1	1:B:31:THR:HB	3	0.05



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2182)	1:B:29:PHE:HD2	1:B:31:THR:HB	3	0.05
(1,2182)	1:B:29:PHE:HD1	1:B:31:THR:HB	18	0.05
(1,2182)	1:B:29:PHE:HD2	1:B:31:THR:HB	18	0.05
(1,2181)	1:A:29:PHE:HD1	1:A:31:THR:HB	7	0.05
(1,2181)	1:A:29:PHE:HD2	1:A:31:THR:HB	7	0.05
(1,2174)	1:B:68:LYS:HA	1:B:68:LYS:HD2	4	0.05
(1,2173)	1:A:68:LYS:HA	1:A:68:LYS:HD2	19	0.05
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	4	0.05
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	4	0.05
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	4	0.05
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	6	0.05
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	6	0.05
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	6	0.05
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	15	0.05
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	15	0.05
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	15	0.05
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	20	0.05
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	20	0.05
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	20	0.05
(1,2094)	1:B:22:ILE:HA	1:B:25:VAL:HG21	18	0.05
(1,2094)	1:B:22:ILE:HA	1:B:25:VAL:HG22	18	0.05
(1,2094)	1:B:22:ILE:HA	1:B:25:VAL:HG23	18	0.05
(1,208)	1:B:16:ASN:HA	1:B:17:GLY:H	5	0.05
(1,208)	1:B:16:ASN:HA	1:B:17:GLY:H	19	0.05
(1,207)	1:A:16:ASN:HA	1:A:17:GLY:H	7	0.05
(1,207)	1:A:16:ASN:HA	1:A:17:GLY:H	9	0.05
(1,207)	1:A:16:ASN:HA	1:A:17:GLY:H	15	0.05
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	17	0.05
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	17	0.05
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	17	0.05
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	20	0.05
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	20	0.05
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	20	0.05
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	5	0.05
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	5	0.05
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	5	0.05
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	6	0.05
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	6	0.05
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	6	0.05
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	7	0.05
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	7	0.05
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	7	0.05



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	8	0.05
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	8	0.05
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	8	0.05
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	11	0.05
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	11	0.05
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	11	0.05
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	3	0.05
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	3	0.05
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	3	0.05
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	12	0.05
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	12	0.05
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	12	0.05
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	16	0.05
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	16	0.05
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	16	0.05
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	20	0.05
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	20	0.05
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	20	0.05
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	5	0.05
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	5	0.05
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	5	0.05
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	7	0.05
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	7	0.05
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	7	0.05
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	19	0.05
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	19	0.05
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	19	0.05
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	2	0.05
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	15	0.05
(1,1814)	1:A:68:LYS:HE2	1:A:69:VAL:HG21	4	0.05
(1,1814)	1:A:68:LYS:HE2	1:A:69:VAL:HG22	4	0.05
(1,1814)	1:A:68:LYS:HE2	1:A:69:VAL:HG23	4	0.05
(1,1814)	1:A:68:LYS:HE3	1:A:69:VAL:HG21	4	0.05
(1,1814)	1:A:68:LYS:HE3	1:A:69:VAL:HG22	4	0.05
(1,1814)	1:A:68:LYS:HE3	1:A:69:VAL:HG23	4	0.05
(1,1811)	1:B:41:LYS:HE2	1:B:44:ILE:HD11	13	0.05
(1,1811)	1:B:41:LYS:HE2	1:B:44:ILE:HD12	13	0.05
(1,1811)	1:B:41:LYS:HE2	1:B:44:ILE:HD13	13	0.05
(1,1811)	1:B:41:LYS:HE3	1:B:44:ILE:HD11	13	0.05
(1,1811)	1:B:41:LYS:HE3	1:B:44:ILE:HD12	13	0.05
(1,1811)	1:B:41:LYS:HE3	1:B:44:ILE:HD13	13	0.05
(1,1810)	1:A:41:LYS:HE2	1:A:44:ILE:HD11	13	0.05



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1810)	1:A:41:LYS:HE2	1:A:44:ILE:HD12	13	0.05
(1,1810)	1:A:41:LYS:HE2	1:A:44:ILE:HD13	13	0.05
(1,1810)	1:A:41:LYS:HE3	1:A:44:ILE:HD11	13	0.05
(1,1810)	1:A:41:LYS:HE3	1:A:44:ILE:HD12	13	0.05
(1,1810)	1:A:41:LYS:HE3	1:A:44:ILE:HD13	13	0.05
(1,1809)	1:B:11:VAL:HG21	1:B:41:LYS:HE2	6	0.05
(1,1809)	1:B:11:VAL:HG21	1:B:41:LYS:HE3	6	0.05
(1,1809)	1:B:11:VAL:HG22	1:B:41:LYS:HE2	6	0.05
(1,1809)	1:B:11:VAL:HG22	1:B:41:LYS:HE3	6	0.05
(1,1809)	1:B:11:VAL:HG23	1:B:41:LYS:HE2	6	0.05
(1,1809)	1:B:11:VAL:HG23	1:B:41:LYS:HE3	6	0.05
(1,1809)	1:B:11:VAL:HG21	1:B:41:LYS:HE2	13	0.05
(1,1809)	1:B:11:VAL:HG21	1:B:41:LYS:HE3	13	0.05
(1,1809)	1:B:11:VAL:HG22	1:B:41:LYS:HE2	13	0.05
(1,1809)	1:B:11:VAL:HG22	1:B:41:LYS:HE3	13	0.05
(1,1809)	1:B:11:VAL:HG23	1:B:41:LYS:HE2	13	0.05
(1,1809)	1:B:11:VAL:HG23	1:B:41:LYS:HE3	13	0.05
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG11	3	0.05
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG12	3	0.05
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG13	3	0.05
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG11	3	0.05
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG12	3	0.05
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG13	3	0.05
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG11	6	0.05
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG12	6	0.05
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG13	6	0.05
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG11	6	0.05
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG12	6	0.05
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG13	6	0.05
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	19	0.05
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	19	0.05
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	19	0.05
(1,1691)	1:B:11:VAL:HG21	1:B:46:THR:HB	14	0.05
(1,1691)	1:B:11:VAL:HG22	1:B:46:THR:HB	14	0.05
(1,1691)	1:B:11:VAL:HG23	1:B:46:THR:HB	14	0.05
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG21	13	0.05
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG22	13	0.05
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG23	13	0.05
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG21	13	0.05
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG22	13	0.05
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG23	13	0.05
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG21	13	0.05



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG22	13	0.05
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG23	13	0.05
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD11	7	0.05
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD12	7	0.05
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD13	7	0.05
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD11	11	0.05
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD12	11	0.05
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD13	11	0.05
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD11	17	0.05
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD12	17	0.05
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD13	17	0.05
(1,161)	1:B:13:GLU:H	1:B:73:PHE:H	19	0.05
(1,1579)	1:B:9:ARG:HD2	1:B:76:GLU:HG2	8	0.05
(1,1579)	1:B:9:ARG:HD2	1:B:76:GLU:HG3	8	0.05
(1,1579)	1:B:9:ARG:HD3	1:B:76:GLU:HG2	8	0.05
(1,1579)	1:B:9:ARG:HD3	1:B:76:GLU:HG3	8	0.05
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	17	0.05
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	17	0.05
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	17	0.05
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	17	0.05
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	17	0.05
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	17	0.05
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	17	0.05
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	17	0.05
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	17	0.05
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	1	0.05
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	1	0.05
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	1	0.05
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	1	0.05
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	1	0.05
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	1	0.05
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	1	0.05
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	1	0.05
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	1	0.05
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	16	0.05
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	16	0.05
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	16	0.05
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	16	0.05
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	16	0.05
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	16	0.05
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	16	0.05
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	16	0.05



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	16	0.05
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	15	0.05
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	15	0.05
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	15	0.05
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	15	0.05
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	15	0.05
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	15	0.05
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	2	0.05
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	2	0.05
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	2	0.05
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	2	0.05
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	2	0.05
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	2	0.05
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	5	0.05
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	5	0.05
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	5	0.05
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	5	0.05
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	5	0.05
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	5	0.05
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	11	0.05
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	11	0.05
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	11	0.05
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	11	0.05
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	11	0.05
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	11	0.05
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	1	0.05
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	1	0.05
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	1	0.05
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	12	0.05
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	12	0.05
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	12	0.05
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	18	0.05
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	18	0.05
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	18	0.05
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	5	0.05
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	5	0.05
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	5	0.05
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	14	0.05
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	14	0.05
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	14	0.05
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	19	0.05
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	19	0.05



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	19	0.05
(1,1413)	1:A:3:ASP:HB2	1:A:53:VAL:H	20	0.05
(1,1358)	1:B:81:LEU:HA	1:B:82:GLU:H	5	0.05
(1,1330)	1:B:78:LEU:HD21	1:B:79:SER:H	19	0.05
(1,1330)	1:B:78:LEU:HD22	1:B:79:SER:H	19	0.05
(1,1330)	1:B:78:LEU:HD23	1:B:79:SER:H	19	0.05
(1,13)	1:A:4:PHE:H	1:A:54:LYS:HA	16	0.05
(1,1212)	1:B:69:VAL:HG11	1:B:71:GLY:H	17	0.05
(1,1212)	1:B:69:VAL:HG12	1:B:71:GLY:H	17	0.05
(1,1212)	1:B:69:VAL:HG13	1:B:71:GLY:H	17	0.05
(1,1196)	1:B:69:VAL:H	1:B:70:GLN:H	6	0.05
(1,1195)	1:A:69:VAL:H	1:A:70:GLN:H	9	0.05
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	9	0.05
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	11	0.05
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	18	0.05
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	4	0.05
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	19	0.05
(1,1150)	1:B:67:ARG:HE	1:B:75:VAL:HB	7	0.05
(1,1150)	1:B:67:ARG:HE	1:B:75:VAL:HB	11	0.05
(1,1106)	1:B:62:LEU:HD11	1:B:66:LEU:H	14	0.05
(1,1106)	1:B:62:LEU:HD12	1:B:66:LEU:H	14	0.05
(1,1106)	1:B:62:LEU:HD13	1:B:66:LEU:H	14	0.05
(1,1105)	1:A:62:LEU:HD11	1:A:66:LEU:H	15	0.05
(1,1105)	1:A:62:LEU:HD12	1:A:66:LEU:H	15	0.05
(1,1105)	1:A:62:LEU:HD13	1:A:66:LEU:H	15	0.05
(1,1104)	1:B:62:LEU:HD11	1:B:65:LYS:H	15	0.05
(1,1104)	1:B:62:LEU:HD12	1:B:65:LYS:H	15	0.05
(1,1104)	1:B:62:LEU:HD13	1:B:65:LYS:H	15	0.05
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	1	0.05
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	1	0.05
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	1	0.05
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	10	0.05
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	10	0.05
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	10	0.05
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	15	0.05
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	15	0.05
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	15	0.05
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	17	0.05
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	17	0.05
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	17	0.05
(1,939)	1:B:54:LYS:HE2	1:B:55:ASN:HD22	4	0.04
(1,939)	1:B:54:LYS:HE3	1:B:55:ASN:HD22	4	0.04



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(1,939) 1:B:54:LYS:HE2 1:B:55:ASN:HD22 20 0.04 (1,939) 1:B:54:LYS:HE3 1:B:55:ASN:HD22 20 0.04 (1,938) 1:A:54:LYS:HE2 1:A:55:ASN:HD22 11 0.04 (1,938) 1:A:54:LYS:HE3 1:A:55:ASN:HD22 11 0.04 (1,938) 1:A:55:ILE:HG12 1:B:52:PHE:H 4 0.04 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 12 0.04 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 16 0.04 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 18 0.04 (1,899) 1:B:47:CYS:HG 1:B:48:ASN:H 1 0.04 (1,899) 1:B:45:PHE:HZ 1:B:48:ASN:H 7 0.04 (1,893) 1:B:47:CYS:HG 1:B:48:ASN:H <td< th=""><th>Key</th><th>Atom-1</th><th>Atom-2</th><th>Model</th><th>Violation (Å)</th></td<>	Key	Atom-1	Atom-2	Model	Violation (Å)
(1,938) 1:A:54:LYS:HE2 1:A:55:ASN:HD22 11 0.04 (1,938) 1:A:54:LYS:HE3 1:A:55:ASN:HD22 11 0.04 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 4 0.04 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 12 0.04 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 16 0.04 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 18 0.04 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 18 0.04 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 18 0.04 (1,899) 1:B:47:CYS:HG 1:B:48:ASN:H 1 0.04 (1,899) 1:B:47:CYS:HG 1:B:48:ASN:H 1 0.04 (1,890) 1:B:47:CYS:HG 1:B:48:ASN:H 7 0.04 (1,833) 1:B:47:CYS:HG 1:B:48:ASN:H 7 0.04 (1,823) 1:B:45:PHE:HZ 1:B:47:CYS:H 7 0.04 (1,823) 1:B:45:PHE:HZ 1:A:47:CYS:H 15	(1,939)	1:B:54:LYS:HE2	1:B:55:ASN:HD22	20	0.04
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(1,761) 1:B:43:GLY:H 1:B:44:ILE:H 19 0.04 (1,725) 1:B:41:LYS:HG2 1:B:42:ASP:H 1 0.04 (1,725) 1:B:41:LYS:HG3 1:B:42:ASP:H 1 0.04 (1,719) 1:B:41:LYS:H 1:B:46:THR:H 15 0.04 (1,719) 1:A:41:LYS:H 1:A:46:THR:H 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 9 0.04	(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	14	0.04
(1,725) 1:B:41:LYS:HG2 1:B:42:ASP:H 1 0.04 (1,725) 1:B:41:LYS:HG3 1:B:42:ASP:H 1 0.04 (1,719) 1:B:41:LYS:H 1:B:46:THR:H 15 0.04 (1,718) 1:A:41:LYS:H 1:A:46:THR:H 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 4 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 4 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 9 0.04	(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	15	0.04
(1,725) 1:B:41:LYS:HG3 1:B:42:ASP:H 1 0.04 (1,719) 1:B:41:LYS:H 1:B:46:THR:H 15 0.04 (1,718) 1:A:41:LYS:H 1:A:46:THR:H 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 4 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 4 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 9 0.04	(1,761)	1:B:43:GLY:H	1:B:44:ILE:H	19	0.04
(1,725) 1:B:41:LYS:HG3 1:B:42:ASP:H 1 0.04 (1,719) 1:B:41:LYS:H 1:B:46:THR:H 15 0.04 (1,718) 1:A:41:LYS:H 1:A:46:THR:H 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 4 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 4 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 9 0.04	(1,725)	1:B:41:LYS:HG2	1:B:42:ASP:H	1	0.04
(1,719) 1:B:41:LYS:H 1:B:46:THR:H 15 0.04 (1,718) 1:A:41:LYS:H 1:A:46:THR:H 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 4 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 4 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04	· ' '	1:B:41:LYS:HG3	1:B:42:ASP:H	1	0.04
(1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 4 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 4 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 9 0.04	(1,719)	1:B:41:LYS:H	1:B:46:THR:H	15	0.04
(1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 2 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 4 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 4 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 9 0.04	(1,718)	1:A:41:LYS:H	1:A:46:THR:H	2	0.04
(1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 4 0.04 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 4 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 9 0.04	(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD1	2	0.04
(1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 4 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 9 0.04	(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD2	2	0.04
(1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 9 0.04	(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD1	4	0.04
(1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 3 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 9 0.04	(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD2	4	0.04
(1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 9 0.04 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 9 0.04	(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD1	3	0.04
(1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 9 0.04	(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD2	3	0.04
	(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD1	9	0.04
	(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD2	9	0.04
1 (-,) 1.2.00.11110.1121 0.01	(1,615)	1:B:35:THR:H	1:B:83:HIS:HE1	5	0.04
(1,563) 1:A:32:ASN:HD21 1:A:33:ILE:HB 12 0.04	(1,563)	1:A:32:ASN:HD21	1:A:33:ILE:HB	12	0.04
(1,563) 1:A:32:ASN:HD21 1:A:33:ILE:HB 17 0.04	· · /	1:A:32:ASN:HD21	1:A:33:ILE:HB	17	0.04
(1,545) 1:A:29:PHE:HD1 1:A:31:THR:H 6 0.04	· · /	1:A:29:PHE:HD1	1:A:31:THR:H	6	0.04
(1,545) 1:A:29:PHE:HD2 1:A:31:THR:H 6 0.04	· /	1:A:29:PHE:HD2	1:A:31:THR:H	6	0.04
(1,545) 1:A:29:PHE:HD1 1:A:31:THR:H 18 0.04	· · /	1:A:29:PHE:HD1	1:A:31:THR:H	18	
(1,545) 1:A:29:PHE:HD2 1:A:31:THR:H 18 0.04	· · /	1:A:29:PHE:HD2	1:A:31:THR:H	18	0.04
(1,541) 1:A:30:ASP:HA 1:A:31:THR:H 14 0.04		1:A:30:ASP:HA	1:A:31:THR:H	14	0.04
(1,5005) 1:B:77:ARG:H 1:B:77:ARG:HG2 7 0.04		1:B:77:ARG:H	1:B:77:ARG:HG2	7	0.04
(1,5005) 1:B:77:ARG:H 1:B:77:ARG:HG3 7 0.04		1:B:77:ARG:H	1:B:77:ARG:HG3	7	0.04
(1,5002) 1:B:69:VAL:HG11 1:B:70:GLN:HE21 14 0.04	(1,5002)	1:B:69:VAL:HG11	1:B:70:GLN:HE21	14	0.04
(1,5002) 1:B:69:VAL:HG11 1:B:70:GLN:HE22 14 0.04			1:B:70:GLN:HE22	14	0.04



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,5002)	1:B:69:VAL:HG12	1:B:70:GLN:HE21	14	0.04
(1,5002)	1:B:69:VAL:HG12	1:B:70:GLN:HE22	14	0.04
(1,5002)	1:B:69:VAL:HG13	1:B:70:GLN:HE21	14	0.04
(1,5002)	1:B:69:VAL:HG13	1:B:70:GLN:HE22	14	0.04
(1,4959)	1:B:59:LEU:HD11	1:B:77:ARG:HG2	16	0.04
(1,4959)	1:B:59:LEU:HD11	1:B:77:ARG:HG3	16	0.04
(1,4959)	1:B:59:LEU:HD12	1:B:77:ARG:HG2	16	0.04
(1,4959)	1:B:59:LEU:HD12	1:B:77:ARG:HG3	16	0.04
(1,4959)	1:B:59:LEU:HD13	1:B:77:ARG:HG2	16	0.04
(1,4959)	1:B:59:LEU:HD13	1:B:77:ARG:HG3	16	0.04
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD21	6	0.04
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD22	6	0.04
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD21	6	0.04
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD22	6	0.04
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD21	9	0.04
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD22	9	0.04
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD21	9	0.04
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD22	9	0.04
(1,4928)	1:B:54:LYS:H	1:B:54:LYS:HG2	8	0.04
(1,4928)	1:B:54:LYS:H	1:B:54:LYS:HG3	8	0.04
(1,4926)	1:B:53:VAL:HG21	1:B:54:LYS:HG2	12	0.04
(1,4926)	1:B:53:VAL:HG21	1:B:54:LYS:HG3	12	0.04
(1,4926)	1:B:53:VAL:HG22	1:B:54:LYS:HG2	12	0.04
(1,4926)	1:B:53:VAL:HG22	1:B:54:LYS:HG3	12	0.04
(1,4926)	1:B:53:VAL:HG23	1:B:54:LYS:HG2	12	0.04
(1,4926)	1:B:53:VAL:HG23	1:B:54:LYS:HG3	12	0.04
(1,4899)	1:B:39:ASN:HD21	1:B:46:THR:HB	4	0.04
(1,4899)	1:B:39:ASN:HD22	1:B:46:THR:HB	4	0.04
(1,4899)	1:B:39:ASN:HD21	1:B:46:THR:HB	8	0.04
(1,4899)	1:B:39:ASN:HD22	1:B:46:THR:HB	8	0.04
(1,4898)	1:B:39:ASN:HD21	1:B:41:LYS:HE2	14	0.04
(1,4898)	1:B:39:ASN:HD21	1:B:41:LYS:HE3	14	0.04
(1,4898)	1:B:39:ASN:HD22	1:B:41:LYS:HE2	14	0.04
(1,4898)	1:B:39:ASN:HD22	1:B:41:LYS:HE3	14	0.04
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB2	6	0.04
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB3	6	0.04
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB2	10	0.04
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB3	10	0.04
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB2	20	0.04
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB3	20	0.04
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	20	0.04
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	20	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	20	0.04
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	20	0.04
(1,4745)	1:B:9:ARG:HG2	1:B:11:VAL:HG21	6	0.04
(1,4745)	1:B:9:ARG:HG2	1:B:11:VAL:HG22	6	0.04
(1,4745)	1:B:9:ARG:HG2	1:B:11:VAL:HG23	6	0.04
(1,4745)	1:B:9:ARG:HG3	1:B:11:VAL:HG21	6	0.04
(1,4745)	1:B:9:ARG:HG3	1:B:11:VAL:HG22	6	0.04
(1,4745)	1:B:9:ARG:HG3	1:B:11:VAL:HG23	6	0.04
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG2	8	0.04
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG3	8	0.04
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG2	18	0.04
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG3	18	0.04
(1,4695)	1:A:67:ARG:HG2	1:A:75:VAL:H	16	0.04
(1,4695)	1:A:67:ARG:HG3	1:A:75:VAL:H	16	0.04
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE1	3	0.04
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE2	3	0.04
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE3	3	0.04
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE1	3	0.04
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE2	3	0.04
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE3	3	0.04
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE1	6	0.04
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE2	6	0.04
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE3	6	0.04
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE1	6	0.04
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE2	6	0.04
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE3	6	0.04
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE1	11	0.04
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE2	11	0.04
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE3	11	0.04
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE1	11	0.04
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE2	11	0.04
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE3	11	0.04
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE1	17	0.04
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE2	17	0.04
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE3	17	0.04
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE1	17	0.04
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE2	17	0.04
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE3	17	0.04
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE1	20	0.04
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE2	20	0.04
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE3	20	0.04
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE1	20	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE2	20	0.04
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE3	20	0.04
(1,4605)	1:A:39:ASN:HD21	1:A:46:THR:HB	12	0.04
(1,4605)	1:A:39:ASN:HD22	1:A:46:THR:HB	12	0.04
(1,4605)	1:A:39:ASN:HD21	1:A:46:THR:HB	13	0.04
(1,4605)	1:A:39:ASN:HD22	1:A:46:THR:HB	13	0.04
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB2	3	0.04
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB3	3	0.04
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB2	3	0.04
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB3	3	0.04
(1,4593)	1:A:37:VAL:HG11	1:A:48:ASN:HD21	2	0.04
(1,4593)	1:A:37:VAL:HG11	1:A:48:ASN:HD22	2	0.04
(1,4593)	1:A:37:VAL:HG12	1:A:48:ASN:HD21	2	0.04
(1,4593)	1:A:37:VAL:HG12	1:A:48:ASN:HD22	2	0.04
(1,4593)	1:A:37:VAL:HG13	1:A:48:ASN:HD21	2	0.04
(1,4593)	1:A:37:VAL:HG13	1:A:48:ASN:HD22	2	0.04
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB2	11	0.04
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB3	11	0.04
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB2	16	0.04
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB3	16	0.04
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB2	17	0.04
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB3	17	0.04
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD11	4	0.04
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD12	4	0.04
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD13	4	0.04
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD11	4	0.04
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD12	4	0.04
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD13	4	0.04
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD11	8	0.04
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD12	8	0.04
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD13	8	0.04
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD11	8	0.04
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD12	8	0.04
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD13	8	0.04
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD11	16	0.04
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD12	16	0.04
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD13	16	0.04
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD11	16	0.04
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD12	16	0.04
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD13	16	0.04
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	2	0.04
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	2	0.04



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	2	0.04
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	2	0.04
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	2	0.04
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	2	0.04
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	4	0.04
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	4	0.04
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	4	0.04
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	4	0.04
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	4	0.04
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	4	0.04
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	7	0.04
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	7	0.04
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	7	0.04
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	7	0.04
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	7	0.04
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	7	0.04
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	9	0.04
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	9	0.04
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	9	0.04
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	9	0.04
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	9	0.04
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	9	0.04
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	10	0.04
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	10	0.04
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	10	0.04
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	10	0.04
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	10	0.04
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	10	0.04
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	17	0.04
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	17	0.04
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	17	0.04
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	17	0.04
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	17	0.04
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	17	0.04
(1,4468)	1:A:16:ASN:HB2	1:A:17:GLY:H	6	0.04
(1,4468)	1:A:16:ASN:HB3	1:A:17:GLY:H	6	0.04
(1,4464)	1:A:15:LYS:HE2	1:A:16:ASN:HD21	5	0.04
(1,4464)	1:A:15:LYS:HE2	1:A:16:ASN:HD22	5	0.04
(1,4464)	1:A:15:LYS:HE3	1:A:16:ASN:HD21	5	0.04
(1,4464)	1:A:15:LYS:HE3	1:A:16:ASN:HD22	5	0.04
(1,4462)	1:A:15:LYS:HD2	1:A:16:ASN:HB2	9	0.04
(1,4462)	1:A:15:LYS:HD2	1:A:16:ASN:HB3	9	0.04



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4462)	1:A:15:LYS:HD3	1:A:16:ASN:HB2	9	0.04
(1,4462)	1:A:15:LYS:HD3	1:A:16:ASN:HB3	9	0.04
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	7	0.04
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	7	0.04
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	7	0.04
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	7	0.04
(1,4397)	1:B:82:GLU:HA	1:B:83:HIS:HD2	11	0.04
(1,4388)	1:A:81:LEU:HB2	1:A:83:HIS:HD2	4	0.04
(1,4388)	1:A:81:LEU:HB3	1:A:83:HIS:HD2	4	0.04
(1,4388)	1:A:81:LEU:HB2	1:A:83:HIS:HD2	17	0.04
(1,4388)	1:A:81:LEU:HB3	1:A:83:HIS:HD2	17	0.04
(1,4387)	1:B:5:LEU:HG	1:B:83:HIS:HD2	14	0.04
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	1	0.04
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	1	0.04
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	1	0.04
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	1	0.04
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	1	0.04
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	1	0.04
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	6	0.04
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	6	0.04
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	6	0.04
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	6	0.04
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	6	0.04
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	6	0.04
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	7	0.04
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	7	0.04
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	7	0.04
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	7	0.04
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	7	0.04
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	7	0.04
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	10	0.04
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	10	0.04
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	10	0.04
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	10	0.04
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	10	0.04
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	10	0.04
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	16	0.04
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	16	0.04
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	16	0.04
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	16	0.04
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	16	0.04
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	16	0.04



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(1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG21 5 0.04 (1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG22 5 0.04 (1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG23 5 0.04 (1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG21 16 0.04 (1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG22 16 0.04 (1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG23 16 0.04 (1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG23 16 0.04 (1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG23 16 0.04 (1,4363) 1:B:73:PHE:HZ 1:B:73:PHE:HE1 11 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE2 12 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE2 12 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE2 1 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE2 1 0.04 (1,4352) 1:A:44:ILE:HG13 1:A	Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG23 5 0.04 (1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG21 16 0.04 (1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG22 16 0.04 (1,4365) 1:B:73:PHE:HZ 1:B:73:PHE:HE1 1 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE1 11 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE2 11 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE2 12 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE2 12 0.04 (1,4353) 1:B:44:ILE:HG13 1:A:73:PHE:HE2 12 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE2 1 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE2 1 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE2 1 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:52:PHE:HE2 1 0.04 (1,4332) 1:A:4:PHE:HB3 1	(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG21	5	0.04
(1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG21 16 0.04 (1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG22 16 0.04 (1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG23 16 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE1 11 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE2 11 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE1 12 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE2 12 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE2 1 0.04 (1,4352) 1:A:44:PHE:HB2 1:A:52:PHE:HE2 2 0.04 (1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE1 1 0.04 (1,4332) 1:A:4:PHE:HB3 1:	(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG22	5	0.04
(1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG22 16 0.04 (1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG23 16 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE1 11 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE2 11 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE1 12 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE2 12 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE2 1 0.04 (1,4332) 1:A:44:PHE:HB2 1:A:55:PHE:HE1 1 0.04 (1,4332) 1:A:4*PHE:HB3	(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG23	5	0.04
(1,4365) 1:B:73:PHE:HZ 1:B:74:THR:HG23 16 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE1 11 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE2 11 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE1 12 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE2 12 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE1 1 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE2 2 0.04 (1,4332) 1:A:4:PHE:HB2 1:A:52:PHE:HE1 1 0.04 (1,4332) 1:A:4:PHE:HB2 1:A:52:PHE:HE1 1 0.04 (1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE1 9 0.04 (1,4332) 1:A:4:PHE:HB3 1:A:5	(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG21	16	0.04
(1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE1 11 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE2 11 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE1 12 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE2 12 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE1 1 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE2 1 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE2 20 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE2 20 0.04 (1,4352) 1:A:44:PHE:HB3 1:A:52:PHE:HE1 1 0.04 (1,4332) 1:A:4:PHE:HB2 1:A:52:PHE:HE2 1 0.04 (1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE1 9 0.04 (1,4332) 1:A:4:PHE:HB2 1:A:52:PHE:HE2 9 0.04 (1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE2 9 0.04 (1,4332) 1:A:4:PHE:HB3 1:A:52	(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG22	16	0.04
(1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE2 11 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE1 12 0.04 (1,4353) 1:B:44:ILE:HG13 1:B:73:PHE:HE2 12 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE1 1 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE2 1 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE1 20 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE2 20 0.04 (1,4352) 1:A:44:ILE:HG13 1:A:73:PHE:HE2 20 0.04 (1,4332) 1:A:44:ILE:HG13 1:A:73:PHE:HE2 20 0.04 (1,4332) 1:A:4:PHE:HB2 1:A:52:PHE:HE1 1 0.04 (1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE2 1 0.04 (1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE1 9 0.04 (1,4332) 1:A:4:PHE:HB3 1:A:52:PHE:HE2 9 0.04 (1,4332) 1:A:4:PHE:HB3 1:A:	(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG23	16	0.04
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(1,4323) 1:B:52:PHE:HD1 1:B:53:VAL:H 11 0.04 (1,4323) 1:B:52:PHE:HD2 1:B:53:VAL:H 11 0.04 (1,4322) 1:A:52:PHE:HD1 1:A:53:VAL:H 4 0.04 (1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 4 0.04 (1,4322) 1:A:52:PHE:HD1 1:A:53:VAL:H 7 0.04 (1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 7 0.04 (1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 7 0.04	(1,4323)	1:B:52:PHE:HD1	1:B:53:VAL:H	3	0.04
(1,4323) 1:B:52:PHE:HD2 1:B:53:VAL:H 11 0.04 (1,4322) 1:A:52:PHE:HD1 1:A:53:VAL:H 4 0.04 (1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 4 0.04 (1,4322) 1:A:52:PHE:HD1 1:A:53:VAL:H 7 0.04 (1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 7 0.04 (1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 7 0.04	(1,4323)	1:B:52:PHE:HD2	1:B:53:VAL:H	3	0.04
(1,4322) 1:A:52:PHE:HD1 1:A:53:VAL:H 4 0.04 (1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 4 0.04 (1,4322) 1:A:52:PHE:HD1 1:A:53:VAL:H 7 0.04 (1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 7 0.04 (1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 7 0.04	(1,4323)	1:B:52:PHE:HD1	1:B:53:VAL:H	11	0.04
(1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 4 0.04 (1,4322) 1:A:52:PHE:HD1 1:A:53:VAL:H 7 0.04 (1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 7 0.04	(1,4323)	1:B:52:PHE:HD2	1:B:53:VAL:H	11	0.04
(1,4322) 1:A:52:PHE:HD1 1:A:53:VAL:H 7 0.04 (1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 7 0.04	(1,4322)	1:A:52:PHE:HD1	1:A:53:VAL:H	4	0.04
(1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 7 0.04	(1,4322)	1:A:52:PHE:HD2	1:A:53:VAL:H	4	0.04
() /	(1,4322)	1:A:52:PHE:HD1	1:A:53:VAL:H	7	0.04
	(1,4322)	1:A:52:PHE:HD2	1:A:53:VAL:H	7	0.04
	(1,4322)	1:A:52:PHE:HD1	1:A:53:VAL:H	16	0.04
(1,4322) 1:A:52:PHE:HD2 1:A:53:VAL:H 16 0.04	(1,4322)	1:A:52:PHE:HD2	1:A:53:VAL:H	16	0.04
(1,4310) 1:A:5:LEU:HA 1:A:52:PHE:HD1 1 0.04	(1,4310)	1:A:5:LEU:HA	1:A:52:PHE:HD1	1	0.04
(1,4310) 1:A:5:LEU:HA 1:A:52:PHE:HD2 1 0.04	(1,4310)	1:A:5:LEU:HA	1:A:52:PHE:HD2	1	0.04
(1,4300) 1:A:5:LEU:HD11 1:A:52:PHE:HD1 5 0.04	(1,4300)	1:A:5:LEU:HD11	1:A:52:PHE:HD1	5	0.04
(1,4300) 1:A:5:LEU:HD11 1:A:52:PHE:HD2 5 0.04	(1,4300)	1:A:5:LEU:HD11	1:A:52:PHE:HD2	5	0.04
(1,4300) 1:A:5:LEU:HD12 1:A:52:PHE:HD1 5 0.04	(1,4300)	1:A:5:LEU:HD12	1:A:52:PHE:HD1	5	0.04
(1,4300) 1:A:5:LEU:HD12 1:A:52:PHE:HD2 5 0.04	(1,4300)	1:A:5:LEU:HD12	1:A:52:PHE:HD2	5	0.04
(1,4300) 1:A:5:LEU:HD13 1:A:52:PHE:HD1 5 0.04	(1,4300)	1:A:5:LEU:HD13	1:A:52:PHE:HD1	5	0.04
(1,4300) 1:A:5:LEU:HD13 1:A:52:PHE:HD2 5 0.04	(1,4300)	1:A:5:LEU:HD13	1:A:52:PHE:HD2	5	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	9	0.04
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	10	0.04
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	13	0.04
(1,4264)	1:A:22:ILE:HD11	1:A:45:PHE:HE1	1	0.04
(1,4264)	1:A:22:ILE:HD11	1:A:45:PHE:HE2	1	0.04
(1,4264)	1:A:22:ILE:HD12	1:A:45:PHE:HE1	1	0.04
(1,4264)	1:A:22:ILE:HD12	1:A:45:PHE:HE2	1	0.04
(1,4264)	1:A:22:ILE:HD13	1:A:45:PHE:HE1	1	0.04
(1,4264)	1:A:22:ILE:HD13	1:A:45:PHE:HE2	1	0.04
(1,4205)	1:B:29:PHE:HD1	1:B:65:LYS:HD2	3	0.04
(1,4205)	1:B:29:PHE:HD2	1:B:65:LYS:HD2	3	0.04
(1,4205)	1:B:29:PHE:HD1	1:B:65:LYS:HD2	9	0.04
(1,4205)	1:B:29:PHE:HD2	1:B:65:LYS:HD2	9	0.04
(1,4205)	1:B:29:PHE:HD1	1:B:65:LYS:HD2	11	0.04
(1,4205)	1:B:29:PHE:HD2	1:B:65:LYS:HD2	11	0.04
(1,4205)	1:B:29:PHE:HD1	1:B:65:LYS:HD2	16	0.04
(1,4205)	1:B:29:PHE:HD2	1:B:65:LYS:HD2	16	0.04
(1,4204)	1:A:29:PHE:HD1	1:A:65:LYS:HD2	10	0.04
(1,4204)	1:A:29:PHE:HD2	1:A:65:LYS:HD2	10	0.04
(1,4187)	1:B:4:PHE:HZ	1:B:6:ALA:HA	11	0.04
(1,4186)	1:A:4:PHE:HZ	1:A:6:ALA:HA	2	0.04
(1,4186)	1:A:4:PHE:HZ	1:A:6:ALA:HA	14	0.04
(1,4165)	1:B:4:PHE:HE1	1:B:55:ASN:HA	18	0.04
(1,4165)	1:B:4:PHE:HE2	1:B:55:ASN:HA	18	0.04
(1,4145)	1:B:4:PHE:HD1	1:B:5:LEU:H	13	0.04
(1,4145)	1:B:4:PHE:HD2	1:B:5:LEU:H	13	0.04
(1,4144)	1:A:4:PHE:HD1	1:A:5:LEU:H	13	0.04
(1,4144)	1:A:4:PHE:HD2	1:A:5:LEU:H	13	0.04
(1,4138)	1:A:4:PHE:HD1	1:A:54:LYS:HA	13	0.04
(1,4138)	1:A:4:PHE:HD2	1:A:54:LYS:HA	13	0.04
(1,4119)	1:B:80:ASN:HA	1:B:81:LEU:HG	4	0.04
(1,4118)	1:A:80:ASN:HA	1:A:81:LEU:HG	5	0.04
(1,4118)	1:A:80:ASN:HA	1:A:81:LEU:HG	17	0.04
(1,4112)	1:A:77:ARG:HG3	1:A:79:SER:HA	11	0.04
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG2	3	0.04
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG3	3	0.04
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	14	0.04
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	14	0.04
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	16	0.04
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	16	0.04
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	19	0.04
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	19	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	11	0.04
(1,4036)	1:A:15:LYS:HA	1:A:17:GLY:H	9	0.04
(1,3986)	1:A:81:LEU:HD11	1:A:83:HIS:HB3	3	0.04
(1,3986)	1:A:81:LEU:HD12	1:A:83:HIS:HB3	3	0.04
(1,3986)	1:A:81:LEU:HD13	1:A:83:HIS:HB3	3	0.04
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD11	6	0.04
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD12	6	0.04
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD13	6	0.04
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD11	6	0.04
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD12	6	0.04
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD13	6	0.04
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD11	6	0.04
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD12	6	0.04
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD13	6	0.04
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD11	20	0.04
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD12	20	0.04
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD13	20	0.04
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD11	20	0.04
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD12	20	0.04
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD13	20	0.04
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD11	20	0.04
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD12	20	0.04
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD13	20	0.04
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD11	1	0.04
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD12	1	0.04
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD13	1	0.04
(1,3927)	1:B:23:THR:H	1:B:26:ILE:HD11	5	0.04
(1,3927)	1:B:23:THR:H	1:B:26:ILE:HD12	5	0.04
(1,3927)	1:B:23:THR:H	1:B:26:ILE:HD13	5	0.04
(1,3889)	1:A:82:GLU:HA	1:A:83:HIS:HB2	4	0.04
(1,3889)	1:A:82:GLU:HA	1:A:83:HIS:HB2	19	0.04
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD21	3	0.04
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD22	3	0.04
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD23	3	0.04
(1,3841)	1:A:80:ASN:HB2	1:A:81:LEU:HD21	10	0.04
(1,3841)	1:A:80:ASN:HB2	1:A:81:LEU:HD22	10	0.04
(1,3841)	1:A:80:ASN:HB2	1:A:81:LEU:HD23	10	0.04
(1,3824)	1:B:9:ARG:HD2	1:B:78:LEU:HD21	15	0.04
(1,3824)	1:B:9:ARG:HD2	1:B:78:LEU:HD22	15	0.04
(1,3824)	1:B:9:ARG:HD2	1:B:78:LEU:HD23	15	0.04
(1,3824)	1:B:9:ARG:HD3	1:B:78:LEU:HD21	15	0.04
(1,3824)	1:B:9:ARG:HD3	1:B:78:LEU:HD22	15	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3824)	1:B:9:ARG:HD3	1:B:78:LEU:HD23	15	0.04
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD11	12	0.04
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD12	12	0.04
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD13	12	0.04
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD11	5	0.04
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD12	5	0.04
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD13	5	0.04
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD11	16	0.04
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD12	16	0.04
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD13	16	0.04
(1,381)	1:B:22:ILE:H	1:B:23:THR:HG1	8	0.04
(1,3797)	1:A:9:ARG:HD2	1:A:78:LEU:HD11	10	0.04
(1,3797)	1:A:9:ARG:HD2	1:A:78:LEU:HD12	10	0.04
(1,3797)	1:A:9:ARG:HD2	1:A:78:LEU:HD13	10	0.04
(1,3797)	1:A:9:ARG:HD3	1:A:78:LEU:HD11	10	0.04
(1,3797)	1:A:9:ARG:HD3	1:A:78:LEU:HD12	10	0.04
(1,3797)	1:A:9:ARG:HD3	1:A:78:LEU:HD13	10	0.04
(1,3792)	1:B:50:MET:HE1	1:B:78:LEU:HD11	13	0.04
(1,3792)	1:B:50:MET:HE1	1:B:78:LEU:HD12	13	0.04
(1,3792)	1:B:50:MET:HE1	1:B:78:LEU:HD13	13	0.04
(1,3792)	1:B:50:MET:HE2	1:B:78:LEU:HD11	13	0.04
(1,3792)	1:B:50:MET:HE2	1:B:78:LEU:HD12	13	0.04
(1,3792)	1:B:50:MET:HE2	1:B:78:LEU:HD13	13	0.04
(1,3792)	1:B:50:MET:HE3	1:B:78:LEU:HD11	13	0.04
(1,3792)	1:B:50:MET:HE3	1:B:78:LEU:HD12	13	0.04
(1,3792)	1:B:50:MET:HE3	1:B:78:LEU:HD13	13	0.04
(1,3764)	1:B:4:PHE:HZ	1:B:77:ARG:HD2	10	0.04
(1,3764)	1:B:4:PHE:HZ	1:B:77:ARG:HD3	10	0.04
(1,3758)	1:B:6:ALA:HB1	1:B:77:ARG:HD2	1	0.04
(1,3758)	1:B:6:ALA:HB1	1:B:77:ARG:HD3	1	0.04
(1,3758)	1:B:6:ALA:HB2	1:B:77:ARG:HD2	1	0.04
(1,3758)	1:B:6:ALA:HB2	1:B:77:ARG:HD3	1	0.04
(1,3758)	1:B:6:ALA:HB3	1:B:77:ARG:HD2	1	0.04
(1,3758)	1:B:6:ALA:HB3	1:B:77:ARG:HD3	1	0.04
(1,3754)	1:B:59:LEU:HD11	1:B:77:ARG:HD2	9	0.04
(1,3754)	1:B:59:LEU:HD11	1:B:77:ARG:HD3	9	0.04
(1,3754)	1:B:59:LEU:HD12	1:B:77:ARG:HD2	9	0.04
(1,3754)	1:B:59:LEU:HD12	1:B:77:ARG:HD3	9	0.04
(1,3754)	1:B:59:LEU:HD13	1:B:77:ARG:HD2	9	0.04
(1,3754)	1:B:59:LEU:HD13	1:B:77:ARG:HD3	9	0.04
(1,3738)	1:B:59:LEU:HD11	1:B:77:ARG:HG2	15	0.04
(1,3738)	1:B:59:LEU:HD12	1:B:77:ARG:HG2	15	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3738)	1:B:59:LEU:HD13	1:B:77:ARG:HG2	15	0.04
(1,3733)	1:A:74:THR:HA	1:A:76:GLU:HG2	19	0.04
(1,3733)	1:A:74:THR:HA	1:A:76:GLU:HG3	19	0.04
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	5	0.04
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	5	0.04
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	5	0.04
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	14	0.04
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	14	0.04
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	14	0.04
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	17	0.04
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	17	0.04
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	17	0.04
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG21	4	0.04
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG22	4	0.04
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG23	4	0.04
(1,3695)	1:A:73:PHE:HA	1:A:74:THR:HG21	10	0.04
(1,3695)	1:A:73:PHE:HA	1:A:74:THR:HG22	10	0.04
(1,3695)	1:A:73:PHE:HA	1:A:74:THR:HG23	10	0.04
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG11	1	0.04
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG12	1	0.04
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG13	1	0.04
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG11	1	0.04
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG12	1	0.04
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG13	1	0.04
(1,3628)	1:B:70:GLN:HG2	1:B:72:VAL:H	5	0.04
(1,3628)	1:B:70:GLN:HG3	1:B:72:VAL:H	5	0.04
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB2	3	0.04
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB3	3	0.04
(1,3594)	1:B:66:LEU:HA	1:B:69:VAL:HB	14	0.04
(1,3593)	1:A:66:LEU:HA	1:A:69:VAL:HB	8	0.04
(1,3591)	1:A:20:ASN:HA	1:A:22:ILE:HB	5	0.04
(1,3591)	1:A:20:ASN:HA	1:A:22:ILE:HB	9	0.04
(1,3591)	1:A:20:ASN:HA	1:A:22:ILE:HB	16	0.04
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG11	14	0.04
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG12	14	0.04
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG13	14	0.04
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG11	14	0.04
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG12	14	0.04
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG13	14	0.04
(1,3562)	1:B:15:LYS:HE2	1:B:18:MET:H	12	0.04
(1,3562)	1:B:15:LYS:HE3	1:B:18:MET:H	12	0.04
(1,3562)	1:B:15:LYS:HE2	1:B:18:MET:H	19	0.04



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(1,3562) 1:B:15:LYS:HE3 1:B:18:MET:H 19 0.04 (1,3561) 1:A:15:LYS:HE2 1:A:18:MET:H 2 0.04 (1,3561) 1:A:15:LYS:HE3 1:A:18:MET:H 2 0.04 (1,3516) 1:B:67:ARG:HD2 1:B:69:VAL:HA 7 0.04 (1,3516) 1:B:67:ARG:HD2 1:B:75:VAL:HG11 2 0.04 (1,3516) 1:B:67:ARG:HD2 1:B:75:VAL:HG13 2 0.04 (1,3516) 1:B:67:ARG:HD3 1:B:75:VAL:HG11 2 0.04 (1,3516) 1:B:67:ARG:HD3 1:B:75:VAL:HG12 2 0.04 (1,3516) 1:B:67:ARG:HD3 1:B:75:VAL:HG12 2 0.04 (1,346) 1:A:21:GLN:HE22 1:A:69:VAL:HG21 11 0.04 (1,346) 1:A:21:GLN:HE22 1:A:69:VAL:HG22 11 0.04 (1,342) 1:A:9:ARG:H 1:A:69:VAL:HG23 11 0.04 (1,3422) 1:A:9:ARG:H 1:A:69:WET:HE2 10 0.04 (1,3422) 1:A:9:ARG:H 1:A:63:MET:HE3	Key	Atom-1	Atom-2	Model	Violation (Å)
(1,356) 1:A:15:LYS:HE3 1:A:18:MET:H 2 0.04 (1,353) 1:B:21:GLN:HE22 1:B:69:VAL:HA 7 0.04 (1,3516) 1:B:67:ARG:HD2 1:B:75:VAL:HG11 2 0.04 (1,3516) 1:B:67:ARG:HD2 1:B:75:VAL:HG12 2 0.04 (1,3516) 1:B:67:ARG:HD3 1:B:75:VAL:HG11 2 0.04 (1,3516) 1:B:67:ARG:HD3 1:B:75:VAL:HG12 2 0.04 (1,3516) 1:B:67:ARG:HD3 1:B:75:VAL:HG12 2 0.04 (1,3451) 1:A:21:GLN:HE22 1:A:69:VAL:HG21 2 0.04 (1,346) 1:A:21:GLN:HE22 1:A:69:VAL:HG22 11 0.04 (1,346) 1:A:21:GLN:HE22 1:A:69:VAL:HG23 11 0.04 (1,3422) 1:A:9:ARG:H 1:A:63:MET:HE1 10 0.04 (1,3422) 1:A:9:ARG:H 1:A:63:MET:HE2 10 0.04 (1,3422) 1:A:9:ARG:H 1:A:63:MET:HE3 13 0.04 (1,3420) 1:A:63:MET:HE1 1:A:7:ARG:H <td>(1,3562)</td> <td>1:B:15:LYS:HE3</td> <td>1:B:18:MET:H</td> <td>19</td> <td>0.04</td>	(1,3562)	1:B:15:LYS:HE3	1:B:18:MET:H	19	0.04
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(1,3413) 1:B:63:MET:HE1 1:B:76:GLU:HA 8 0.04 (1,3413) 1:B:63:MET:HE2 1:B:76:GLU:HA 8 0.04 (1,3413) 1:B:63:MET:HE3 1:B:76:GLU:HA 8 0.04 (1,3412) 1:A:63:MET:HE1 1:A:76:GLU:HA 7 0.04 (1,3412) 1:A:63:MET:HE2 1:A:76:GLU:HA 7 0.04 (1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE2 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 17 0.04	(1,3413)	1:B:63:MET:HE2	1:B:76:GLU:HA	6	0.04
(1,3413) 1:B:63:MET:HE2 1:B:76:GLU:HA 8 0.04 (1,3413) 1:B:63:MET:HE3 1:B:76:GLU:HA 8 0.04 (1,3412) 1:A:63:MET:HE1 1:A:76:GLU:HA 7 0.04 (1,3412) 1:A:63:MET:HE2 1:A:76:GLU:HA 7 0.04 (1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 7 0.04 (1,3412) 1:A:63:MET:HE1 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE1 1:A:76:GLU:HA 17 0.04	(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	6	0.04
(1,3413) 1:B:63:MET:HE3 1:B:76:GLU:HA 8 0.04 (1,3412) 1:A:63:MET:HE1 1:A:76:GLU:HA 7 0.04 (1,3412) 1:A:63:MET:HE2 1:A:76:GLU:HA 7 0.04 (1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 7 0.04 (1,3412) 1:A:63:MET:HE1 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE2 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 17 0.04	(1,3413)	1:B:63:MET:HE1	1:B:76:GLU:HA	8	0.04
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(1,3412) 1:A:63:MET:HE2 1:A:76:GLU:HA 7 0.04 (1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 7 0.04 (1,3412) 1:A:63:MET:HE1 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE2 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE1 1:A:76:GLU:HA 17 0.04	(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	8	0.04
(1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 7 0.04 (1,3412) 1:A:63:MET:HE1 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE2 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE1 1:A:76:GLU:HA 17 0.04	(1,3412)	1:A:63:MET:HE1	1:A:76:GLU:HA	7	0.04
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(1,3412) 1:A:63:MET:HE1 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE2 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE1 1:A:76:GLU:HA 17 0.04	(1,3412)	1:A:63:MET:HE3	1:A:76:GLU:HA	7	0.04
(1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE1 1:A:76:GLU:HA 17 0.04	(1,3412)	1:A:63:MET:HE1	1:A:76:GLU:HA	16	0.04
(1,3412) 1:A:63:MET:HE3 1:A:76:GLU:HA 16 0.04 (1,3412) 1:A:63:MET:HE1 1:A:76:GLU:HA 17 0.04	(1,3412)	1:A:63:MET:HE2	1:A:76:GLU:HA	16	0.04
	(1,3412)	1:A:63:MET:HE3	1:A:76:GLU:HA	16	0.04
	(1,3412)	1:A:63:MET:HE1	1:A:76:GLU:HA	17	0.04
	('	1:A:63:MET:HE2	1:A:76:GLU:HA	17	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3412)	1:A:63:MET:HE3	1:A:76:GLU:HA	17	0.04
(1,3412)	1:A:63:MET:HE1	1:A:76:GLU:HA	20	0.04
(1,3412)	1:A:63:MET:HE2	1:A:76:GLU:HA	20	0.04
(1,3412)	1:A:63:MET:HE3	1:A:76:GLU:HA	20	0.04
(1,3410)	1:A:63:MET:HE1	1:A:77:ARG:HA	10	0.04
(1,3410)	1:A:63:MET:HE2	1:A:77:ARG:HA	10	0.04
(1,3410)	1:A:63:MET:HE3	1:A:77:ARG:HA	10	0.04
(1,3410)	1:A:63:MET:HE1	1:A:77:ARG:HA	11	0.04
(1,3410)	1:A:63:MET:HE2	1:A:77:ARG:HA	11	0.04
(1,3410)	1:A:63:MET:HE3	1:A:77:ARG:HA	11	0.04
(1,3410)	1:A:63:MET:HE1	1:A:77:ARG:HA	15	0.04
(1,3410)	1:A:63:MET:HE2	1:A:77:ARG:HA	15	0.04
(1,3410)	1:A:63:MET:HE3	1:A:77:ARG:HA	15	0.04
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	18	0.04
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	18	0.04
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	18	0.04
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE1	8	0.04
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE2	8	0.04
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE3	8	0.04
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE1	19	0.04
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE2	19	0.04
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE3	19	0.04
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE1	19	0.04
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE2	19	0.04
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE3	19	0.04
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE1	19	0.04
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE2	19	0.04
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE3	19	0.04
(1,3287)	1:A:61:THR:HG21	1:A:65:LYS:HE2	8	0.04
(1,3287)	1:A:61:THR:HG21	1:A:65:LYS:HE3	8	0.04
(1,3287)	1:A:61:THR:HG22	1:A:65:LYS:HE2	8	0.04
(1,3287)	1:A:61:THR:HG22	1:A:65:LYS:HE3	8	0.04
(1,3287)	1:A:61:THR:HG23	1:A:65:LYS:HE2	8	0.04
(1,3287)	1:A:61:THR:HG23	1:A:65:LYS:HE3	8	0.04
(1,3224)	1:B:6:ALA:HB1	1:B:59:LEU:HD21	17	0.04
(1,3224)	1:B:6:ALA:HB1	1:B:59:LEU:HD22	17	0.04
(1,3224)	1:B:6:ALA:HB1	1:B:59:LEU:HD23	17	0.04
(1,3224)	1:B:6:ALA:HB2	1:B:59:LEU:HD21	17	0.04
(1,3224)	1:B:6:ALA:HB2	1:B:59:LEU:HD22	17	0.04
(1,3224)	1:B:6:ALA:HB2	1:B:59:LEU:HD23	17	0.04
(1,3224)	1:B:6:ALA:HB3	1:B:59:LEU:HD21	17	0.04
(1,3224)	1:B:6:ALA:HB3	1:B:59:LEU:HD22	17	0.04



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(1,3212) 1:B:	6:ALA:HB3 6:ALA:HB1	1:B:59:LEU:HD23	17	0.04
()	6. A I A . H B 1		11	0.04
(1,3212) 1:B	U.ALA.IIDI	1:B:59:LEU:HD11	7	0.04
	6:ALA:HB1	1:B:59:LEU:HD12	7	0.04
(1,3212) 1:B:	6:ALA:HB1	1:B:59:LEU:HD13	7	0.04
(1,3212) 1:B:	:6:ALA:HB2	1:B:59:LEU:HD11	7	0.04
(1,3212) 1:B:	:6:ALA:HB2	1:B:59:LEU:HD12	7	0.04
(1,3212) 1:B:	:6:ALA:HB2	1:B:59:LEU:HD13	7	0.04
(1,3212) 1:B:	:6:ALA:HB3	1:B:59:LEU:HD11	7	0.04
(1,3212) 1:B:	:6:ALA:HB3	1:B:59:LEU:HD12	7	0.04
(1,3212) 1:B:	:6:ALA:HB3	1:B:59:LEU:HD13	7	0.04
(1,3211) 1:A:	:6:ALA:HB1	1:A:59:LEU:HD11	15	0.04
(1,3211) 1:A	:6:ALA:HB1	1:A:59:LEU:HD12	15	0.04
(1,3211) 1:A	:6:ALA:HB1	1:A:59:LEU:HD13	15	0.04
(1,3211) 1:A	:6:ALA:HB2	1:A:59:LEU:HD11	15	0.04
(1,3211) 1:A	:6:ALA:HB2	1:A:59:LEU:HD12	15	0.04
(1,3211) 1:A	:6:ALA:HB2	1:A:59:LEU:HD13	15	0.04
(1,3211) 1:A	:6:ALA:HB3	1:A:59:LEU:HD11	15	0.04
(1,3211) 1:A	:6:ALA:HB3	1:A:59:LEU:HD12	15	0.04
(1,3211) 1:A	:6:ALA:HB3	1:A:59:LEU:HD13	15	0.04
(1,3186) 1:I	B:58:LYS:H	1:B:58:LYS:HD2	14	0.04
(1,3186) 1:I	B:58:LYS:H	1:B:58:LYS:HD3	14	0.04
(1,3185) 1:A	A:58:LYS:H	1:A:58:LYS:HD2	10	0.04
(1,3185) 1:A	A:58:LYS:H	1:A:58:LYS:HD3	10	0.04
(1,3176) 1:B:	30:ASP:HB2	1:B:58:LYS:HD2	3	0.04
(1,3176) 1:B:	30:ASP:HB2	1:B:58:LYS:HD3	3	0.04
(1,3176) 1:B:	30:ASP:HB3	1:B:58:LYS:HD2	3	0.04
(1,3176) 1:B:	30:ASP:HB3	1:B:58:LYS:HD3	3	0.04
(1,3130) 1:B:	4:PHE:HD1	1:B:56:THR:HG21	13	0.04
(1,3130) 1:B:	4:PHE:HD1	1:B:56:THR:HG22	13	0.04
(1,3130) 1:B:	4:PHE:HD1	1:B:56:THR:HG23	13	0.04
(1,3130) 1:B:	4:PHE:HD2	1:B:56:THR:HG21	13	0.04
(1,3130) 1:B:	4:PHE:HD2	1:B:56:THR:HG22	13	0.04
(1,3130) 1:B:	4:PHE:HD2	1:B:56:THR:HG23	13	0.04
(1,3130) 1:B:	4:PHE:HD1	1:B:56:THR:HG21	17	0.04
(1,3130) 1:B:	4:PHE:HD1	1:B:56:THR:HG22	17	0.04
(1,3130) 1:B:	4:PHE:HD1	1:B:56:THR:HG23	17	0.04
(1,3130) 1:B:	4:PHE:HD2	1:B:56:THR:HG21	17	0.04
	4:PHE:HD2	1:B:56:THR:HG22	17	0.04
(1,3130) 1:B:	4:PHE:HD2	1:B:56:THR:HG23	17	0.04
(1,3102) 1:B	:54:LYS:HA	1:B:54:LYS:HE2	14	0.04
(1,3102) 1:B	:54:LYS:HA	1:B:54:LYS:HE3	14	0.04
	:54:LYS:HA	1:B:54:LYS:HD2	2	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD3	2	0.04
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD2	18	0.04
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD3	18	0.04
(1,3037)	1:A:53:VAL:HG21	1:A:58:LYS:HA	6	0.04
(1,3037)	1:A:53:VAL:HG22	1:A:58:LYS:HA	6	0.04
(1,3037)	1:A:53:VAL:HG23	1:A:58:LYS:HA	6	0.04
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG11	13	0.04
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG12	13	0.04
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG13	13	0.04
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG11	18	0.04
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG12	18	0.04
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG13	18	0.04
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	12	0.04
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	12	0.04
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	12	0.04
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	12	0.04
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	12	0.04
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	12	0.04
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	19	0.04
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	19	0.04
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	19	0.04
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	19	0.04
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	19	0.04
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	19	0.04
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	3	0.04
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	3	0.04
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	3	0.04
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	3	0.04
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	3	0.04
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	3	0.04
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	4	0.04
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	4	0.04
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	4	0.04
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	4	0.04
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	4	0.04
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	4	0.04
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	13	0.04
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	13	0.04
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	13	0.04
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	13	0.04
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	13	0.04
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	13	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD11	12	0.04
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD12	12	0.04
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD13	12	0.04
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	16	0.04
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	16	0.04
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	16	0.04
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	16	0.04
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	16	0.04
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	16	0.04
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	16	0.04
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	16	0.04
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	16	0.04
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	17	0.04
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	17	0.04
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	17	0.04
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	17	0.04
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	17	0.04
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	17	0.04
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	17	0.04
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	17	0.04
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	17	0.04
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD11	1	0.04
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD12	1	0.04
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD13	1	0.04
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD11	1	0.04
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD12	1	0.04
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD13	1	0.04
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD21	6	0.04
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD22	6	0.04
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD23	6	0.04
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD21	6	0.04
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD22	6	0.04
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD23	6	0.04
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD21	6	0.04
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD22	6	0.04
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD23	6	0.04
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG21	20	0.04
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG22	20	0.04
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG23	20	0.04
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG21	2	0.04
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG22	2	0.04
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG23	2	0.04



 $Continued\ from\ previous\ page...$

(1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG21 14 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG22 14 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG21 15 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG22 15 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG22 15 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG21 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG21 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG22 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG22 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG23 18 0.04 (1,2881) 1:A:3:ILE:HG21 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:3:ILE:HG21 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:3:ILE:HG22 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:3:ILE:HG23 <td< th=""><th>Key</th><th>Atom-1</th><th>Atom-2</th><th>Model</th><th>Violation (Å)</th></td<>	Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG23 14 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG21 15 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG22 15 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG23 15 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG23 15 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG21 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG21 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG22 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG23 18 0.04 (1,2881) 1:A:8:ILE:HG21 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:8:ILE:HG21 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:8:ILE:HG21 1:A:62:LEU:HD13 19 0.04 (1,2881) 1:A:8:ILE:HG21 1:A:62:LEU:HD13 19 0.04 (1,2881) 1:A:8:ILE:HG22 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:8:ILE:HG23 1:A:62:LEU:HD12 19 0.04 (1,2816) 1:B:50:MET:HE1 1:B:51:ILE:HG13 2 0.04 (1,2816) 1:B:50:MET:HE2 1:B:51:ILE:HG13 5 0.04 (1,2816) 1:B:50:MET:HE2 1:B:51:ILE:HG13 5 0.04 (1,2816) 1:B:50:MET:HE2 1:B:51:ILE:HG13 5 0.04 (1,2816) 1:B:50:MET:HE2 1:B:51:ILE:HG13 6 0.04 (1,2816) 1:B:50:MET:HE2 1:B:51:ILE:HG13 5 0.04 (1,2816) 1:B:50:MET:HE2 1:B:51:ILE:HG13 10 0.04 (1,2816) 1:B:50:MET:HE2 1:B:51:ILE:HG13 11 0.04	(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG21	14	0.04
(1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG21 15 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG22 15 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG23 15 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG21 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG21 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG22 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG22 18 0.04 (1,2881) 1:A:8:ILE:HG21 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:8:ILE:HG21 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:8:ILE:HG21 1:A:62:LEU:HD12 19 0.04 (1,2881) 1:A:8:ILE:HG21 1:A:62:LEU:HD13 19 0.04 (1,2881) 1:A:8:ILE:HG22 1:A:62:LEU:HD13 19 0.04 (1,2881) 1:A:8:ILE:HG23 1:A:62:LEU:HD13 19 0.04 (1,2881) 1:A:8:ILE:HG23 1:A:62:LEU:HD13 19 0.04 (1,2881) 1:A:8:ILE:HG23 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:8:ILE:HG23 1:A:62:LEU:HD13 19 0.04 (1,2881) 1:A:8:ILE:HG23 1:A:62:LEU:HD13 19 0.04 (1,2816) 1:B:50:MET:HE1 1:B:51:ILE:HG13 2 0.04 (1,2816) 1:B:50:MET:HE2 1:B:51:ILE:HG13 2 0.04 (1,2816) 1:B:50:MET:HE2 1:B:51:ILE:HG13 2 0.04 (1,2816) 1:B:50:MET:HE3 1:B:51:ILE:HG13 5 0.04 (1,2816) 1:B:50:MET:HE3 1:B:51:ILE:HG13 1 1 0.	(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG22	14	0.04
(1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG22 15 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG21 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG21 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG22 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG22 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG23 18 0.04 (1,2881) 1:A:8:ILE:HG21 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:8:ILE:HG21 1:A:62:LEU:HD12 19 0.04 (1,2881) 1:A:8:ILE:HG21 1:A:62:LEU:HD13 19 0.04 (1,2881) 1:A:8:ILE:HG22 1:A:62:LEU:HD13 19 0.04 (1,2881) 1:A:8:ILE:HG22 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:8:ILE:HG22 1:A:62:LEU:HD13 19 0.04 (1,2881) 1:A:8:ILE:HG23 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:8:ILE:HG23 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:8:ILE:HG23 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:8:ILE:HG23 1:A:62:LEU:HD12 19 0.04 (1,2816) 1:B:50:MET:HE1 1:B:51:ILE:HG13 2 0.04 (1,2816) 1:B:50:MET:HE1 1:B:51:ILE:HG13 2 0.04 (1,2816) 1:B:50:MET:HE2 1:B:51:ILE:HG13 2 0.04 (1,2816) 1:B:50:MET:HE3 1:B:51:ILE:HG13 5 0.04 (1,2816) 1:B:50:MET:HE3 1:B:51:ILE:HG13 1 1 0.04 (1,2816) 1:B:50:MET:HE3 1:B:51:ILE:HG13	(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG23	14	0.04
(1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG22 15 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG23 15 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG21 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG21 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG22 18 0.04 (1,2889) 1:A:31:THR:HB 1:A:51:ILE:HG23 18 0.04 (1,2881) 1:A:31:THR:HB 1:A:51:ILE:HG23 18 0.04 (1,2881) 1:A:8:ILE:HG21 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:8:ILE:HG21 1:A:62:LEU:HD12 19 0.04 (1,2881) 1:A:8:ILE:HG21 1:A:62:LEU:HD13 19 0.04 (1,2881) 1:A:8:ILE:HG22 1:A:62:LEU:HD13 19 0.04 (1,2881) 1:A:8:ILE:HG22 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:8:ILE:HG22 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:8:ILE:HG22 1:A:62:LEU:HD13 19 0.04 (1,2881) 1:A:8:ILE:HG23 1:A:62:LEU:HD13 19 0.04 (1,2881) 1:A:8:ILE:HG23 1:A:62:LEU:HD13 19 0.04 (1,2881) 1:A:8:ILE:HG23 1:A:62:LEU:HD11 19 0.04 (1,2881) 1:A:8:ILE:HG23 1:A:62:LEU:HD12 19 0.04 (1,2881) 1:A:8:ILE:HG23 1:A:62:LEU:HD12 19 0.04 (1,2881) 1:A:8:ILE:HG33 1:A:62:LEU:HD12 19 0.04 (1,2816) 1:B:50:MET:HE1 1:B:51:ILE:HG13 2 0.04 (1,2816) 1:B:50:MET:HE2 1:B:51:ILE:HG13 2 0.04 (1,2816) 1:B:50:MET:HE2 1:B:51:ILE:HG13 2 0.04 (1,2816) 1:B:50:MET:HE2 1:B:51:ILE:HG13 5 0.04 (1,2816) 1:B:50:MET:HE3 1:B:51:ILE:HG13 1	(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG21	15	0.04
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(1,2815) 1:A:50:MET:HE3 1:A:51:ILE:HG13 3 0.04	· · /	1:A:50:MET:HE2	1:A:51:ILE:HG13	3	0.04
	(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	3	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	12	0.04
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	12	0.04
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	12	0.04
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	17	0.04
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	17	0.04
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	17	0.04
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	18	0.04
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	18	0.04
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	18	0.04
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	2	0.04
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	4	0.04
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	7	0.04
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	9	0.04
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	13	0.04
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	18	0.04
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	19	0.04
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	20	0.04
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD21	10	0.04
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD22	10	0.04
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD23	10	0.04
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD21	10	0.04
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD22	10	0.04
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD23	10	0.04
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD21	10	0.04
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD22	10	0.04
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD23	10	0.04
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD21	7	0.04
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD22	7	0.04
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD23	7	0.04
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD21	7	0.04
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD22	7	0.04
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD23	7	0.04
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD21	7	0.04
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD22	7	0.04
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD23	7	0.04
(1,2668)	1:B:23:THR:HG1	1:B:47:CYS:HB3	11	0.04
(1,2668)	1:B:23:THR:HG1	1:B:47:CYS:HB3	17	0.04
(1,2667)	1:A:23:THR:HG1	1:A:47:CYS:HB3	3	0.04
(1,2667)	1:A:23:THR:HG1	1:A:47:CYS:HB3	6	0.04
(1,2667)	1:A:23:THR:HG1	1:A:47:CYS:HB3	8	0.04
(1,2667)	1:A:23:THR:HG1	1:A:47:CYS:HB3	12	0.04
(1,2667)	1:A:23:THR:HG1	1:A:47:CYS:HB3	13	0.04



 $Continued\ from\ previous\ page...$

(1,2639) 1:A:46:THR:HG21 1:A:47:CYS:H 12 0.04 (1,2639) 1:A:46:THR:HG22 1:A:47:CYS:H 12 0.04 (1,2639) 1:A:46:THR:HG23 1:A:47:CYS:H 12 0.04 (1,2612) 1:B:44:ILE:HB 1:B:46:THR:HG21 3 0.04 (1,2612) 1:B:44:ILE:HB 1:B:46:THR:HG22 3 0.04 (1,2612) 1:B:44:ILE:HB 1:B:46:THR:HG23 3 0.04 (1,2612) 1:B:44:ILE:HB 1:B:46:THR:HG21 11 0.04 (1,2612) 1:B:44:ILE:HB 1:B:46:THR:HG22 11 0.04 (1,2612) 1:B:44:ILE:HB 1:B:46:THR:HG23 11 0.04 (1,2611) 1:A:44:ILE:HB 1:A:46:THR:HG23 18 0.04 (1,2611) 1:A:44:ILE:HB 1:A:46:THR:HG23 18 0.04 (1,2611) 1:A:44:ILE:HB 1:A:46:THR:HG23 19 0.04 (1,2611) 1:A:44:ILE:HB 1:A:46:THR:HG23 19 0.04 (1,2595) 1:A:44:ILE:H 1:A:44:ILE	:
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(1,2611) 1:A:44:ILE:HB 1:A:46:THR:HG23 18 0.04 (1,2611) 1:A:44:ILE:HB 1:A:46:THR:HG21 19 0.04 (1,2611) 1:A:44:ILE:HB 1:A:46:THR:HG22 19 0.04 (1,2611) 1:A:44:ILE:HB 1:A:46:THR:HG23 19 0.04 (1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD11 7 0.04 (1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD12 7 0.04 (1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD13 7 0.04	:
(1,2611) 1:A:44:ILE:HB 1:A:46:THR:HG21 19 0.04 (1,2611) 1:A:44:ILE:HB 1:A:46:THR:HG22 19 0.04 (1,2611) 1:A:44:ILE:HB 1:A:46:THR:HG23 19 0.04 (1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD11 7 0.04 (1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD12 7 0.04 (1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD13 7 0.04	:
(1,2611) 1:A:44:ILE:HB 1:A:46:THR:HG22 19 0.04 (1,2611) 1:A:44:ILE:HB 1:A:46:THR:HG23 19 0.04 (1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD11 7 0.04 (1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD12 7 0.04 (1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD13 7 0.04	:
(1,2611) 1:A:44:ILE:HB 1:A:46:THR:HG23 19 0.04 (1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD11 7 0.04 (1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD12 7 0.04 (1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD13 7 0.04	:
(1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD11 7 0.04 (1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD12 7 0.04 (1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD13 7 0.04	
(1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD12 7 0.04 (1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD13 7 0.04	:
(1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD13 7 0.04	
(1,2595) 1:A:44:ILE:H 1:A:44:ILE:HD13 7 0.04	
(1,2590) 1:B:44:ILE:HD11 1:B:73:PHE:HD1 7 0.04	
(1,2590) 1:B:44:ILE:HD11 1:B:73:PHE:HD2 7 0.04	:
(1,2590) 1:B:44:ILE:HD12 1:B:73:PHE:HD1 7 0.04	:
(1,2590) 1:B:44:ILE:HD12 1:B:73:PHE:HD2 7 0.04	:
(1,2590) 1:B:44:ILE:HD13 1:B:73:PHE:HD1 7 0.04	:
(1,2590) 1:B:44:ILE:HD13 1:B:73:PHE:HD2 7 0.04	
(1,2586) 1:B:13:GLU:HA 1:B:44:ILE:HD11 12 0.04	:
(1,2586) 1:B:13:GLU:HA 1:B:44:ILE:HD12 12 0.04	:
(1,2586) 1:B:13:GLU:HA 1:B:44:ILE:HD13 12 0.04	:
(1,2585) 1:A:13:GLU:HA 1:A:44:ILE:HD11 10 0.04	:
(1,2585) 1:A:13:GLU:HA 1:A:44:ILE:HD12 10 0.04	:
(1,2585) 1:A:13:GLU:HA 1:A:44:ILE:HD13 10 0.04	:
(1,2584) 1:B:44:ILE:HD11 1:B:46:THR:HB 8 0.04	:
(1,2584) 1:B:44:ILE:HD12 1:B:46:THR:HB 8 0.04	:
(1,2584) 1:B:44:ILE:HD13 1:B:46:THR:HB 8 0.04	:
(1,2584) 1:B:44:ILE:HD11 1:B:46:THR:HB 19 0.04	:
(1,2584) 1:B:44:ILE:HD12 1:B:46:THR:HB 19 0.04	:
(1,2584) 1:B:44:ILE:HD13 1:B:46:THR:HB 19 0.04	
(1,2583) 1:A:44:ILE:HD11 1:A:46:THR:HB 7 0.04	:
(1,2583) 1:A:44:ILE:HD12 1:A:46:THR:HB 7 0.04	:
(1,2583) 1:A:44:ILE:HD13 1:A:46:THR:HB 7 0.04	:
(1,2583) 1:A:44:ILE:HD11 1:A:46:THR:HB 18 0.04	:
(1,2583) 1:A:44:ILE:HD12 1:A:46:THR:HB 18 0.04	
(1,2583) 1:A:44:ILE:HD13 1:A:46:THR:HB 18 0.04	



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2575)	1:A:44:ILE:HG21	1:A:45:PHE:H	16	0.04
(1,2575)	1:A:44:ILE:HG22	1:A:45:PHE:H	16	0.04
(1,2575)	1:A:44:ILE:HG23	1:A:45:PHE:H	16	0.04
(1,2552)	1:B:44:ILE:HG13	1:B:45:PHE:H	6	0.04
(1,2552)	1:B:44:ILE:HG13	1:B:45:PHE:H	8	0.04
(1,2552)	1:B:44:ILE:HG13	1:B:45:PHE:H	18	0.04
(1,2537)	1:A:44:ILE:HG12	1:A:45:PHE:H	15	0.04
(1,2501)	1:A:15:LYS:H	1:A:40:ALA:HB1	4	0.04
(1,2501)	1:A:15:LYS:H	1:A:40:ALA:HB2	4	0.04
(1,2501)	1:A:15:LYS:H	1:A:40:ALA:HB3	4	0.04
(1,2501)	1:A:15:LYS:H	1:A:40:ALA:HB1	19	0.04
(1,2501)	1:A:15:LYS:H	1:A:40:ALA:HB2	19	0.04
(1,2501)	1:A:15:LYS:H	1:A:40:ALA:HB3	19	0.04
(1,2486)	1:B:40:ALA:HA	1:B:45:PHE:HA	5	0.04
(1,2486)	1:B:40:ALA:HA	1:B:45:PHE:HA	11	0.04
(1,2486)	1:B:40:ALA:HA	1:B:45:PHE:HA	19	0.04
(1,2485)	1:A:40:ALA:HA	1:A:45:PHE:HA	14	0.04
(1,2485)	1:A:40:ALA:HA	1:A:45:PHE:HA	15	0.04
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD21	4	0.04
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD22	4	0.04
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD23	4	0.04
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD21	10	0.04
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD22	10	0.04
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD23	10	0.04
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD21	19	0.04
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD22	19	0.04
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD23	19	0.04
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD21	11	0.04
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD22	11	0.04
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD23	11	0.04
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD21	12	0.04
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD22	12	0.04
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD23	12	0.04
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD21	13	0.04
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD22	13	0.04
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD23	13	0.04
(1,2448)	1:B:23:THR:HG1	1:B:38:LEU:HD21	19	0.04
(1,2448)	1:B:23:THR:HG1	1:B:38:LEU:HD22	19	0.04
(1,2448)	1:B:23:THR:HG1	1:B:38:LEU:HD23	19	0.04
(1,2424)	1:B:38:LEU:HD11	1:B:39:ASN:H	6	0.04
(1,2424)	1:B:38:LEU:HD12	1:B:39:ASN:H	6	0.04
(1,2424)	1:B:38:LEU:HD13	1:B:39:ASN:H	6	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2424)	1:B:38:LEU:HD11	1:B:39:ASN:H	10	0.04
(1,2424)	1:B:38:LEU:HD12	1:B:39:ASN:H	10	0.04
(1,2424)	1:B:38:LEU:HD13	1:B:39:ASN:H	10	0.04
(1,2423)	1:A:38:LEU:HD11	1:A:39:ASN:H	15	0.04
(1,2423)	1:A:38:LEU:HD12	1:A:39:ASN:H	15	0.04
(1,2423)	1:A:38:LEU:HD13	1:A:39:ASN:H	15	0.04
(1,2387)	1:A:37:VAL:HG21	1:A:38:LEU:H	3	0.04
(1,2387)	1:A:37:VAL:HG22	1:A:38:LEU:H	3	0.04
(1,2387)	1:A:37:VAL:HG23	1:A:38:LEU:H	3	0.04
(1,2380)	1:B:37:VAL:HG21	1:B:48:ASN:HD22	6	0.04
(1,2380)	1:B:37:VAL:HG22	1:B:48:ASN:HD22	6	0.04
(1,2380)	1:B:37:VAL:HG23	1:B:48:ASN:HD22	6	0.04
(1,2380)	1:B:37:VAL:HG21	1:B:48:ASN:HD22	20	0.04
(1,2380)	1:B:37:VAL:HG22	1:B:48:ASN:HD22	20	0.04
(1,2380)	1:B:37:VAL:HG23	1:B:48:ASN:HD22	20	0.04
(1,2345)	1:A:37:VAL:HG11	1:A:48:ASN:HB3	14	0.04
(1,2345)	1:A:37:VAL:HG12	1:A:48:ASN:HB3	14	0.04
(1,2345)	1:A:37:VAL:HG13	1:A:48:ASN:HB3	14	0.04
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	19	0.04
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	19	0.04
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	19	0.04
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	13	0.04
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	13	0.04
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	13	0.04
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	15	0.04
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	15	0.04
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	15	0.04
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	20	0.04
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	20	0.04
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	20	0.04
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	2	0.04
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	2	0.04
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	2	0.04
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	13	0.04
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	13	0.04
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	13	0.04
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	9	0.04
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	9	0.04
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	9	0.04
(1,2282)	1:B:36:ILE:HG21	1:B:37:VAL:HB	11	0.04
(1,2282)	1:B:36:ILE:HG22	1:B:37:VAL:HB	11	0.04
(1,2282)	1:B:36:ILE:HG23	1:B:37:VAL:HB	11	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2282)	1:B:36:ILE:HG21	1:B:37:VAL:HB	14	0.04
(1,2282)	1:B:36:ILE:HG22	1:B:37:VAL:HB	14	0.04
(1,2282)	1:B:36:ILE:HG23	1:B:37:VAL:HB	14	0.04
(1,2258)	1:B:35:THR:HB	1:B:50:MET:HB2	1	0.04
(1,2257)	1:A:35:THR:HB	1:A:50:MET:HB2	17	0.04
(1,2182)	1:B:29:PHE:HD1	1:B:31:THR:HB	5	0.04
(1,2182)	1:B:29:PHE:HD2	1:B:31:THR:HB	5	0.04
(1,2182)	1:B:29:PHE:HD1	1:B:31:THR:HB	6	0.04
(1,2182)	1:B:29:PHE:HD2	1:B:31:THR:HB	6	0.04
(1,2182)	1:B:29:PHE:HD1	1:B:31:THR:HB	7	0.04
(1,2182)	1:B:29:PHE:HD2	1:B:31:THR:HB	7	0.04
(1,2182)	1:B:29:PHE:HD1	1:B:31:THR:HB	8	0.04
(1,2182)	1:B:29:PHE:HD2	1:B:31:THR:HB	8	0.04
(1,2182)	1:B:29:PHE:HD1	1:B:31:THR:HB	20	0.04
(1,2182)	1:B:29:PHE:HD2	1:B:31:THR:HB	20	0.04
(1,2181)	1:A:29:PHE:HD1	1:A:31:THR:HB	2	0.04
(1,2181)	1:A:29:PHE:HD2	1:A:31:THR:HB	2	0.04
(1,2181)	1:A:29:PHE:HD1	1:A:31:THR:HB	17	0.04
(1,2181)	1:A:29:PHE:HD2	1:A:31:THR:HB	17	0.04
(1,2181)	1:A:29:PHE:HD1	1:A:31:THR:HB	19	0.04
(1,2181)	1:A:29:PHE:HD2	1:A:31:THR:HB	19	0.04
(1,2176)	1:B:25:VAL:HA	1:B:28:LYS:HE2	9	0.04
(1,2176)	1:B:25:VAL:HA	1:B:28:LYS:HE3	9	0.04
(1,2147)	1:A:23:THR:HG21	1:A:27:SER:HB2	4	0.04
(1,2147)	1:A:23:THR:HG22	1:A:27:SER:HB2	4	0.04
(1,2147)	1:A:23:THR:HG23	1:A:27:SER:HB2	4	0.04
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	9	0.04
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	9	0.04
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	9	0.04
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	7	0.04
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	7	0.04
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	7	0.04
(1,2088)	1:B:25:VAL:HG11	1:B:27:SER:H	1	0.04
(1,2088)	1:B:25:VAL:HG12	1:B:27:SER:H	1	0.04
(1,2088)	1:B:25:VAL:HG13	1:B:27:SER:H	1	0.04
(1,2088)	1:B:25:VAL:HG11	1:B:27:SER:H	7	0.04
(1,2088)	1:B:25:VAL:HG12	1:B:27:SER:H	7	0.04
(1,2088)	1:B:25:VAL:HG13	1:B:27:SER:H	7	0.04
(1,2088)	1:B:25:VAL:HG11	1:B:27:SER:H	18	0.04
(1,2088)	1:B:25:VAL:HG12	1:B:27:SER:H	18	0.04
(1,2088)	1:B:25:VAL:HG13	1:B:27:SER:H	18	0.04
(1,2087)	1:A:25:VAL:HG11	1:A:27:SER:H	14	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2087)	1:A:25:VAL:HG12	1:A:27:SER:H	14	0.04
(1,2087)	1:A:25:VAL:HG13	1:A:27:SER:H	14	0.04
(1,2087)	1:A:25:VAL:HG11	1:A:27:SER:H	15	0.04
(1,2087)	1:A:25:VAL:HG12	1:A:27:SER:H	15	0.04
(1,2087)	1:A:25:VAL:HG13	1:A:27:SER:H	15	0.04
(1,207)	1:A:16:ASN:HA	1:A:17:GLY:H	3	0.04
(1,207)	1:A:16:ASN:HA	1:A:17:GLY:H	10	0.04
(1,207)	1:A:16:ASN:HA	1:A:17:GLY:H	14	0.04
(1,207)	1:A:16:ASN:HA	1:A:17:GLY:H	18	0.04
(1,207)	1:A:16:ASN:HA	1:A:17:GLY:H	19	0.04
(1,207)	1:A:16:ASN:HA	1:A:17:GLY:H	20	0.04
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	9	0.04
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	9	0.04
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	9	0.04
(1,2018)	1:B:22:ILE:HD11	1:B:23:THR:HA	19	0.04
(1,2018)	1:B:22:ILE:HD12	1:B:23:THR:HA	19	0.04
(1,2018)	1:B:22:ILE:HD13	1:B:23:THR:HA	19	0.04
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	3	0.04
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	3	0.04
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	3	0.04
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	13	0.04
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	13	0.04
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	13	0.04
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	18	0.04
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	18	0.04
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	18	0.04
(1,1932)	1:A:21:GLN:HE21	1:A:22:ILE:HA	15	0.04
(1,1837)	1:A:18:MET:HA	1:A:21:GLN:HG2	4	0.04
(1,1837)	1:A:18:MET:HA	1:A:21:GLN:HG3	4	0.04
(1,1812)	1:A:25:VAL:HG21	1:A:65:LYS:HE2	12	0.04
(1,1812)	1:A:25:VAL:HG21	1:A:65:LYS:HE3	12	0.04
(1,1812)	1:A:25:VAL:HG22	1:A:65:LYS:HE2	12	0.04
(1,1812)	1:A:25:VAL:HG22	1:A:65:LYS:HE3	12	0.04
(1,1812)	1:A:25:VAL:HG23	1:A:65:LYS:HE2	12	0.04
(1,1812)	1:A:25:VAL:HG23	1:A:65:LYS:HE3	12	0.04
(1,1811)	1:B:41:LYS:HE2	1:B:44:ILE:HD11	9	0.04
(1,1811)	1:B:41:LYS:HE2	1:B:44:ILE:HD12	9	0.04
(1,1811)	1:B:41:LYS:HE2	1:B:44:ILE:HD13	9	0.04
(1,1811)	1:B:41:LYS:HE3	1:B:44:ILE:HD11	9	0.04
(1,1811)	1:B:41:LYS:HE3	1:B:44:ILE:HD12	9	0.04
(1,1811)	1:B:41:LYS:HE3	1:B:44:ILE:HD13	9	0.04
(1,1808)	1:A:11:VAL:HG21	1:A:41:LYS:HE2	1	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1808)	1:A:11:VAL:HG21	1:A:41:LYS:HE3	1	0.04
(1,1808)	1:A:11:VAL:HG22	1:A:41:LYS:HE2	1	0.04
(1,1808)	1:A:11:VAL:HG22	1:A:41:LYS:HE3	1	0.04
(1,1808)	1:A:11:VAL:HG23	1:A:41:LYS:HE2	1	0.04
(1,1808)	1:A:11:VAL:HG23	1:A:41:LYS:HE3	1	0.04
(1,1797)	1:B:15:LYS:HG2	1:B:18:MET:HE1	6	0.04
(1,1797)	1:B:15:LYS:HG2	1:B:18:MET:HE2	6	0.04
(1,1797)	1:B:15:LYS:HG2	1:B:18:MET:HE3	6	0.04
(1,1797)	1:B:15:LYS:HG3	1:B:18:MET:HE1	6	0.04
(1,1797)	1:B:15:LYS:HG3	1:B:18:MET:HE2	6	0.04
(1,1797)	1:B:15:LYS:HG3	1:B:18:MET:HE3	6	0.04
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG11	2	0.04
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG12	2	0.04
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG13	2	0.04
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG11	2	0.04
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG12	2	0.04
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG13	2	0.04
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG11	3	0.04
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG12	3	0.04
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG13	3	0.04
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG11	3	0.04
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG12	3	0.04
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG13	3	0.04
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG11	10	0.04
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG12	10	0.04
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG13	10	0.04
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG11	10	0.04
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG12	10	0.04
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG13	10	0.04
(1,172)	1:B:13:GLU:HG2	1:B:15:LYS:H	20	0.04
(1,172)	1:B:13:GLU:HG3	1:B:15:LYS:H	20	0.04
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	5	0.04
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	5	0.04
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	5	0.04
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	19	0.04
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	19	0.04
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	19	0.04
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	7	0.04
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	7	0.04
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	7	0.04
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	7	0.04
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	7	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG23	7	0.04
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	7	0.04
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	7	0.04
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	7	0.04
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	15	0.04
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	15	0.04
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	15	0.04
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	15	0.04
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	15	0.04
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG23	15	0.04
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	15	0.04
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	15	0.04
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	15	0.04
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD11	2	0.04
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD12	2	0.04
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD13	2	0.04
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD11	10	0.04
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD12	10	0.04
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD13	10	0.04
(1,1577)	1:B:9:ARG:HD2	1:B:11:VAL:HB	1	0.04
(1,1577)	1:B:9:ARG:HD3	1:B:11:VAL:HB	1	0.04
(1,1572)	1:B:9:ARG:HG3	1:B:10:ILE:H	19	0.04
(1,1552)	1:B:8:ILE:HD11	1:B:77:ARG:HA	3	0.04
(1,1552)	1:B:8:ILE:HD12	1:B:77:ARG:HA	3	0.04
(1,1552)	1:B:8:ILE:HD13	1:B:77:ARG:HA	3	0.04
(1,1552)	1:B:8:ILE:HD11	1:B:77:ARG:HA	19	0.04
(1,1552)	1:B:8:ILE:HD12	1:B:77:ARG:HA	19	0.04
(1,1552)	1:B:8:ILE:HD13	1:B:77:ARG:HA	19	0.04
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	15	0.04
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	15	0.04
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	15	0.04
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	15	0.04
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	15	0.04
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	15	0.04
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	15	0.04
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	15	0.04
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	15	0.04
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	5	0.04
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	5	0.04
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	5	0.04
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	5	0.04
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	5	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	5	0.04
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	13	0.04
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	13	0.04
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	13	0.04
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	13	0.04
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	13	0.04
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	13	0.04
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	17	0.04
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	17	0.04
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	17	0.04
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	17	0.04
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	17	0.04
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	17	0.04
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	20	0.04
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	20	0.04
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	20	0.04
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	20	0.04
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	20	0.04
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	20	0.04
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	16	0.04
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	16	0.04
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	16	0.04
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	16	0.04
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	16	0.04
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	16	0.04
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	6	0.04
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	6	0.04
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	6	0.04
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	10	0.04
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	10	0.04
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	10	0.04
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	17	0.04
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	17	0.04
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	17	0.04
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	20	0.04
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	20	0.04
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	20	0.04
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	8	0.04
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	8	0.04
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	8	0.04
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	13	0.04
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	13	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	13	0.04
(1,1414)	1:B:3:ASP:HB2	1:B:53:VAL:H	16	0.04
(1,1378)	1:B:40:ALA:H	1:B:41:LYS:HD2	10	0.04
(1,1378)	1:B:40:ALA:H	1:B:41:LYS:HD3	10	0.04
(1,1356)	1:B:82:GLU:H	1:B:82:GLU:HG2	1	0.04
(1,1356)	1:B:82:GLU:H	1:B:82:GLU:HG3	1	0.04
(1,1356)	1:B:82:GLU:H	1:B:82:GLU:HG2	18	0.04
(1,1356)	1:B:82:GLU:H	1:B:82:GLU:HG3	18	0.04
(1,1309)	1:A:77:ARG:H	1:A:77:ARG:HD2	9	0.04
(1,1309)	1:A:77:ARG:H	1:A:77:ARG:HD3	9	0.04
(1,1223)	1:A:69:VAL:HG21	1:A:72:VAL:H	5	0.04
(1,1223)	1:A:69:VAL:HG22	1:A:72:VAL:H	5	0.04
(1,1223)	1:A:69:VAL:HG23	1:A:72:VAL:H	5	0.04
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	3	0.04
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	6	0.04
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	7	0.04
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	10	0.04
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	12	0.04
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	13	0.04
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	1	0.04
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	2	0.04
(1,1150)	1:B:67:ARG:HE	1:B:75:VAL:HB	13	0.04
(1,1105)	1:A:62:LEU:HD11	1:A:66:LEU:H	10	0.04
(1,1105)	1:A:62:LEU:HD12	1:A:66:LEU:H	10	0.04
(1,1105)	1:A:62:LEU:HD13	1:A:66:LEU:H	10	0.04
(1,1105)	1:A:62:LEU:HD11	1:A:66:LEU:H	14	0.04
(1,1105)	1:A:62:LEU:HD12	1:A:66:LEU:H	14	0.04
(1,1105)	1:A:62:LEU:HD13	1:A:66:LEU:H	14	0.04
(1,1104)	1:B:62:LEU:HD11	1:B:65:LYS:H	9	0.04
(1,1104)	1:B:62:LEU:HD12	1:B:65:LYS:H	9	0.04
(1,1104)	1:B:62:LEU:HD13	1:B:65:LYS:H	9	0.04
(1,1104)	1:B:62:LEU:HD11	1:B:65:LYS:H	11	0.04
(1,1104)	1:B:62:LEU:HD12	1:B:65:LYS:H	11	0.04
(1,1104)	1:B:62:LEU:HD13	1:B:65:LYS:H	11	0.04
(1,1094)	1:B:65:LYS:H	1:B:68:LYS:HE2	18	0.04
(1,1094)	1:B:65:LYS:H	1:B:68:LYS:HE3	18	0.04
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	9	0.04
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	9	0.04
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	9	0.04
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	18	0.04
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	18	0.04
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	18	0.04



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1020)	1:A:58:LYS:HZ1	1:A:61:THR:H	11	0.04
(1,1020)	1:A:58:LYS:HZ2	1:A:61:THR:H	11	0.04
(1,1020)	1:A:58:LYS:HZ3	1:A:61:THR:H	11	0.04
(1,1020)	1:A:58:LYS:HZ1	1:A:61:THR:H	15	0.04
(1,1020)	1:A:58:LYS:HZ2	1:A:61:THR:H	15	0.04
(1,1020)	1:A:58:LYS:HZ3	1:A:61:THR:H	15	0.04
(1,909)	1:B:3:ASP:HB3	1:B:53:VAL:H	1	0.03
(1,899)	1:B:51:ILE:HG12	1:B:52:PHE:H	3	0.03
(1,899)	1:B:51:ILE:HG12	1:B:52:PHE:H	8	0.03
(1,898)	1:A:51:ILE:HG12	1:A:52:PHE:H	9	0.03
(1,898)	1:A:51:ILE:HG12	1:A:52:PHE:H	17	0.03
(1,839)	1:B:48:ASN:HD21	1:B:78:LEU:HD21	15	0.03
(1,839)	1:B:48:ASN:HD21	1:B:78:LEU:HD22	15	0.03
(1,839)	1:B:48:ASN:HD21	1:B:78:LEU:HD23	15	0.03
(1,838)	1:A:48:ASN:HD21	1:A:78:LEU:HD21	6	0.03
(1,838)	1:A:48:ASN:HD21	1:A:78:LEU:HD22	6	0.03
(1,838)	1:A:48:ASN:HD21	1:A:78:LEU:HD23	6	0.03
(1,832)	1:A:47:CYS:HG	1:A:48:ASN:H	20	0.03
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	14	0.03
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	7	0.03
(1,822)	1:A:45:PHE:HZ	1:A:47:CYS:H	11	0.03
(1,761)	1:B:43:GLY:H	1:B:44:ILE:H	10	0.03
(1,726)	1:A:41:LYS:HB2	1:A:42:ASP:H	15	0.03
(1,726)	1:A:41:LYS:HB3	1:A:42:ASP:H	15	0.03
(1,719)	1:B:41:LYS:H	1:B:46:THR:H	5	0.03
(1,719)	1:B:41:LYS:H	1:B:46:THR:H	6	0.03
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD1	3	0.03
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD2	3	0.03
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD1	19	0.03
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD2	19	0.03
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD1	14	0.03
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD2	14	0.03
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD1	18	0.03
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD2	18	0.03
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD1	19	0.03
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD2	19	0.03
(1,668)	1:A:39:ASN:H	1:A:48:ASN:H	18	0.03
(1,615)	1:B:35:THR:H	1:B:83:HIS:HE1	3	0.03
(1,615)	1:B:35:THR:H	1:B:83:HIS:HE1	19	0.03
(1,570)	1:A:32:ASN:HD22	1:B:16:ASN:HA	3	0.03
(1,563)	1:A:32:ASN:HD21	1:A:33:ILE:HB	13	0.03
(1,563)	1:A:32:ASN:HD21	1:A:33:ILE:HB	18	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD11	2	0.03
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD12	2	0.03
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD13	2	0.03
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD11	9	0.03
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD12	9	0.03
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD13	9	0.03
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD11	17	0.03
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD12	17	0.03
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD13	17	0.03
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD11	1	0.03
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD12	1	0.03
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD13	1	0.03
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD11	4	0.03
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD12	4	0.03
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD13	4	0.03
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD11	9	0.03
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD12	9	0.03
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD13	9	0.03
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD11	14	0.03
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD12	14	0.03
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD13	14	0.03
(1,546)	1:B:29:PHE:HD1	1:B:31:THR:H	3	0.03
(1,546)	1:B:29:PHE:HD2	1:B:31:THR:H	3	0.03
(1,542)	1:B:30:ASP:HA	1:B:31:THR:H	15	0.03
(1,5014)	1:B:81:LEU:H	1:B:82:GLU:HG2	15	0.03
(1,5014)	1:B:81:LEU:H	1:B:82:GLU:HG3	15	0.03
(1,5013)	1:B:80:ASN:HB2	1:B:81:LEU:HD21	18	0.03
(1,5013)	1:B:80:ASN:HB2	1:B:81:LEU:HD22	18	0.03
(1,5013)	1:B:80:ASN:HB2	1:B:81:LEU:HD23	18	0.03
(1,5013)	1:B:80:ASN:HB3	1:B:81:LEU:HD21	18	0.03
(1,5013)	1:B:80:ASN:HB3	1:B:81:LEU:HD22	18	0.03
(1,5013)	1:B:80:ASN:HB3	1:B:81:LEU:HD23	18	0.03
(1,5005)	1:B:77:ARG:H	1:B:77:ARG:HG2	3	0.03
(1,5005)	1:B:77:ARG:H	1:B:77:ARG:HG3	3	0.03
(1,5005)	1:B:77:ARG:H	1:B:77:ARG:HG2	12	0.03
(1,5005)	1:B:77:ARG:H	1:B:77:ARG:HG3	12	0.03
(1,5002)	1:B:69:VAL:HG11	1:B:70:GLN:HE21	12	0.03
(1,5002)	1:B:69:VAL:HG11	1:B:70:GLN:HE22	12	0.03
(1,5002)	1:B:69:VAL:HG12	1:B:70:GLN:HE21	12	0.03
(1,5002)	1:B:69:VAL:HG12	1:B:70:GLN:HE22	12	0.03
(1,5002)	1:B:69:VAL:HG13	1:B:70:GLN:HE21	12	0.03
(1,5002)	1:B:69:VAL:HG13	1:B:70:GLN:HE22	12	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4988)	1:B:66:LEU:HB2	1:B:75:VAL:HG11	20	0.03
(1,4988)	1:B:66:LEU:HB2	1:B:75:VAL:HG12	20	0.03
(1,4988)	1:B:66:LEU:HB2	1:B:75:VAL:HG13	20	0.03
(1,4988)	1:B:66:LEU:HB3	1:B:75:VAL:HG11	20	0.03
(1,4988)	1:B:66:LEU:HB3	1:B:75:VAL:HG12	20	0.03
(1,4988)	1:B:66:LEU:HB3	1:B:75:VAL:HG13	20	0.03
(1,4936)	1:B:54:LYS:HE2	1:B:55:ASN:HD21	20	0.03
(1,4936)	1:B:54:LYS:HE2	1:B:55:ASN:HD22	20	0.03
(1,4936)	1:B:54:LYS:HE3	1:B:55:ASN:HD21	20	0.03
(1,4936)	1:B:54:LYS:HE3	1:B:55:ASN:HD22	20	0.03
(1,4935)	1:B:54:LYS:HD2	1:B:55:ASN:HD21	13	0.03
(1,4935)	1:B:54:LYS:HD2	1:B:55:ASN:HD22	13	0.03
(1,4935)	1:B:54:LYS:HD3	1:B:55:ASN:HD21	13	0.03
(1,4935)	1:B:54:LYS:HD3	1:B:55:ASN:HD22	13	0.03
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD21	3	0.03
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD22	3	0.03
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD21	3	0.03
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD22	3	0.03
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD21	17	0.03
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD22	17	0.03
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD21	17	0.03
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD22	17	0.03
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD21	18	0.03
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD22	18	0.03
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD21	18	0.03
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD22	18	0.03
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE1	5	0.03
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE2	5	0.03
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE3	5	0.03
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE1	5	0.03
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE2	5	0.03
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE3	5	0.03
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE1	10	0.03
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE2	10	0.03
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE3	10	0.03
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE1	10	0.03
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE2	10	0.03
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE3	10	0.03
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE1	20	0.03
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE2	20	0.03
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE3	20	0.03
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE1	20	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE2	20	0.03
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE3	20	0.03
(1,4906)	1:B:42:ASP:HB2	1:B:44:ILE:HG12	3	0.03
(1,4906)	1:B:42:ASP:HB3	1:B:44:ILE:HG12	3	0.03
(1,4906)	1:B:42:ASP:HB2	1:B:44:ILE:HG12	8	0.03
(1,4906)	1:B:42:ASP:HB3	1:B:44:ILE:HG12	8	0.03
(1,4906)	1:B:42:ASP:HB2	1:B:44:ILE:HG12	10	0.03
(1,4906)	1:B:42:ASP:HB3	1:B:44:ILE:HG12	10	0.03
(1,4898)	1:B:39:ASN:HD21	1:B:41:LYS:HE2	3	0.03
(1,4898)	1:B:39:ASN:HD21	1:B:41:LYS:HE3	3	0.03
(1,4898)	1:B:39:ASN:HD22	1:B:41:LYS:HE2	3	0.03
(1,4898)	1:B:39:ASN:HD22	1:B:41:LYS:HE3	3	0.03
(1,4898)	1:B:39:ASN:HD21	1:B:41:LYS:HE2	15	0.03
(1,4898)	1:B:39:ASN:HD21	1:B:41:LYS:HE3	15	0.03
(1,4898)	1:B:39:ASN:HD22	1:B:41:LYS:HE2	15	0.03
(1,4898)	1:B:39:ASN:HD22	1:B:41:LYS:HE3	15	0.03
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB2	12	0.03
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB3	12	0.03
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD11	3	0.03
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD12	3	0.03
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD13	3	0.03
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD11	3	0.03
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD12	3	0.03
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD13	3	0.03
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD11	13	0.03
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD12	13	0.03
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD13	13	0.03
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD11	13	0.03
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD12	13	0.03
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD13	13	0.03
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD11	15	0.03
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD12	15	0.03
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD13	15	0.03
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD11	15	0.03
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD12	15	0.03
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD13	15	0.03
(1,4850)	1:B:29:PHE:HZ	1:B:65:LYS:HD2	11	0.03
(1,4850)	1:B:29:PHE:HZ	1:B:65:LYS:HD3	11	0.03
(1,4833)	1:B:28:LYS:HA	1:B:28:LYS:HG2	12	0.03
(1,4833)	1:B:28:LYS:HA	1:B:28:LYS:HG3	12	0.03
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG2	7	0.03
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	7	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	7	0.03
	1:B:25:VAL:HG22	1:B:28:LYS:HG3	7	0.03
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	7	0.03
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	7	0.03
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG2	8	0.03
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	8	0.03
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	8	0.03
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG3	8	0.03
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	8	0.03
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	8	0.03
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG2	16	0.03
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	16	0.03
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	16	0.03
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG3	16	0.03
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	16	0.03
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	16	0.03
(1,4775)	1:B:16:ASN:HB2	1:B:17:GLY:H	16	0.03
(1,4775)	1:B:16:ASN:HB3	1:B:17:GLY:H	16	0.03
(1,4771)	1:B:15:LYS:HD2	1:B:16:ASN:HD21	17	0.03
(1,4771)	1:B:15:LYS:HD2	1:B:16:ASN:HD22	17	0.03
(1,4771)	1:B:15:LYS:HD3	1:B:16:ASN:HD21	17	0.03
(1,4771)	1:B:15:LYS:HD3	1:B:16:ASN:HD22	17	0.03
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG2	6	0.03
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG3	6	0.03
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG2	16	0.03
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG3	16	0.03
(1,4689)	1:A:66:LEU:HB2	1:A:75:VAL:HG11	2	0.03
(1,4689)	1:A:66:LEU:HB2	1:A:75:VAL:HG12	2	0.03
(1,4689)	1:A:66:LEU:HB2	1:A:75:VAL:HG13	2	0.03
(1,4689)	1:A:66:LEU:HB3	1:A:75:VAL:HG11	2	0.03
(1,4689)	1:A:66:LEU:HB3	1:A:75:VAL:HG12	2	0.03
(1,4689)	1:A:66:LEU:HB3	1:A:75:VAL:HG13	2	0.03
(1,4679)	1:A:63:MET:HE1	1:A:77:ARG:HB2	9	0.03
(1,4679)	1:A:63:MET:HE1	1:A:77:ARG:HB3	9	0.03
(1,4679)	1:A:63:MET:HE2	1:A:77:ARG:HB2	9	0.03
(1,4679)	1:A:63:MET:HE2	1:A:77:ARG:HB3	9	0.03
(1,4679)	1:A:63:MET:HE3	1:A:77:ARG:HB2	9	0.03
(1,4679)	1:A:63:MET:HE3	1:A:77:ARG:HB3	9	0.03
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE1	4	0.03
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE2	4	0.03
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE3	4	0.03
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE1	4	0.03



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` '	1:A:48:ASN:HD22			
(1 4000)	1.71.10.71011.111222	1:A:50:MET:HE2	4	0.03
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE3	4	0.03
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE1	5	0.03
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE2	5	0.03
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE3	5	0.03
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE1	5	0.03
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE2	5	0.03
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE3	5	0.03
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE1	7	0.03
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE2	7	0.03
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE3	7	0.03
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE1	7	0.03
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE2	7	0.03
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE3	7	0.03
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE1	19	0.03
	1:A:48:ASN:HD21	1:A:50:MET:HE2	19	0.03
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE3	19	0.03
· · /	1:A:48:ASN:HD22	1:A:50:MET:HE1	19	0.03
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE2	19	0.03
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE3	19	0.03
(1,4613)	1:A:42:ASP:HB2	1:A:44:ILE:HG12	11	0.03
(1,4613)	1:A:42:ASP:HB3	1:A:44:ILE:HG12	11	0.03
(1,4606)	1:A:39:ASN:HD21	1:A:46:THR:HG21	14	0.03
(1,4606)	1:A:39:ASN:HD21	1:A:46:THR:HG22	14	0.03
(1,4606)	1:A:39:ASN:HD21	1:A:46:THR:HG23	14	0.03
(1,4606)	1:A:39:ASN:HD22	1:A:46:THR:HG21	14	0.03
(1,4606)	1:A:39:ASN:HD22	1:A:46:THR:HG22	14	0.03
(1,4606)	1:A:39:ASN:HD22	1:A:46:THR:HG23	14	0.03
(1,4604)	1:A:39:ASN:HD21	1:A:41:LYS:HE2	7	0.03
(1,4604)	1:A:39:ASN:HD21	1:A:41:LYS:HE3	7	0.03
(1,4604)	1:A:39:ASN:HD22	1:A:41:LYS:HE2	7	0.03
(1,4604)	1:A:39:ASN:HD22	1:A:41:LYS:HE3	7	0.03
(1,4604)	1:A:39:ASN:HD21	1:A:41:LYS:HE2	11	0.03
(1,4604)	1:A:39:ASN:HD21	1:A:41:LYS:HE3	11	0.03
(1,4604)	1:A:39:ASN:HD22	1:A:41:LYS:HE2	11	0.03
(1,4604)	1:A:39:ASN:HD22	1:A:41:LYS:HE3	11	0.03
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB2	4	0.03
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB3	4	0.03
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB2	15	0.03
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB3	15	0.03
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB2	20	0.03
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB3	20	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD11	17	0.03
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD12	17	0.03
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD13	17	0.03
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD11	17	0.03
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD12	17	0.03
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD13	17	0.03
(1,4560)	1:A:31:THR:HG21	1:A:58:LYS:HE2	7	0.03
(1,4560)	1:A:31:THR:HG21	1:A:58:LYS:HE3	7	0.03
(1,4560)	1:A:31:THR:HG22	1:A:58:LYS:HE2	7	0.03
(1,4560)	1:A:31:THR:HG22	1:A:58:LYS:HE3	7	0.03
(1,4560)	1:A:31:THR:HG23	1:A:58:LYS:HE2	7	0.03
(1,4560)	1:A:31:THR:HG23	1:A:58:LYS:HE3	7	0.03
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	11	0.03
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	11	0.03
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	11	0.03
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	11	0.03
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	11	0.03
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	11	0.03
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	18	0.03
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	18	0.03
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	18	0.03
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	18	0.03
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	18	0.03
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	18	0.03
(1,4514)	1:A:24:GLY:HA2	1:A:28:LYS:HE2	1	0.03
(1,4514)	1:A:24:GLY:HA2	1:A:28:LYS:HE3	1	0.03
(1,4514)	1:A:24:GLY:HA3	1:A:28:LYS:HE2	1	0.03
(1,4514)	1:A:24:GLY:HA3	1:A:28:LYS:HE3	1	0.03
(1,4496)	1:A:20:ASN:HB2	1:A:21:GLN:HE21	13	0.03
(1,4496)	1:A:20:ASN:HB3	1:A:21:GLN:HE21	13	0.03
(1,4477)	1:A:18:MET:H	1:B:32:ASN:HD21	4	0.03
(1,4477)	1:A:18:MET:H	1:B:32:ASN:HD22	4	0.03
(1,4468)	1:A:16:ASN:HB2	1:A:17:GLY:H	5	0.03
(1,4468)	1:A:16:ASN:HB3	1:A:17:GLY:H	5	0.03
(1,4457)	1:A:15:LYS:HB2	1:A:18:MET:HB2	4	0.03
(1,4457)	1:A:15:LYS:HB2	1:A:18:MET:HB3	4	0.03
(1,4457)	1:A:15:LYS:HB3	1:A:18:MET:HB2	4	0.03
(1,4457)	1:A:15:LYS:HB3	1:A:18:MET:HB3	4	0.03
(1,4457)	1:A:15:LYS:HB2	1:A:18:MET:HB2	17	0.03
(1,4457)	1:A:15:LYS:HB2	1:A:18:MET:HB3	17	0.03
(1,4457)	1:A:15:LYS:HB3	1:A:18:MET:HB2	17	0.03
	1:A:15:LYS:HB3	1:A:18:MET:HB3	17	



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Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,4397)	1:B:82:GLU:HA	1:B:83:HIS:HD2	13	0.03
(1,4389)	1:B:81:LEU:HB2	1:B:83:HIS:HD2	4	0.03
(1,4389)	1:B:81:LEU:HB3	1:B:83:HIS:HD2	4	0.03
(1,4389)	1:B:81:LEU:HB2	1:B:83:HIS:HD2	5	0.03
(1,4389)	1:B:81:LEU:HB3	1:B:83:HIS:HD2	5	0.03
(1,4389)	1:B:81:LEU:HB2	1:B:83:HIS:HD2	19	0.03
(1,4389)	1:B:81:LEU:HB3	1:B:83:HIS:HD2	19	0.03
(1,4388)	1:A:81:LEU:HB2	1:A:83:HIS:HD2	6	0.03
(1,4388)	1:A:81:LEU:HB3	1:A:83:HIS:HD2	6	0.03
(1,4388)	1:A:81:LEU:HB2	1:A:83:HIS:HD2	11	0.03
(1,4388)	1:A:81:LEU:HB3	1:A:83:HIS:HD2	11	0.03
(1,4388)	1:A:81:LEU:HB2	1:A:83:HIS:HD2	16	0.03
(1,4388)	1:A:81:LEU:HB3	1:A:83:HIS:HD2	16	0.03
(1,4387)	1:B:5:LEU:HG	1:B:83:HIS:HD2	3	0.03
(1,4386)	1:A:5:LEU:HG	1:A:83:HIS:HD2	5	0.03
(1,4386)	1:A:5:LEU:HG	1:A:83:HIS:HD2	10	0.03
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	13	0.03
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	13	0.03
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	13	0.03
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	13	0.03
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	13	0.03
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	13	0.03
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG11	14	0.03
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG12	14	0.03
(1,4375)	1:B:4:PHE:HE1	1:B:53:VAL:HG13	14	0.03
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG11	14	0.03
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG12	14	0.03
(1,4375)	1:B:4:PHE:HE2	1:B:53:VAL:HG13	14	0.03
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG21	12	0.03
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG22	12	0.03
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG23	12	0.03
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG21	7	0.03
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG22	7	0.03
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG23	7	0.03
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG21	9	0.03
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG22	9	0.03
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG23	9	0.03
(1,4353)	1:B:44:ILE:HG13	1:B:73:PHE:HE1	15	0.03
(1,4353)	1:B:44:ILE:HG13	1:B:73:PHE:HE2	15	0.03
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE1	5	0.03
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE2	5	0.03
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE1	5	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE2	5	0.03
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE1	7	0.03
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE2	7	0.03
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE1	7	0.03
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE2	7	0.03
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE1	8	0.03
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE2	8	0.03
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE1	8	0.03
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE2	8	0.03
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE1	18	0.03
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE2	18	0.03
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE1	18	0.03
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE2	18	0.03
(1,4329)	1:B:5:LEU:HD21	1:B:52:PHE:HE1	18	0.03
(1,4329)	1:B:5:LEU:HD21	1:B:52:PHE:HE2	18	0.03
(1,4329)	1:B:5:LEU:HD22	1:B:52:PHE:HE1	18	0.03
(1,4329)	1:B:5:LEU:HD22	1:B:52:PHE:HE2	18	0.03
(1,4329)	1:B:5:LEU:HD23	1:B:52:PHE:HE1	18	0.03
(1,4329)	1:B:5:LEU:HD23	1:B:52:PHE:HE2	18	0.03
(1,4329)	1:B:5:LEU:HD21	1:B:52:PHE:HE1	19	0.03
(1,4329)	1:B:5:LEU:HD21	1:B:52:PHE:HE2	19	0.03
(1,4329)	1:B:5:LEU:HD22	1:B:52:PHE:HE1	19	0.03
(1,4329)	1:B:5:LEU:HD22	1:B:52:PHE:HE2	19	0.03
(1,4329)	1:B:5:LEU:HD23	1:B:52:PHE:HE1	19	0.03
(1,4329)	1:B:5:LEU:HD23	1:B:52:PHE:HE2	19	0.03
(1,4323)	1:B:52:PHE:HD1	1:B:53:VAL:H	10	0.03
(1,4323)	1:B:52:PHE:HD2	1:B:53:VAL:H	10	0.03
(1,4323)	1:B:52:PHE:HD1	1:B:53:VAL:H	16	0.03
(1,4323)	1:B:52:PHE:HD2	1:B:53:VAL:H	16	0.03
(1,4323)	1:B:52:PHE:HD1	1:B:53:VAL:H	18	0.03
(1,4323)	1:B:52:PHE:HD2	1:B:53:VAL:H	18	0.03
(1,4323)	1:B:52:PHE:HD1	1:B:53:VAL:H	20	0.03
(1,4323)	1:B:52:PHE:HD2	1:B:53:VAL:H	20	0.03
(1,4311)	1:B:5:LEU:HA	1:B:52:PHE:HD1	15	0.03
(1,4311)	1:B:5:LEU:HA	1:B:52:PHE:HD2	15	0.03
(1,4297)	1:B:45:PHE:HZ	1:B:71:GLY:HA3	14	0.03
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	1	0.03
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	8	0.03
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	16	0.03
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	17	0.03
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	20	0.03
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE1	13	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE2	13	0.03
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE1	13	0.03
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE2	13	0.03
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE1	13	0.03
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE2	13	0.03
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE1	17	0.03
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE2	17	0.03
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE1	17	0.03
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE2	17	0.03
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE1	17	0.03
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE2	17	0.03
(1,4234)	1:A:45:PHE:HD1	1:A:47:CYS:HG	2	0.03
(1,4234)	1:A:45:PHE:HD2	1:A:47:CYS:HG	2	0.03
(1,4205)	1:B:29:PHE:HD1	1:B:65:LYS:HD2	7	0.03
(1,4205)	1:B:29:PHE:HD2	1:B:65:LYS:HD2	7	0.03
(1,4205)	1:B:29:PHE:HD1	1:B:65:LYS:HD2	8	0.03
(1,4205)	1:B:29:PHE:HD2	1:B:65:LYS:HD2	8	0.03
(1,4204)	1:A:29:PHE:HD1	1:A:65:LYS:HD2	9	0.03
(1,4204)	1:A:29:PHE:HD2	1:A:65:LYS:HD2	9	0.03
(1,4204)	1:A:29:PHE:HD1	1:A:65:LYS:HD2	19	0.03
(1,4204)	1:A:29:PHE:HD2	1:A:65:LYS:HD2	19	0.03
(1,4187)	1:B:4:PHE:HZ	1:B:6:ALA:HA	9	0.03
(1,4187)	1:B:4:PHE:HZ	1:B:6:ALA:HA	15	0.03
(1,4186)	1:A:4:PHE:HZ	1:A:6:ALA:HA	3	0.03
(1,4186)	1:A:4:PHE:HZ	1:A:6:ALA:HA	4	0.03
(1,4186)	1:A:4:PHE:HZ	1:A:6:ALA:HA	5	0.03
(1,4186)	1:A:4:PHE:HZ	1:A:6:ALA:HA	11	0.03
(1,4186)	1:A:4:PHE:HZ	1:A:6:ALA:HA	12	0.03
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	19	0.03
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	19	0.03
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	19	0.03
(1,4147)	1:B:4:PHE:H	1:B:4:PHE:HD1	7	0.03
(1,4147)	1:B:4:PHE:H	1:B:4:PHE:HD2	7	0.03
(1,4147)	1:B:4:PHE:H	1:B:4:PHE:HD1	17	0.03
(1,4147)	1:B:4:PHE:H	1:B:4:PHE:HD2	17	0.03
(1,4144)	1:A:4:PHE:HD1	1:A:5:LEU:H	9	0.03
(1,4144)	1:A:4:PHE:HD2	1:A:5:LEU:H	9	0.03
(1,4144)	1:A:4:PHE:HD1	1:A:5:LEU:H	20	0.03
(1,4144)	1:A:4:PHE:HD2	1:A:5:LEU:H	20	0.03
(1,4133)	1:B:4:PHE:HD1	1:B:59:LEU:HD21	11	0.03
(1,4133)	1:B:4:PHE:HD1	1:B:59:LEU:HD22	11	0.03
(1,4133)	1:B:4:PHE:HD1	1:B:59:LEU:HD23	11	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4133)	1:B:4:PHE:HD2	1:B:59:LEU:HD21	11	0.03
(1,4133)	1:B:4:PHE:HD2	1:B:59:LEU:HD22	11	0.03
(1,4133)	1:B:4:PHE:HD2	1:B:59:LEU:HD23	11	0.03
(1,4129)	1:B:83:HIS:HA	1:B:83:HIS:HD2	14	0.03
(1,4127)	1:B:83:HIS:HA	1:B:83:HIS:HB3	16	0.03
(1,4119)	1:B:80:ASN:HA	1:B:81:LEU:HG	2	0.03
(1,4119)	1:B:80:ASN:HA	1:B:81:LEU:HG	6	0.03
(1,4118)	1:A:80:ASN:HA	1:A:81:LEU:HG	1	0.03
(1,4118)	1:A:80:ASN:HA	1:A:81:LEU:HG	13	0.03
(1,4113)	1:B:77:ARG:HG3	1:B:79:SER:HA	20	0.03
(1,4112)	1:A:77:ARG:HG3	1:A:79:SER:HA	18	0.03
(1,4111)	1:B:79:SER:HA	1:B:81:LEU:HG	12	0.03
(1,4110)	1:A:79:SER:HA	1:A:81:LEU:HG	7	0.03
(1,4108)	1:A:79:SER:HA	1:A:81:LEU:HD21	12	0.03
(1,4108)	1:A:79:SER:HA	1:A:81:LEU:HD22	12	0.03
(1,4108)	1:A:79:SER:HA	1:A:81:LEU:HD23	12	0.03
(1,4086)	1:A:73:PHE:HA	1:A:75:VAL:HG21	11	0.03
(1,4086)	1:A:73:PHE:HA	1:A:75:VAL:HG22	11	0.03
(1,4086)	1:A:73:PHE:HA	1:A:75:VAL:HG23	11	0.03
(1,4053)	1:B:41:LYS:HG2	1:B:42:ASP:HA	3	0.03
(1,4053)	1:B:41:LYS:HG3	1:B:42:ASP:HA	3	0.03
(1,4053)	1:B:41:LYS:HG2	1:B:42:ASP:HA	4	0.03
(1,4053)	1:B:41:LYS:HG3	1:B:42:ASP:HA	4	0.03
(1,4053)	1:B:41:LYS:HG2	1:B:42:ASP:HA	16	0.03
(1,4053)	1:B:41:LYS:HG3	1:B:42:ASP:HA	16	0.03
(1,4049)	1:B:41:LYS:HA	1:B:41:LYS:HD2	2	0.03
(1,4049)	1:B:41:LYS:HA	1:B:41:LYS:HD3	2	0.03
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG2	5	0.03
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG3	5	0.03
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG2	17	0.03
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG3	17	0.03
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG2	18	0.03
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG3	18	0.03
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	3	0.03
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	3	0.03
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	6	0.03
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	6	0.03
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	8	0.03
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	8	0.03
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	11	0.03
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	11	0.03
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	13	0.03



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Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	13	0.03
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	17	0.03
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	17	0.03
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	18	0.03
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	18	0.03
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	18	0.03
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	19	0.03
(1,4036)	1:A:15:LYS:HA	1:A:17:GLY:H	15	0.03
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD11	4	0.03
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD12	4	0.03
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD13	4	0.03
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD11	4	0.03
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD12	4	0.03
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD13	4	0.03
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD11	4	0.03
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD12	4	0.03
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD13	4	0.03
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD11	8	0.03
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD12	8	0.03
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD13	8	0.03
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD11	12	0.03
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD12	12	0.03
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD13	12	0.03
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD11	16	0.03
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD12	16	0.03
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD13	16	0.03
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD11	19	0.03
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD12	19	0.03
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD13	19	0.03
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD11	3	0.03
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD12	3	0.03
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD13	3	0.03
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD11	15	0.03
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD12	15	0.03
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD13	15	0.03
(1,3916)	1:B:18:MET:HE1	1:B:72:VAL:HG21	6	0.03
(1,3916)	1:B:18:MET:HE1	1:B:72:VAL:HG22	6	0.03
(1,3916)	1:B:18:MET:HE1	1:B:72:VAL:HG23	6	0.03
(1,3916)	1:B:18:MET:HE2	1:B:72:VAL:HG21	6	0.03
(1,3916)	1:B:18:MET:HE2	1:B:72:VAL:HG22	6	0.03
(1,3916)	1:B:18:MET:HE2	1:B:72:VAL:HG23	6	0.03
(1,3916)	1:B:18:MET:HE3	1:B:72:VAL:HG21	6	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3916)	1:B:18:MET:HE3	1:B:72:VAL:HG22	6	0.03
(1,3916)	1:B:18:MET:HE3	1:B:72:VAL:HG23	6	0.03
(1,3916)	1:B:18:MET:HE1	1:B:72:VAL:HG21	15	0.03
(1,3916)	1:B:18:MET:HE1	1:B:72:VAL:HG22	15	0.03
(1,3916)	1:B:18:MET:HE1	1:B:72:VAL:HG23	15	0.03
(1,3916)	1:B:18:MET:HE2	1:B:72:VAL:HG21	15	0.03
(1,3916)	1:B:18:MET:HE2	1:B:72:VAL:HG22	15	0.03
(1,3916)	1:B:18:MET:HE2	1:B:72:VAL:HG23	15	0.03
(1,3916)	1:B:18:MET:HE3	1:B:72:VAL:HG21	15	0.03
(1,3916)	1:B:18:MET:HE3	1:B:72:VAL:HG22	15	0.03
(1,3916)	1:B:18:MET:HE3	1:B:72:VAL:HG23	15	0.03
(1,3890)	1:B:82:GLU:HA	1:B:83:HIS:HB2	20	0.03
(1,3889)	1:A:82:GLU:HA	1:A:83:HIS:HB2	5	0.03
(1,3889)	1:A:82:GLU:HA	1:A:83:HIS:HB2	20	0.03
(1,3888)	1:B:8:ILE:H	1:B:81:LEU:HD21	6	0.03
(1,3888)	1:B:8:ILE:H	1:B:81:LEU:HD22	6	0.03
(1,3888)	1:B:8:ILE:H	1:B:81:LEU:HD23	6	0.03
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD21	15	0.03
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD22	15	0.03
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD23	15	0.03
(1,3858)	1:B:50:MET:HG2	1:B:81:LEU:HD11	8	0.03
(1,3858)	1:B:50:MET:HG2	1:B:81:LEU:HD12	8	0.03
(1,3858)	1:B:50:MET:HG2	1:B:81:LEU:HD13	8	0.03
(1,3845)	1:A:80:ASN:HB3	1:A:81:LEU:HD21	9	0.03
(1,3845)	1:A:80:ASN:HB3	1:A:81:LEU:HD22	9	0.03
(1,3845)	1:A:80:ASN:HB3	1:A:81:LEU:HD23	9	0.03
(1,3842)	1:B:80:ASN:HB2	1:B:81:LEU:HD21	12	0.03
(1,3842)	1:B:80:ASN:HB2	1:B:81:LEU:HD22	12	0.03
(1,3842)	1:B:80:ASN:HB2	1:B:81:LEU:HD23	12	0.03
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD21	11	0.03
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD22	11	0.03
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD23	11	0.03
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD21	11	0.03
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD22	11	0.03
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD23	11	0.03
(1,3821)	1:A:9:ARG:HB2	1:A:78:LEU:HD21	2	0.03
(1,3821)	1:A:9:ARG:HB2	1:A:78:LEU:HD22	2	0.03
(1,3821)	1:A:9:ARG:HB2	1:A:78:LEU:HD23	2	0.03
(1,3821)	1:A:9:ARG:HB3	1:A:78:LEU:HD21	2	0.03
(1,3821)	1:A:9:ARG:HB3	1:A:78:LEU:HD22	2	0.03
(1,3821)	1:A:9:ARG:HB3	1:A:78:LEU:HD23	2	0.03
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD11	7	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD12	7	0.03
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD13	7	0.03
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD11	8	0.03
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD12	8	0.03
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD13	8	0.03
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD11	2	0.03
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD12	2	0.03
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD13	2	0.03
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD11	19	0.03
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD12	19	0.03
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD13	19	0.03
(1,3810)	1:B:48:ASN:HD21	1:B:78:LEU:HD11	19	0.03
(1,3810)	1:B:48:ASN:HD21	1:B:78:LEU:HD12	19	0.03
(1,3810)	1:B:48:ASN:HD21	1:B:78:LEU:HD13	19	0.03
(1,381)	1:B:22:ILE:H	1:B:23:THR:HG1	16	0.03
(1,3809)	1:A:48:ASN:HD21	1:A:78:LEU:HD11	13	0.03
(1,3809)	1:A:48:ASN:HD21	1:A:78:LEU:HD12	13	0.03
(1,3809)	1:A:48:ASN:HD21	1:A:78:LEU:HD13	13	0.03
(1,380)	1:A:22:ILE:H	1:A:23:THR:HG1	11	0.03
(1,380)	1:A:22:ILE:H	1:A:23:THR:HG1	15	0.03
(1,380)	1:A:22:ILE:H	1:A:23:THR:HG1	16	0.03
(1,3792)	1:B:50:MET:HE1	1:B:78:LEU:HD11	5	0.03
(1,3792)	1:B:50:MET:HE1	1:B:78:LEU:HD12	5	0.03
(1,3792)	1:B:50:MET:HE1	1:B:78:LEU:HD13	5	0.03
(1,3792)	1:B:50:MET:HE2	1:B:78:LEU:HD11	5	0.03
(1,3792)	1:B:50:MET:HE2	1:B:78:LEU:HD12	5	0.03
(1,3792)	1:B:50:MET:HE2	1:B:78:LEU:HD13	5	0.03
(1,3792)	1:B:50:MET:HE3	1:B:78:LEU:HD11	5	0.03
(1,3792)	1:B:50:MET:HE3	1:B:78:LEU:HD12	5	0.03
(1,3792)	1:B:50:MET:HE3	1:B:78:LEU:HD13	5	0.03
(1,3791)	1:A:50:MET:HE1	1:A:78:LEU:HD11	13	0.03
(1,3791)	1:A:50:MET:HE1	1:A:78:LEU:HD12	13	0.03
(1,3791)	1:A:50:MET:HE1	1:A:78:LEU:HD13	13	0.03
(1,3791)	1:A:50:MET:HE2	1:A:78:LEU:HD11	13	0.03
(1,3791)	1:A:50:MET:HE2	1:A:78:LEU:HD12	13	0.03
(1,3791)	1:A:50:MET:HE2	1:A:78:LEU:HD13	13	0.03
(1,3791)	1:A:50:MET:HE3	1:A:78:LEU:HD11	13	0.03
(1,3791)	1:A:50:MET:HE3	1:A:78:LEU:HD12	13	0.03
(1,3791)	1:A:50:MET:HE3	1:A:78:LEU:HD13	13	0.03
(1,3764)	1:B:4:PHE:HZ	1:B:77:ARG:HD2	17	0.03
(1,3764)	1:B:4:PHE:HZ	1:B:77:ARG:HD3	17	0.03
(1,3754)	1:B:59:LEU:HD11	1:B:77:ARG:HD2	17	0.03



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	1:B:59:LEU:HD11	4 D BE ADOLIDA		
(1,3754)		1:B:77:ARG:HD3	17	0.03
1 \ /	1:B:59:LEU:HD12	1:B:77:ARG:HD2	17	0.03
(1,3754)	1:B:59:LEU:HD12	1:B:77:ARG:HD3	17	0.03
(1,3754)	1:B:59:LEU:HD13	1:B:77:ARG:HD2	17	0.03
(1,3754)	1:B:59:LEU:HD13	1:B:77:ARG:HD3	17	0.03
(1,3753)	1:A:59:LEU:HD11	1:A:77:ARG:HD2	13	0.03
(1,3753)	1:A:59:LEU:HD11	1:A:77:ARG:HD3	13	0.03
(1,3753)	1:A:59:LEU:HD12	1:A:77:ARG:HD2	13	0.03
(1,3753)	1:A:59:LEU:HD12	1:A:77:ARG:HD3	13	0.03
(1,3753)	1:A:59:LEU:HD13	1:A:77:ARG:HD2	13	0.03
(1,3753)	1:A:59:LEU:HD13	1:A:77:ARG:HD3	13	0.03
(1,3753)	1:A:59:LEU:HD11	1:A:77:ARG:HD2	19	0.03
(1,3753)	1:A:59:LEU:HD11	1:A:77:ARG:HD3	19	0.03
(1,3753)	1:A:59:LEU:HD12	1:A:77:ARG:HD2	19	0.03
(1,3753)	1:A:59:LEU:HD12	1:A:77:ARG:HD3	19	0.03
(1,3753)	1:A:59:LEU:HD13	1:A:77:ARG:HD2	19	0.03
(1,3753)	1:A:59:LEU:HD13	1:A:77:ARG:HD3	19	0.03
(1,3734)	1:B:74:THR:HA	1:B:76:GLU:HG2	18	0.03
(1,3734)	1:B:74:THR:HA	1:B:76:GLU:HG3	18	0.03
(1,3734)	1:B:74:THR:HA	1:B:76:GLU:HG2	20	0.03
(1,3734)	1:B:74:THR:HA	1:B:76:GLU:HG3	20	0.03
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	13	0.03
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	13	0.03
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	13	0.03
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	3	0.03
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	3	0.03
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	3	0.03
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG21	9	0.03
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG22	9	0.03
(1,3701)	1:A:11:VAL:H	1:A:74:THR:HG23	9	0.03
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG21	7	0.03
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG22	7	0.03
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG23	7	0.03
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG21	7	0.03
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG22	7	0.03
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG23	7	0.03
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG21	11	0.03
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG22	11	0.03
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG23	11	0.03
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG21	11	0.03
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG22	11	0.03
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG23	11	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG21	19	0.03
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG22	19	0.03
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG23	19	0.03
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG21	19	0.03
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG22	19	0.03
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG23	19	0.03
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG21	17	0.03
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG22	17	0.03
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG23	17	0.03
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG11	7	0.03
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG12	7	0.03
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG13	7	0.03
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG11	8	0.03
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG12	8	0.03
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG13	8	0.03
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG11	9	0.03
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG12	9	0.03
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG13	9	0.03
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG11	20	0.03
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG12	20	0.03
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG13	20	0.03
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG11	10	0.03
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG12	10	0.03
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG13	10	0.03
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG11	12	0.03
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG12	12	0.03
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG13	12	0.03
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG11	15	0.03
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG12	15	0.03
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG13	15	0.03
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB2	19	0.03
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB3	19	0.03
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB2	20	0.03
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB3	20	0.03
(1,3594)	1:B:66:LEU:HA	1:B:69:VAL:HB	9	0.03
(1,3593)	1:A:66:LEU:HA	1:A:69:VAL:HB	17	0.03
(1,3592)	1:B:20:ASN:HA	1:B:22:ILE:HB	17	0.03
(1,3592)	1:B:20:ASN:HA	1:B:22:ILE:HB	18	0.03
(1,3563)	1:A:67:ARG:H	1:A:68:LYS:HE2	14	0.03
(1,3563)	1:A:67:ARG:H	1:A:68:LYS:HE3	14	0.03
(1,3562)	1:B:15:LYS:HE2	1:B:18:MET:H	15	0.03
(1,3562)	1:B:15:LYS:HE3	1:B:18:MET:H	15	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3561)	1:A:15:LYS:HE2	1:A:18:MET:H	10	0.03
(1,3561)	1:A:15:LYS:HE3	1:A:18:MET:H	10	0.03
(1,3560)	1:B:15:LYS:HE2	1:B:16:ASN:HD21	16	0.03
(1,3560)	1:B:15:LYS:HE3	1:B:16:ASN:HD21	16	0.03
(1,3559)	1:A:15:LYS:HE2	1:A:16:ASN:HD21	5	0.03
(1,3559)	1:A:15:LYS:HE3	1:A:16:ASN:HD21	5	0.03
(1,3529)	1:A:68:LYS:HA	1:A:68:LYS:HG3	3	0.03
(1,3421)	1:B:63:MET:HE1	1:B:77:ARG:H	3	0.03
(1,3421)	1:B:63:MET:HE2	1:B:77:ARG:H	3	0.03
(1,3421)	1:B:63:MET:HE3	1:B:77:ARG:H	3	0.03
(1,3421)	1:B:63:MET:HE1	1:B:77:ARG:H	7	0.03
(1,3421)	1:B:63:MET:HE2	1:B:77:ARG:H	7	0.03
(1,3421)	1:B:63:MET:HE3	1:B:77:ARG:H	7	0.03
(1,3421)	1:B:63:MET:HE1	1:B:77:ARG:H	10	0.03
(1,3421)	1:B:63:MET:HE2	1:B:77:ARG:H	10	0.03
(1,3421)	1:B:63:MET:HE3	1:B:77:ARG:H	10	0.03
(1,3421)	1:B:63:MET:HE1	1:B:77:ARG:H	13	0.03
(1,3421)	1:B:63:MET:HE2	1:B:77:ARG:H	13	0.03
(1,3421)	1:B:63:MET:HE3	1:B:77:ARG:H	13	0.03
(1,3421)	1:B:63:MET:HE1	1:B:77:ARG:H	17	0.03
(1,3421)	1:B:63:MET:HE2	1:B:77:ARG:H	17	0.03
(1,3421)	1:B:63:MET:HE3	1:B:77:ARG:H	17	0.03
(1,3420)	1:A:63:MET:HE1	1:A:77:ARG:H	8	0.03
(1,3420)	1:A:63:MET:HE2	1:A:77:ARG:H	8	0.03
(1,3420)	1:A:63:MET:HE3	1:A:77:ARG:H	8	0.03
(1,3420)	1:A:63:MET:HE1	1:A:77:ARG:H	16	0.03
(1,3420)	1:A:63:MET:HE2	1:A:77:ARG:H	16	0.03
(1,3420)	1:A:63:MET:HE3	1:A:77:ARG:H	16	0.03
(1,342)	1:A:21:GLN:HE22	1:A:69:VAL:HG11	10	0.03
(1,342)	1:A:21:GLN:HE22	1:A:69:VAL:HG12	10	0.03
(1,342)	1:A:21:GLN:HE22	1:A:69:VAL:HG13	10	0.03
(1,3413)	1:B:63:MET:HE1	1:B:76:GLU:HA	11	0.03
(1,3413)	1:B:63:MET:HE2	1:B:76:GLU:HA	11	0.03
(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	11	0.03
(1,3412)	1:A:63:MET:HE1	1:A:76:GLU:HA	2	0.03
(1,3412)	1:A:63:MET:HE2	1:A:76:GLU:HA	2	0.03
(1,3412)	1:A:63:MET:HE3	1:A:76:GLU:HA	2	0.03
(1,3412)	1:A:63:MET:HE1	1:A:76:GLU:HA	10	0.03
(1,3412)	1:A:63:MET:HE2	1:A:76:GLU:HA	10	0.03
(1,3412)	1:A:63:MET:HE3	1:A:76:GLU:HA	10	0.03
(1,3411)	1:B:63:MET:HE1	1:B:77:ARG:HA	17	0.03
(1,3411)	1:B:63:MET:HE2	1:B:77:ARG:HA	17	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3411)	1:B:63:MET:HE3	1:B:77:ARG:HA	17	0.03
(1,3410)	1:A:63:MET:HE1	1:A:77:ARG:HA	13	0.03
(1,3410)	1:A:63:MET:HE2	1:A:77:ARG:HA	13	0.03
(1,3410)	1:A:63:MET:HE3	1:A:77:ARG:HA	13	0.03
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE1	18	0.03
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE2	18	0.03
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE3	18	0.03
(1,3287)	1:A:61:THR:HG21	1:A:65:LYS:HE2	10	0.03
(1,3287)	1:A:61:THR:HG21	1:A:65:LYS:HE3	10	0.03
(1,3287)	1:A:61:THR:HG22	1:A:65:LYS:HE2	10	0.03
(1,3287)	1:A:61:THR:HG22	1:A:65:LYS:HE3	10	0.03
(1,3287)	1:A:61:THR:HG23	1:A:65:LYS:HE2	10	0.03
(1,3287)	1:A:61:THR:HG23	1:A:65:LYS:HE3	10	0.03
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD21	19	0.03
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD22	19	0.03
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD23	19	0.03
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD21	19	0.03
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD22	19	0.03
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD23	19	0.03
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD21	19	0.03
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD22	19	0.03
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD23	19	0.03
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD21	20	0.03
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD22	20	0.03
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD23	20	0.03
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD21	20	0.03
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD22	20	0.03
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD23	20	0.03
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD21	20	0.03
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD22	20	0.03
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD23	20	0.03
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD11	18	0.03
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD12	18	0.03
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD13	18	0.03
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD11	18	0.03
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD12	18	0.03
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD13	18	0.03
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD11	18	0.03
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD12	18	0.03
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD13	18	0.03
(1,3185)	1:A:58:LYS:H	1:A:58:LYS:HD2	7	0.03
(1,3185)	1:A:58:LYS:H	1:A:58:LYS:HD3	7	0.03



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Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG21	17	0.03
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG22	17	0.03
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG23	17	0.03
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG21	17	0.03
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG22	17	0.03
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG23	17	0.03
(1,3105)	1:A:54:LYS:H	1:A:54:LYS:HE2	7	0.03
(1,3105)	1:A:54:LYS:H	1:A:54:LYS:HE3	7	0.03
(1,3098)	1:B:15:LYS:HD2	1:B:16:ASN:HD21	14	0.03
(1,3098)	1:B:15:LYS:HD3	1:B:16:ASN:HD21	14	0.03
(1,3097)	1:A:15:LYS:HD2	1:A:16:ASN:HD21	20	0.03
(1,3097)	1:A:15:LYS:HD3	1:A:16:ASN:HD21	20	0.03
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD2	9	0.03
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD3	9	0.03
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD2	16	0.03
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD3	16	0.03
(1,3091)	1:A:54:LYS:HA	1:A:54:LYS:HD2	2	0.03
(1,3091)	1:A:54:LYS:HA	1:A:54:LYS:HD3	2	0.03
(1,3091)	1:A:54:LYS:HA	1:A:54:LYS:HD2	3	0.03
(1,3091)	1:A:54:LYS:HA	1:A:54:LYS:HD3	3	0.03
(1,3091)	1:A:54:LYS:HA	1:A:54:LYS:HD2	5	0.03
(1,3091)	1:A:54:LYS:HA	1:A:54:LYS:HD3	5	0.03
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG11	16	0.03
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG12	16	0.03
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG13	16	0.03
(1,3006)	1:B:53:VAL:HG11	1:B:55:ASN:H	20	0.03
(1,3006)	1:B:53:VAL:HG12	1:B:55:ASN:H	20	0.03
(1,3006)	1:B:53:VAL:HG13	1:B:55:ASN:H	20	0.03
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	2	0.03
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	2	0.03
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	2	0.03
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	2	0.03
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	2	0.03
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	2	0.03
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG11	3	0.03
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG12	3	0.03
(1,2990)	1:B:4:PHE:HB2	1:B:53:VAL:HG13	3	0.03
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG11	3	0.03
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG12	3	0.03
(1,2990)	1:B:4:PHE:HB3	1:B:53:VAL:HG13	3	0.03
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	5	0.03
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	5	0.03



 $Continued\ from\ previous\ page...$

Key	$egin{aligned} Atom-1 \end{aligned}$	Atom-2	Model	Violation (Å)
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	5	0.03
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	5	0.03
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	5	0.03
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	5	0.03
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD11	1	0.03
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD12	1	0.03
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD13	1	0.03
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD11	15	0.03
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD12	15	0.03
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD13	15	0.03
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	12	0.03
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	12	0.03
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	12	0.03
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	12	0.03
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	12	0.03
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	12	0.03
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	12	0.03
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	12	0.03
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	12	0.03
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	17	0.03
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	17	0.03
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	17	0.03
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	17	0.03
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	17	0.03
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	17	0.03
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	17	0.03
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	17	0.03
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	17	0.03
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD11	6	0.03
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD12	6	0.03
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD13	6	0.03
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD11	6	0.03
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD12	6	0.03
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD13	6	0.03
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD11	8	0.03
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD12	8	0.03
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD13	8	0.03
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD11	8	0.03
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD12	8	0.03
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD13	8	0.03
(1,2924)	1:B:51:ILE:HD11	1:B:62:LEU:HD21	17	0.03
(1,2924)	1:B:51:ILE:HD11	1:B:62:LEU:HD22	17	0.03



 $Continued\ from\ previous\ page...$

Key	$egin{aligned} ext{Atom-1} \end{aligned}$	Atom-2	Model	Violation (Å)
(1,2924)	1:B:51:ILE:HD11	1:B:62:LEU:HD23	17	0.03
(1,2924)	1:B:51:ILE:HD12	1:B:62:LEU:HD21	17	0.03
(1,2924)	1:B:51:ILE:HD12	1:B:62:LEU:HD22	17	0.03
(1,2924)	1:B:51:ILE:HD12	1:B:62:LEU:HD23	17	0.03
(1,2924)	1:B:51:ILE:HD13	1:B:62:LEU:HD21	17	0.03
(1,2924)	1:B:51:ILE:HD13	1:B:62:LEU:HD22	17	0.03
(1,2924)	1:B:51:ILE:HD13	1:B:62:LEU:HD23	17	0.03
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG21	5	0.03
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG22	5	0.03
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG23	5	0.03
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG21	18	0.03
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG22	18	0.03
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG23	18	0.03
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG21	7	0.03
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG22	7	0.03
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG23	7	0.03
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG21	12	0.03
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG22	12	0.03
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG23	12	0.03
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD11	7	0.03
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD12	7	0.03
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD13	7	0.03
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD11	7	0.03
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD12	7	0.03
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD13	7	0.03
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD11	7	0.03
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD12	7	0.03
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD13	7	0.03
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD11	13	0.03
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD12	13	0.03
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD13	13	0.03
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD11	13	0.03
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD12	13	0.03
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD13	13	0.03
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD11	13	0.03
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD12	13	0.03
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD13	13	0.03
(1,2816)	1:B:50:MET:HE1	1:B:51:ILE:HG13	1	0.03
(1,2816)	1:B:50:MET:HE2	1:B:51:ILE:HG13	1	0.03
(1,2816)	1:B:50:MET:HE3	1:B:51:ILE:HG13	1	0.03
(1,2816)	1:B:50:MET:HE1	1:B:51:ILE:HG13	4	0.03
(1,2816)	1:B:50:MET:HE2	1:B:51:ILE:HG13	4	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2816)	1:B:50:MET:HE3	1:B:51:ILE:HG13	4	0.03
(1,2816)	1:B:50:MET:HE1	1:B:51:ILE:HG13	7	0.03
(1,2816)	1:B:50:MET:HE2	1:B:51:ILE:HG13	7	0.03
(1,2816)	1:B:50:MET:HE3	1:B:51:ILE:HG13	7	0.03
(1,2816)	1:B:50:MET:HE1	1:B:51:ILE:HG13	14	0.03
(1,2816)	1:B:50:MET:HE2	1:B:51:ILE:HG13	14	0.03
(1,2816)	1:B:50:MET:HE3	1:B:51:ILE:HG13	14	0.03
(1,2816)	1:B:50:MET:HE1	1:B:51:ILE:HG13	19	0.03
(1,2816)	1:B:50:MET:HE2	1:B:51:ILE:HG13	19	0.03
(1,2816)	1:B:50:MET:HE3	1:B:51:ILE:HG13	19	0.03
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	8	0.03
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	8	0.03
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	8	0.03
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	15	0.03
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	15	0.03
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	15	0.03
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	20	0.03
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	20	0.03
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	20	0.03
(1,2792)	1:B:8:ILE:H	1:B:50:MET:HG3	3	0.03
(1,2792)	1:B:8:ILE:H	1:B:50:MET:HG3	9	0.03
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	10	0.03
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	12	0.03
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	16	0.03
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	20	0.03
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	8	0.03
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	15	0.03
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD21	2	0.03
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD22	2	0.03
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD23	2	0.03
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD21	2	0.03
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD22	2	0.03
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD23	2	0.03
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD21	2	0.03
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD22	2	0.03
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD23	2	0.03
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD21	14	0.03
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD22	14	0.03
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD23	14	0.03
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD21	14	0.03
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD22	14	0.03
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD23	14	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD21	14	0.03
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD22	14	0.03
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD23	14	0.03
(1,2668)	1:B:23:THR:HG1	1:B:47:CYS:HB3	7	0.03
(1,2667)	1:A:23:THR:HG1	1:A:47:CYS:HB3	14	0.03
(1,2667)	1:A:23:THR:HG1	1:A:47:CYS:HB3	20	0.03
(1,2640)	1:B:46:THR:HG21	1:B:47:CYS:H	19	0.03
(1,2640)	1:B:46:THR:HG22	1:B:47:CYS:H	19	0.03
(1,2640)	1:B:46:THR:HG23	1:B:47:CYS:H	19	0.03
(1,2639)	1:A:46:THR:HG21	1:A:47:CYS:H	13	0.03
(1,2639)	1:A:46:THR:HG22	1:A:47:CYS:H	13	0.03
(1,2639)	1:A:46:THR:HG23	1:A:47:CYS:H	13	0.03
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG21	8	0.03
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG22	8	0.03
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG23	8	0.03
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	10	0.03
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	10	0.03
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	10	0.03
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	14	0.03
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	14	0.03
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	14	0.03
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD11	4	0.03
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD12	4	0.03
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD13	4	0.03
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD11	8	0.03
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD12	8	0.03
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD13	8	0.03
(1,2591)	1:A:44:ILE:HD11	1:A:73:PHE:HZ	4	0.03
(1,2591)	1:A:44:ILE:HD12	1:A:73:PHE:HZ	4	0.03
(1,2591)	1:A:44:ILE:HD13	1:A:73:PHE:HZ	4	0.03
(1,2586)	1:B:13:GLU:HA	1:B:44:ILE:HD11	1	0.03
(1,2586)	1:B:13:GLU:HA	1:B:44:ILE:HD12	1	0.03
(1,2586)	1:B:13:GLU:HA	1:B:44:ILE:HD13	1	0.03
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD11	1	0.03
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD12	1	0.03
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD13	1	0.03
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD11	14	0.03
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD12	14	0.03
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD13	14	0.03
(1,2584)	1:B:44:ILE:HD11	1:B:46:THR:HB	3	0.03
(1,2584)	1:B:44:ILE:HD12	1:B:46:THR:HB	3	0.03
(1,2584)	1:B:44:ILE:HD13	1:B:46:THR:HB	3	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2583)	1:A:44:ILE:HD11	1:A:46:THR:HB	3	0.03
(1,2583)	1:A:44:ILE:HD12	1:A:46:THR:HB	3	0.03
(1,2583)	1:A:44:ILE:HD13	1:A:46:THR:HB	3	0.03
(1,2583)	1:A:44:ILE:HD11	1:A:46:THR:HB	8	0.03
(1,2583)	1:A:44:ILE:HD12	1:A:46:THR:HB	8	0.03
(1,2583)	1:A:44:ILE:HD13	1:A:46:THR:HB	8	0.03
(1,2576)	1:B:44:ILE:HG21	1:B:45:PHE:H	7	0.03
(1,2576)	1:B:44:ILE:HG22	1:B:45:PHE:H	7	0.03
(1,2576)	1:B:44:ILE:HG23	1:B:45:PHE:H	7	0.03
(1,2575)	1:A:44:ILE:HG21	1:A:45:PHE:H	2	0.03
(1,2575)	1:A:44:ILE:HG22	1:A:45:PHE:H	2	0.03
(1,2575)	1:A:44:ILE:HG23	1:A:45:PHE:H	2	0.03
(1,2571)	1:A:14:ASP:H	1:A:44:ILE:HG21	7	0.03
(1,2571)	1:A:14:ASP:H	1:A:44:ILE:HG22	7	0.03
(1,2571)	1:A:14:ASP:H	1:A:44:ILE:HG23	7	0.03
(1,2525)	1:A:13:GLU:HA	1:A:44:ILE:HB	7	0.03
(1,2524)	1:B:14:ASP:HB3	1:B:43:GLY:HA3	19	0.03
(1,2486)	1:B:40:ALA:HA	1:B:45:PHE:HA	3	0.03
(1,2485)	1:A:40:ALA:HA	1:A:45:PHE:HA	20	0.03
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD21	5	0.03
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD22	5	0.03
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD23	5	0.03
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD21	9	0.03
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD22	9	0.03
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD23	9	0.03
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD21	15	0.03
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD22	15	0.03
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD23	15	0.03
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD21	2	0.03
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD22	2	0.03
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD23	2	0.03
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD21	8	0.03
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD22	8	0.03
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD23	8	0.03
(1,2432)	1:A:38:LEU:HD21	1:B:35:THR:HG21	5	0.03
(1,2432)	1:A:38:LEU:HD21	1:B:35:THR:HG22	5	0.03
(1,2432)	1:A:38:LEU:HD21	1:B:35:THR:HG23	5	0.03
(1,2432)	1:A:38:LEU:HD22	1:B:35:THR:HG21	5	0.03
(1,2432)	1:A:38:LEU:HD22	1:B:35:THR:HG22	5	0.03
(1,2432)	1:A:38:LEU:HD22	1:B:35:THR:HG23	5	0.03
(1,2432)	1:A:38:LEU:HD23	1:B:35:THR:HG21	5	0.03
(1,2432)	1:A:38:LEU:HD23	1:B:35:THR:HG22	5	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2432)	1:A:38:LEU:HD23	1:B:35:THR:HG23	5	0.03
(1,2432)	1:A:38:LEU:HD21	1:B:35:THR:HG21	19	0.03
(1,2432)	1:A:38:LEU:HD21	1:B:35:THR:HG22	19	0.03
(1,2432)	1:A:38:LEU:HD21	1:B:35:THR:HG23	19	0.03
(1,2432)	1:A:38:LEU:HD22	1:B:35:THR:HG21	19	0.03
(1,2432)	1:A:38:LEU:HD22	1:B:35:THR:HG22	19	0.03
(1,2432)	1:A:38:LEU:HD22	1:B:35:THR:HG23	19	0.03
(1,2432)	1:A:38:LEU:HD23	1:B:35:THR:HG21	19	0.03
(1,2432)	1:A:38:LEU:HD23	1:B:35:THR:HG22	19	0.03
(1,2432)	1:A:38:LEU:HD23	1:B:35:THR:HG23	19	0.03
(1,2424)	1:B:38:LEU:HD11	1:B:39:ASN:H	5	0.03
(1,2424)	1:B:38:LEU:HD12	1:B:39:ASN:H	5	0.03
(1,2424)	1:B:38:LEU:HD13	1:B:39:ASN:H	5	0.03
(1,2424)	1:B:38:LEU:HD11	1:B:39:ASN:H	8	0.03
(1,2424)	1:B:38:LEU:HD12	1:B:39:ASN:H	8	0.03
(1,2424)	1:B:38:LEU:HD13	1:B:39:ASN:H	8	0.03
(1,2424)	1:B:38:LEU:HD11	1:B:39:ASN:H	9	0.03
(1,2424)	1:B:38:LEU:HD12	1:B:39:ASN:H	9	0.03
(1,2424)	1:B:38:LEU:HD13	1:B:39:ASN:H	9	0.03
(1,2423)	1:A:38:LEU:HD11	1:A:39:ASN:H	10	0.03
(1,2423)	1:A:38:LEU:HD12	1:A:39:ASN:H	10	0.03
(1,2423)	1:A:38:LEU:HD13	1:A:39:ASN:H	10	0.03
(1,2400)	1:B:38:LEU:HD11	1:B:47:CYS:HG	6	0.03
(1,2400)	1:B:38:LEU:HD12	1:B:47:CYS:HG	6	0.03
(1,2400)	1:B:38:LEU:HD13	1:B:47:CYS:HG	6	0.03
(1,2400)	1:B:38:LEU:HD11	1:B:47:CYS:HG	8	0.03
(1,2400)	1:B:38:LEU:HD12	1:B:47:CYS:HG	8	0.03
(1,2400)	1:B:38:LEU:HD13	1:B:47:CYS:HG	8	0.03
(1,2388)	1:B:37:VAL:HG21	1:B:38:LEU:H	7	0.03
(1,2388)	1:B:37:VAL:HG22	1:B:38:LEU:H	7	0.03
(1,2388)	1:B:37:VAL:HG23	1:B:38:LEU:H	7	0.03
(1,2387)	1:A:37:VAL:HG21	1:A:38:LEU:H	7	0.03
(1,2387)	1:A:37:VAL:HG22	1:A:38:LEU:H	7	0.03
(1,2387)	1:A:37:VAL:HG23	1:A:38:LEU:H	7	0.03
(1,2379)	1:A:37:VAL:HG21	1:A:48:ASN:HD22	3	0.03
(1,2379)	1:A:37:VAL:HG22	1:A:48:ASN:HD22	3	0.03
(1,2379)	1:A:37:VAL:HG23	1:A:48:ASN:HD22	3	0.03
(1,235)	1:B:15:LYS:HG2	1:B:19:THR:H	2	0.03
(1,235)	1:B:15:LYS:HG3	1:B:19:THR:H	2	0.03
(1,235)	1:B:15:LYS:HG2	1:B:19:THR:H	8	0.03
(1,235)	1:B:15:LYS:HG3	1:B:19:THR:H	8	0.03
(1,2346)	1:B:37:VAL:HG11	1:B:48:ASN:HB3	8	0.03



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(1.9246)		$\mathbf{Atom-2}$	Model	Violation (Å)
(1,4040)	1:B:37:VAL:HG12	1:B:48:ASN:HB3	8	0.03
(1,2346)	1:B:37:VAL:HG13	1:B:48:ASN:HB3	8	0.03
(1,234)	1:A:15:LYS:HG2	1:A:19:THR:H	1	0.03
(1,234)	1:A:15:LYS:HG3	1:A:19:THR:H	1	0.03
(1,234)	1:A:15:LYS:HG2	1:A:19:THR:H	20	0.03
(1,234)	1:A:15:LYS:HG3	1:A:19:THR:H	20	0.03
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD11	1	0.03
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD12	1	0.03
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD13	1	0.03
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	7	0.03
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	7	0.03
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	7	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	4	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	4	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	4	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	8	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	8	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	8	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	14	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	14	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	14	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	16	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	16	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	16	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	18	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	18	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	18	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	19	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	19	0.03
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	19	0.03
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	5	0.03
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	5	0.03
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	5	0.03
(1,2282)	1:B:36:ILE:HG21	1:B:37:VAL:HB	2	0.03
(1,2282)	1:B:36:ILE:HG22	1:B:37:VAL:HB	2	0.03
(1,2282)	1:B:36:ILE:HG23	1:B:37:VAL:HB	2	0.03
(1,2281)	1:A:36:ILE:HG21	1:A:37:VAL:HB	5	0.03
(1,2281)	1:A:36:ILE:HG22	1:A:37:VAL:HB	5	0.03
(1,2281)	1:A:36:ILE:HG23	1:A:37:VAL:HB	5	0.03
(1,2258)	1:B:35:THR:HB	1:B:50:MET:HB2	6	0.03
(1,2258)	1:B:35:THR:HB	1:B:50:MET:HB2	10	0.03
(1,2257)	1:A:35:THR:HB	1:A:50:MET:HB2	11	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2248)	1:B:33:ILE:HD11	1:B:34:ARG:H	15	0.03
(1,2248)	1:B:33:ILE:HD12	1:B:34:ARG:H	15	0.03
(1,2248)	1:B:33:ILE:HD13	1:B:34:ARG:H	15	0.03
(1,2247)	1:A:33:ILE:HD11	1:A:34:ARG:H	11	0.03
(1,2247)	1:A:33:ILE:HD12	1:A:34:ARG:H	11	0.03
(1,2247)	1:A:33:ILE:HD13	1:A:34:ARG:H	11	0.03
(1,2243)	1:A:20:ASN:HD21	1:B:33:ILE:HD11	13	0.03
(1,2243)	1:A:20:ASN:HD21	1:B:33:ILE:HD12	13	0.03
(1,2243)	1:A:20:ASN:HD21	1:B:33:ILE:HD13	13	0.03
(1,2188)	1:B:31:THR:HG21	1:B:51:ILE:HD11	19	0.03
(1,2188)	1:B:31:THR:HG21	1:B:51:ILE:HD12	19	0.03
(1,2188)	1:B:31:THR:HG21	1:B:51:ILE:HD13	19	0.03
(1,2188)	1:B:31:THR:HG22	1:B:51:ILE:HD11	19	0.03
(1,2188)	1:B:31:THR:HG22	1:B:51:ILE:HD12	19	0.03
(1,2188)	1:B:31:THR:HG22	1:B:51:ILE:HD13	19	0.03
(1,2188)	1:B:31:THR:HG23	1:B:51:ILE:HD11	19	0.03
(1,2188)	1:B:31:THR:HG23	1:B:51:ILE:HD12	19	0.03
(1,2188)	1:B:31:THR:HG23	1:B:51:ILE:HD13	19	0.03
(1,2182)	1:B:29:PHE:HD1	1:B:31:THR:HB	15	0.03
(1,2182)	1:B:29:PHE:HD2	1:B:31:THR:HB	15	0.03
(1,2181)	1:A:29:PHE:HD1	1:A:31:THR:HB	9	0.03
(1,2181)	1:A:29:PHE:HD2	1:A:31:THR:HB	9	0.03
(1,2181)	1:A:29:PHE:HD1	1:A:31:THR:HB	11	0.03
(1,2181)	1:A:29:PHE:HD2	1:A:31:THR:HB	11	0.03
(1,2181)	1:A:29:PHE:HD1	1:A:31:THR:HB	18	0.03
(1,2181)	1:A:29:PHE:HD2	1:A:31:THR:HB	18	0.03
(1,2176)	1:B:25:VAL:HA	1:B:28:LYS:HE2	2	0.03
(1,2176)	1:B:25:VAL:HA	1:B:28:LYS:HE3	2	0.03
(1,2175)	1:A:25:VAL:HA	1:A:28:LYS:HE2	8	0.03
(1,2175)	1:A:25:VAL:HA	1:A:28:LYS:HE3	8	0.03
(1,217)	1:B:18:MET:H	1:B:18:MET:HG3	3	0.03
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	8	0.03
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	8	0.03
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	8	0.03
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	14	0.03
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	14	0.03
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	14	0.03
(1,2099)	1:A:25:VAL:HG21	1:A:29:PHE:HD1	13	0.03
(1,2099)	1:A:25:VAL:HG21	1:A:29:PHE:HD2	13	0.03
(1,2099)	1:A:25:VAL:HG22	1:A:29:PHE:HD1	13	0.03
(1,2099)	1:A:25:VAL:HG22	1:A:29:PHE:HD2	13	0.03
(1,2099)	1:A:25:VAL:HG23	1:A:29:PHE:HD1	13	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
	1:A:25:VAL:HG23	1:A:29:PHE:HD2	13	0.03
(1,2088)	1:B:25:VAL:HG11	1:B:27:SER:H	3	0.03
(1,2088)	1:B:25:VAL:HG12	1:B:27:SER:H	3	0.03
(1,2088)	1:B:25:VAL:HG13	1:B:27:SER:H	3	0.03
(1,2088)	1:B:25:VAL:HG11	1:B:27:SER:H	19	0.03
(1,2088)	1:B:25:VAL:HG12	1:B:27:SER:H	19	0.03
(1,2088)	1:B:25:VAL:HG13	1:B:27:SER:H	19	0.03
(1,2087)	1:A:25:VAL:HG11	1:A:27:SER:H	10	0.03
(1,2087)	1:A:25:VAL:HG12	1:A:27:SER:H	10	0.03
(1,2087)	1:A:25:VAL:HG13	1:A:27:SER:H	10	0.03
(1,2087)	1:A:25:VAL:HG11	1:A:27:SER:H	19	0.03
(1,2087)	1:A:25:VAL:HG12	1:A:27:SER:H	19	0.03
(1,2087)	1:A:25:VAL:HG13	1:A:27:SER:H	19	0.03
(1,208)	1:B:16:ASN:HA	1:B:17:GLY:H	3	0.03
(1,208)	1:B:16:ASN:HA	1:B:17:GLY:H	9	0.03
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	9	0.03
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	9	0.03
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	9	0.03
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	13	0.03
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	13	0.03
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	13	0.03
(1,2007)	1:A:22:ILE:HD11	1:A:69:VAL:HG21	20	0.03
(1,2007)	1:A:22:ILE:HD11	1:A:69:VAL:HG22	20	0.03
(1,2007)	1:A:22:ILE:HD11	1:A:69:VAL:HG23	20	0.03
(1,2007)	1:A:22:ILE:HD12	1:A:69:VAL:HG21	20	0.03
(1,2007)	1:A:22:ILE:HD12	1:A:69:VAL:HG22	20	0.03
(1,2007)	1:A:22:ILE:HD12	1:A:69:VAL:HG23	20	0.03
(1,2007)	1:A:22:ILE:HD13	1:A:69:VAL:HG21	20	0.03
(1,2007)	1:A:22:ILE:HD13	1:A:69:VAL:HG22	20	0.03
(1,2007)	1:A:22:ILE:HD13	1:A:69:VAL:HG23	20	0.03
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	5	0.03
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	5	0.03
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	5	0.03
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	10	0.03
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	10	0.03
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	10	0.03
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	11	0.03
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	11	0.03
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	11	0.03
(1,1970)	1:A:20:ASN:H	1:A:22:ILE:HG13	12	0.03
(1,1936)	1:A:19:THR:HG21	1:A:22:ILE:HB	13	0.03
(1,1936)	1:A:19:THR:HG22	1:A:22:ILE:HB	13	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1936)	1:A:19:THR:HG23	1:A:22:ILE:HB	13	0.03
	1:A:18:MET:HE1	1:A:71:GLY:HA2	8	0.03
(1,1860)	1:A:18:MET:HE2	1:A:71:GLY:HA2	8	0.03
(1,1860)	1:A:18:MET:HE3	1:A:71:GLY:HA2	8	0.03
(1,1860)	1:A:18:MET:HE1	1:A:71:GLY:HA2	11	0.03
(1,1860)	1:A:18:MET:HE2	1:A:71:GLY:HA2	11	0.03
(1,1860)	1:A:18:MET:HE3	1:A:71:GLY:HA2	11	0.03
(1,181)	1:A:15:LYS:H	1:A:44:ILE:HA	19	0.03
(1,1809)	1:B:11:VAL:HG21	1:B:41:LYS:HE2	4	0.03
(1,1809)	1:B:11:VAL:HG21	1:B:41:LYS:HE3	4	0.03
(1,1809)	1:B:11:VAL:HG22	1:B:41:LYS:HE2	4	0.03
(1,1809)	1:B:11:VAL:HG22	1:B:41:LYS:HE3	4	0.03
(1,1809)	1:B:11:VAL:HG23	1:B:41:LYS:HE2	4	0.03
(1,1809)	1:B:11:VAL:HG23	1:B:41:LYS:HE3	4	0.03
(1,1797)	1:B:15:LYS:HG2	1:B:18:MET:HE1	1	0.03
(1,1797)	1:B:15:LYS:HG2	1:B:18:MET:HE2	1	0.03
(1,1797)	1:B:15:LYS:HG2	1:B:18:MET:HE3	1	0.03
(1,1797)	1:B:15:LYS:HG3	1:B:18:MET:HE1	1	0.03
(1,1797)	1:B:15:LYS:HG3	1:B:18:MET:HE2	1	0.03
(1,1797)	1:B:15:LYS:HG3	1:B:18:MET:HE3	1	0.03
(1,1797)	1:B:15:LYS:HG2	1:B:18:MET:HE1	9	0.03
(1,1797)	1:B:15:LYS:HG2	1:B:18:MET:HE2	9	0.03
(1,1797)	1:B:15:LYS:HG2	1:B:18:MET:HE3	9	0.03
(1,1797)	1:B:15:LYS:HG3	1:B:18:MET:HE1	9	0.03
(1,1797)	1:B:15:LYS:HG3	1:B:18:MET:HE2	9	0.03
(1,1797)	1:B:15:LYS:HG3	1:B:18:MET:HE3	9	0.03
(1,1793)	1:B:15:LYS:HB3	1:B:16:ASN:HB2	2	0.03
(1,1775)	1:B:13:GLU:HG2	1:B:44:ILE:HA	11	0.03
(1,1775)	1:B:13:GLU:HG3	1:B:44:ILE:HA	11	0.03
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG11	17	0.03
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG12	17	0.03
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG13	17	0.03
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG11	17	0.03
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG12	17	0.03
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG13	17	0.03
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG11	15	0.03
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG12	15	0.03
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG13	15	0.03
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG11	15	0.03
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG12	15	0.03
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG13	15	0.03
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG11	18	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG12	18	0.03
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG13	18	0.03
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG11	18	0.03
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG12	18	0.03
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG13	18	0.03
(1,175)	1:A:15:LYS:H	1:A:18:MET:HG2	20	0.03
(1,171)	1:A:13:GLU:HG2	1:A:15:LYS:H	6	0.03
(1,171)	1:A:13:GLU:HG3	1:A:15:LYS:H	6	0.03
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	2	0.03
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	2	0.03
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	2	0.03
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	15	0.03
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	15	0.03
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	15	0.03
(1,1690)	1:A:11:VAL:HG21	1:A:46:THR:HB	5	0.03
(1,1690)	1:A:11:VAL:HG22	1:A:46:THR:HB	5	0.03
(1,1690)	1:A:11:VAL:HG23	1:A:46:THR:HB	5	0.03
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	13	0.03
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	13	0.03
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	13	0.03
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	13	0.03
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	13	0.03
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG23	13	0.03
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	13	0.03
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	13	0.03
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	13	0.03
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	16	0.03
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	16	0.03
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	16	0.03
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	16	0.03
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	16	0.03
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG23	16	0.03
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	16	0.03
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	16	0.03
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	16	0.03
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	17	0.03
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	17	0.03
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	17	0.03
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	17	0.03
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	17	0.03
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG23	17	0.03
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	17	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	17	0.03
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	17	0.03
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG21	6	0.03
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG22	6	0.03
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG23	6	0.03
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG21	6	0.03
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG22	6	0.03
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG23	6	0.03
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG21	6	0.03
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG22	6	0.03
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG23	6	0.03
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG21	7	0.03
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG22	7	0.03
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG23	7	0.03
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG21	7	0.03
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG22	7	0.03
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG23	7	0.03
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG21	7	0.03
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG22	7	0.03
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG23	7	0.03
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG21	9	0.03
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG22	9	0.03
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG23	9	0.03
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG21	9	0.03
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG22	9	0.03
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG23	9	0.03
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG21	9	0.03
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG22	9	0.03
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG23	9	0.03
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG21	11	0.03
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG22	11	0.03
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG23	11	0.03
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG21	11	0.03
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG22	11	0.03
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG23	11	0.03
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG21	11	0.03
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG22	11	0.03
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG23	11	0.03
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG21	20	0.03
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG22	20	0.03
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG23	20	0.03
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG21	20	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG22	20	0.03
, ,	1:A:11:VAL:HG22	1:A:46:THR:HG23	20	0.03
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG21	20	0.03
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG22	20	0.03
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG23	20	0.03
(1,167)	1:A:15:LYS:H	1:A:18:MET:HE1	5	0.03
(1,167)	1:A:15:LYS:H	1:A:18:MET:HE2	5	0.03
(1,167)	1:A:15:LYS:H	1:A:18:MET:HE3	5	0.03
(1,1666)	1:A:10:ILE:HD11	1:A:11:VAL:H	4	0.03
(1,1666)	1:A:10:ILE:HD12	1:A:11:VAL:H	4	0.03
(1,1666)	1:A:10:ILE:HD13	1:A:11:VAL:H	4	0.03
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD11	7	0.03
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD12	7	0.03
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD13	7	0.03
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD11	10	0.03
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD12	10	0.03
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD13	10	0.03
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD11	12	0.03
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD12	12	0.03
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD13	12	0.03
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD11	14	0.03
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD12	14	0.03
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD13	14	0.03
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD11	3	0.03
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD12	3	0.03
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD13	3	0.03
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD11	18	0.03
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD12	18	0.03
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD13	18	0.03
(1,1577)	1:B:9:ARG:HD2	1:B:11:VAL:HB	14	0.03
(1,1577)	1:B:9:ARG:HD3	1:B:11:VAL:HB	14	0.03
(1,1576)	1:A:9:ARG:HD2	1:A:11:VAL:HB	12	0.03
(1,1576)	1:A:9:ARG:HD3	1:A:11:VAL:HB	12	0.03
(1,1576)	1:A:9:ARG:HD2	1:A:11:VAL:HB	19	0.03
(1,1576)	1:A:9:ARG:HD3	1:A:11:VAL:HB	19	0.03
(1,1572)	1:B:9:ARG:HG3	1:B:10:ILE:H	6	0.03
(1,1558)	1:B:24:GLY:H	1:B:26:ILE:HD11	9	0.03
(1,1558)	1:B:24:GLY:H	1:B:26:ILE:HD12	9	0.03
(1,1558)	1:B:24:GLY:H	1:B:26:ILE:HD13	9	0.03
(1,1551)	1:A:8:ILE:HD11	1:A:77:ARG:HA	7	0.03
(1,1551)	1:A:8:ILE:HD12	1:A:77:ARG:HA	7	0.03
(1,1551)	1:A:8:ILE:HD13	1:A:77:ARG:HA	7	0.03



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Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	1	0.03
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	1	0.03
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	1	0.03
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	1	0.03
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	1	0.03
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	1	0.03
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	1	0.03
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	1	0.03
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	1	0.03
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	5	0.03
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	5	0.03
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	5	0.03
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	5	0.03
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	5	0.03
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	5	0.03
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	5	0.03
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	5	0.03
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	5	0.03
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	3	0.03
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	3	0.03
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	3	0.03
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	3	0.03
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	3	0.03
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	3	0.03
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	3	0.03
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	3	0.03
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	3	0.03
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	5	0.03
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	5	0.03
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	5	0.03
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	5	0.03
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	5	0.03
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	5	0.03
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	5	0.03
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	5	0.03
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	5	0.03
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	6	0.03
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	6	0.03
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	6	0.03
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	6	0.03
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	6	0.03
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	6	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	14	0.03
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	14	0.03
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	14	0.03
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	14	0.03
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	14	0.03
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	14	0.03
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	3	0.03
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	3	0.03
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	3	0.03
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	3	0.03
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	3	0.03
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	3	0.03
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	6	0.03
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	6	0.03
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	6	0.03
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	6	0.03
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	6	0.03
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	6	0.03
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	9	0.03
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	9	0.03
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	9	0.03
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	9	0.03
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	9	0.03
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	9	0.03
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	12	0.03
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	12	0.03
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	12	0.03
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	12	0.03
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	12	0.03
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	12	0.03
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	17	0.03
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	17	0.03
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	17	0.03
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	17	0.03
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	17	0.03
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	17	0.03
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	19	0.03
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	19	0.03
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	19	0.03
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	19	0.03
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	19	0.03
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	19	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	20	0.03
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	20	0.03
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	20	0.03
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	20	0.03
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	20	0.03
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	20	0.03
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	3	0.03
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	3	0.03
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	3	0.03
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	11	0.03
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	11	0.03
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	11	0.03
(1,1414)	1:B:3:ASP:HB2	1:B:53:VAL:H	18	0.03
(1,1378)	1:B:40:ALA:H	1:B:41:LYS:HD2	1	0.03
(1,1378)	1:B:40:ALA:H	1:B:41:LYS:HD3	1	0.03
(1,1378)	1:B:40:ALA:H	1:B:41:LYS:HD2	4	0.03
(1,1378)	1:B:40:ALA:H	1:B:41:LYS:HD3	4	0.03
(1,1330)	1:B:78:LEU:HD21	1:B:79:SER:H	7	0.03
(1,1330)	1:B:78:LEU:HD22	1:B:79:SER:H	7	0.03
(1,1330)	1:B:78:LEU:HD23	1:B:79:SER:H	7	0.03
(1,1245)	1:A:74:THR:H	1:A:75:VAL:HG21	10	0.03
(1,1245)	1:A:74:THR:H	1:A:75:VAL:HG22	10	0.03
(1,1245)	1:A:74:THR:H	1:A:75:VAL:HG23	10	0.03
(1,1224)	1:B:69:VAL:HG21	1:B:72:VAL:H	3	0.03
(1,1224)	1:B:69:VAL:HG22	1:B:72:VAL:H	3	0.03
(1,1224)	1:B:69:VAL:HG23	1:B:72:VAL:H	3	0.03
(1,1212)	1:B:69:VAL:HG11	1:B:71:GLY:H	11	0.03
(1,1212)	1:B:69:VAL:HG12	1:B:71:GLY:H	11	0.03
(1,1212)	1:B:69:VAL:HG13	1:B:71:GLY:H	11	0.03
(1,1211)	1:A:69:VAL:HG11	1:A:71:GLY:H	14	0.03
(1,1211)	1:A:69:VAL:HG12	1:A:71:GLY:H	14	0.03
(1,1211)	1:A:69:VAL:HG13	1:A:71:GLY:H	14	0.03
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	4	0.03
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	5	0.03
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	9	0.03
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	17	0.03
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	18	0.03
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	20	0.03
(1,1158)	1:B:68:LYS:H	1:B:75:VAL:HG21	7	0.03
(1,1158)	1:B:68:LYS:H	1:B:75:VAL:HG22	7	0.03
(1,1158)	1:B:68:LYS:H	1:B:75:VAL:HG23	7	0.03
(1,1149)	1:A:67:ARG:HE	1:A:75:VAL:HB	3	0.03



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1106)	1:B:62:LEU:HD11	1:B:66:LEU:H	4	0.03
(1,1106)	1:B:62:LEU:HD12	1:B:66:LEU:H	4	0.03
(1,1106)	1:B:62:LEU:HD13	1:B:66:LEU:H	4	0.03
(1,1106)	1:B:62:LEU:HD11	1:B:66:LEU:H	12	0.03
(1,1106)	1:B:62:LEU:HD12	1:B:66:LEU:H	12	0.03
(1,1106)	1:B:62:LEU:HD13	1:B:66:LEU:H	12	0.03
(1,1106)	1:B:62:LEU:HD11	1:B:66:LEU:H	20	0.03
(1,1106)	1:B:62:LEU:HD12	1:B:66:LEU:H	20	0.03
(1,1106)	1:B:62:LEU:HD13	1:B:66:LEU:H	20	0.03
(1,1105)	1:A:62:LEU:HD11	1:A:66:LEU:H	2	0.03
(1,1105)	1:A:62:LEU:HD12	1:A:66:LEU:H	2	0.03
(1,1105)	1:A:62:LEU:HD13	1:A:66:LEU:H	2	0.03
(1,1105)	1:A:62:LEU:HD11	1:A:66:LEU:H	3	0.03
(1,1105)	1:A:62:LEU:HD12	1:A:66:LEU:H	3	0.03
(1,1105)	1:A:62:LEU:HD13	1:A:66:LEU:H	3	0.03
(1,1104)	1:B:62:LEU:HD11	1:B:65:LYS:H	6	0.03
(1,1104)	1:B:62:LEU:HD12	1:B:65:LYS:H	6	0.03
(1,1104)	1:B:62:LEU:HD13	1:B:65:LYS:H	6	0.03
(1,1104)	1:B:62:LEU:HD11	1:B:65:LYS:H	7	0.03
(1,1104)	1:B:62:LEU:HD12	1:B:65:LYS:H	7	0.03
(1,1104)	1:B:62:LEU:HD13	1:B:65:LYS:H	7	0.03
(1,1104)	1:B:62:LEU:HD11	1:B:65:LYS:H	10	0.03
(1,1104)	1:B:62:LEU:HD12	1:B:65:LYS:H	10	0.03
(1,1104)	1:B:62:LEU:HD13	1:B:65:LYS:H	10	0.03
(1,1104)	1:B:62:LEU:HD11	1:B:65:LYS:H	14	0.03
(1,1104)	1:B:62:LEU:HD12	1:B:65:LYS:H	14	0.03
(1,1104)	1:B:62:LEU:HD13	1:B:65:LYS:H	14	0.03
(1,1103)	1:A:62:LEU:HD11	1:A:65:LYS:H	2	0.03
(1,1103)	1:A:62:LEU:HD12	1:A:65:LYS:H	2	0.03
(1,1103)	1:A:62:LEU:HD13	1:A:65:LYS:H	2	0.03
(1,1103)	1:A:62:LEU:HD11	1:A:65:LYS:H	6	0.03
(1,1103)	1:A:62:LEU:HD12	1:A:65:LYS:H	6	0.03
(1,1103)	1:A:62:LEU:HD13	1:A:65:LYS:H	6	0.03
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	2	0.03
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	2	0.03
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	2	0.03
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	19	0.03
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	19	0.03
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	19	0.03
(1,939)	1:B:54:LYS:HE2	1:B:55:ASN:HD22	15	0.02
(1,939)	1:B:54:LYS:HE3	1:B:55:ASN:HD22	15	0.02
(1,909)	1:B:3:ASP:HB3	1:B:53:VAL:H	17	0.02



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(1,908) 1:A:3:ASP:HB3 1:A:53:VAL:H 7 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 1 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 5 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 10 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 10 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 13 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 17 0.02 (1,898) 1:A:51:ILE:HG12 1:B:52:PHE:H 19 0.02 (1,839) 1:B:48:ASN:HD21 1:B:78:LEU:HD21 8 0.02 (1,839) 1:B:48:ASN:HD21 1:B:78:LEU:HD22 8 0.02 (1,839) 1:B:48:ASN:HD21 1:B:78:LEU:HD22 8 0.02 (1,839) 1:B:48:ASN:HD21 1:B:78:LEU:HD23 8 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD23 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD22 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD22 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD23 14 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 18 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 18 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 4 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 4 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 4 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 10 0.02 (1,833) 1:B:9:ARG:HE 1:B:11:VAL:HG21 5 0.02 (1,711) 1:B:44:ILE:H 11 1.A:44:ILE:H 12 1.00 (1,714) 1:B:44:ILE:H 11 1.A:44:ILE:H 12 1.00 (1,714) 1:B:44:ILE:H 11 1.A:44:ILE:H 11 1.A:44:ILE:H 11 1.A:44:ILE:H 11 1.A:44:ILE:H 11 1.A:44:ILE:H 11 1.A:44:ILE:H 11 1.A:44:	Key	Atom-1	Atom-2	Model	Violation (Å)
(1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 5 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 5 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 10 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 17 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 17 0.02 (1,898) 1:B:51:ILE:HG12 1:B:52:PHE:H 17 0.02 (1,898) 1:A:51:ILE:HG12 1:A:52:PHE:H 16 0.02 (1,848) 1:A:51:ILE:HG12 1:A:52:PHE:H 16 0.02 (1,848) 1:A:51:ILE:HG12 1:B:78:LEU:HD21 8 0.02 (1,839) 1:B:48:ASN:HD21 1:B:78:LEU:HD22 8 0.02 (1,839) 1:B:48:ASN:HD21 1:B:78:LEU:HD22 8 0.02 (1,839) 1:B:48:ASN:HD21 1:B:78:LEU:HD23 8 0.02 (1,838) 1:B:48:ASN:HD21 1:A:78:LEU:HD23 8 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD23 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD22 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD22 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD23 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD23 14 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 3 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 4 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 4 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 6 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 10 0.02 (1,833) 1:B:9:ARG:HE 1:B:11:VAL:HG21 5 0.02 (1,833) 1:B:9:ARG:HE 1:B:11:VAL:HG22 5 0.02 (1,83) 1:B:9:ARG:HE 1:B:11:VAL:HG22 5 0.02 (1,83) 1:B:9:ARG:HE 1:B:11:VAL:HG23 5 0.02 (1,771) 1:B:44:ILE:H 1:A:44:ILE:HG23 5 0.02 (1,774) 1:B:44:ILYS:H 1:B:45:PHE:HD1 1 0.02 (1,776) 1:B:41:LYS:H 1:B:45:PHE:HD1 1 0.02	(1,908)	1:A:3:ASP:HB3	1:A:53:VAL:H	7	0.02
(1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 10 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 13 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 17 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 17 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 17 0.02 (1,899) 1:B:51:ILE:HG12 1:A:52:PHE:H 17 0.02 (1,899) 1:B:51:ILE:HG12 1:A:52:PHE:H 17 0.02 (1,840) 1:A:49:ARG:HE 1:A:10:ILE:H 19 0.02 (1,831) 1:B:48:ASN:HD21 1:B:78:LEU:HD21 8 0.02 (1,839) 1:B:48:ASN:HD21 1:B:78:LEU:HD22 8 0.02 (1,839) 1:B:48:ASN:HD21 1:B:78:LEU:HD22 8 0.02 (1,839) 1:B:48:ASN:HD21 1:A:78:LEU:HD23 8 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD23 8 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD23 14 0.02 (1,838) 1:A:47:CYS:HG 1:B:48:ASN:H 18 0.02 (1,832) 1:A:47:CYS:HG 1:B:48:ASN:H 3 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 3 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 4 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 6 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 10 0.02 (1,833) 1:B:9:ARG:HE 1:B:11:VAL:HG21 5 0.02 (1,833) 1:B:9:ARG:HE 1:B:11:VAL:HG23 5 0.02 (1,83) 1:B:9:ARG:HE 1:B:11:VAL:HG23 5 0.02 (1,711) 1:B:44:ILE:HB 1:B:44:ILE:HG21 15 0.02 (1,744) 1:A:44:ILE:HB 1:A:44:ILE:HG21 15 0.02 (1,744) 1:A:44:ILE:H 1:A:44:ILE:HG21 15 0.02 (1,746) 1:B:41:IVS:H 1:B:45:PHE:HD1 1 1 0.02 (1,746) 1:A:41:IVS:H 1:B:45:PHE:HD1 1 1 0.02 (1,746) 1:A:41:IVS:H 1:A:45:PHE:HD1	(1,908)	1:A:3:ASP:HB3	1:A:53:VAL:H	16	0.02
(1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 13 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 17 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 17 0.02 (1,898) 1:A:51:ILE:HG12 1:A:52:PHE:H 16 0.02 (1,84) 1:A:9-ARG:HE 1-A:10:ILE:H 19 0.02 (1,839) 1:B:48:ASN:HD21 1:B:78:LEU:HD21 8 0.02 (1,839) 1:B:48:ASN:HD21 1:B:78:LEU:HD22 8 0.02 (1,839) 1:B:48:ASN:HD21 1:B:78:LEU:HD22 8 0.02 (1,839) 1:B:48:ASN:HD21 1:B:78:LEU:HD23 8 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD21 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD21 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD22 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD22 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD22 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD23 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD23 14 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 18 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 4 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 10 0.02 (1,833) 1:B:9:ARG:HE 1:B:11:VAL:HG21 5 0.02 (1,833) 1:B:9:ARG:HE 1:B:11:VAL:HG21 5 0.02 (1,833) 1:B:9:ARG:HE 1:B:11:VAL:HG23 5 0.02 (1,711) 1:B:44:ILE:HB 1:B:44:ILE:HG21 15 0.02 (1,714) 1:B:44:ILYS:H 1:B:44:ILE:HG21 15 0.02 (1,719) 1:B:41:LYS:H 1:A:44:ILE:HG21 15 0.02 (1,719) 1:B:41:LYS:H 1:A:44:ILE:HG21 15 0.02 (1,719) 1:B:41:LYS:H 1:A:44:ILE:HG21 15 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 1 1 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 1 1 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 1 1 0.02 (1,716) 1:A:41:LYS:H	(1,899)	1:B:51:ILE:HG12	1:B:52:PHE:H	1	0.02
(1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 17 0.02 (1,899) 1:B:51:ILE:HG12 1:B:52:PHE:H 17 0.02 (1,898) 1:A:51:ILE:HG12 1:B:52:PHE:H 16 0.02 (1,84) 1:A:9:ARG:HE 1:A:10:ILE:H 19 0.02 (1,839) 1:B:48:ASN:HD21 1:B:78:LEU:HD21 8 0.02 (1,839) 1:B:48:ASN:HD21 1:B:78:LEU:HD22 8 0.02 (1,839) 1:B:48:ASN:HD21 1:B:78:LEU:HD22 8 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD23 8 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD23 8 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD23 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD21 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD22 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD22 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD23 14 0.02 (1,838) 1:A:48:ASN:HD21 1:A:78:LEU:HD23 14 0.02 (1,832) 1:A:47:CYS:HG 1:B:48:ASN:H 18 0.02 (1,832) 1:A:47:CYS:HG 1:B:48:ASN:H 4 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 6 0.02 (1,832) 1:A:47:CYS:HG 1:A:48:ASN:H 10 0.02 (1,833) 1:B:9:ARG:HE 1:B:11:VAL:HG21 5 0.02 (1,833) 1:B:9:ARG:HE 1:B:11:VAL:HG21 5 0.02 (1,833) 1:B:9:ARG:HE 1:B:11:VAL:HG22 5 0.02 (1,83) 1:B:9:ARG:HE 1:B:11:VAL:HG23 5 0.02 (1,710) 1:B:44:ILE:H 1:A:44:ILE:H 1 0.02 (1,711) 1:B:44:ILE:H 1:A:44:ILE:H 1 0.02 (1,711) 1:B:44:ILE:H 1:A:44:ILE:H 1 0.02 (1,711) 1:B:44:ILYS:H 1:B:44:ILE:H 1 1 0.02 (1,711) 1:B:44:ILYS:H 1:A:44:ILE:H 1 1 0.02 (1,716) 1:A:44:ILYS:H 1:A:45:PHE:HD1 1 1 0.02 (1,716) 1:A:41:IYS:H 1:A:45:PHE:HD1 1 1 0.02 (1,716)	(1,899)	1:B:51:ILE:HG12	1:B:52:PHE:H	5	0.02
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(1,744) 1:A:44:ILE:H 1:A:44:ILE:HG23 15 0.02 (1,719) 1:B:41:LYS:H 1:B:46:THR:H 14 0.02 (1,719) 1:B:41:LYS:H 1:B:46:THR:H 16 0.02 (1,718) 1:A:41:LYS:H 1:A:46:THR:H 10 0.02 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 5 0.02 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 5 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 13 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 13 0.02 (1,614) 1:A:35:THR:H 1:A:83:HIS:HE1 15 0.02 (1,565) 1:B:32:ASN:HA 1:B:32:ASN:HD21 19 0.02	(1,744)	1:A:44:ILE:H	1:A:44:ILE:HG21	15	0.02
(1,719) 1:B:41:LYS:H 1:B:46:THR:H 14 0.02 (1,719) 1:B:41:LYS:H 1:B:46:THR:H 16 0.02 (1,718) 1:A:41:LYS:H 1:A:46:THR:H 10 0.02 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 5 0.02 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 5 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 13 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 13 0.02 (1,614) 1:A:35:THR:H 1:A:83:HIS:HE1 15 0.02 (1,565) 1:B:32:ASN:HA 1:B:32:ASN:HD21 19 0.02	(1,744)	1:A:44:ILE:H	1:A:44:ILE:HG22	15	0.02
(1,719) 1:B:41:LYS:H 1:B:46:THR:H 16 0.02 (1,718) 1:A:41:LYS:H 1:A:46:THR:H 10 0.02 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 5 0.02 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 5 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 13 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 13 0.02 (1,614) 1:A:35:THR:H 1:A:83:HIS:HE1 15 0.02 (1,565) 1:B:32:ASN:HA 1:B:32:ASN:HD21 19 0.02	(1,744)	1:A:44:ILE:H	1:A:44:ILE:HG23	15	0.02
(1,718) 1:A:41:LYS:H 1:A:46:THR:H 10 0.02 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 5 0.02 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 5 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 13 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 13 0.02 (1,614) 1:A:35:THR:H 1:A:83:HIS:HE1 15 0.02 (1,565) 1:B:32:ASN:HA 1:B:32:ASN:HD21 19 0.02	(1,719)	1:B:41:LYS:H	1:B:46:THR:H	14	0.02
(1,718) 1:A:41:LYS:H 1:A:46:THR:H 10 0.02 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD1 5 0.02 (1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 5 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 13 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 13 0.02 (1,614) 1:A:35:THR:H 1:A:83:HIS:HE1 15 0.02 (1,565) 1:B:32:ASN:HA 1:B:32:ASN:HD21 19 0.02	(1,719)	1:B:41:LYS:H	1:B:46:THR:H	16	0.02
(1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 5 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 13 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 13 0.02 (1,614) 1:A:35:THR:H 1:A:83:HIS:HE1 15 0.02 (1,565) 1:B:32:ASN:HA 1:B:32:ASN:HD21 19 0.02		1:A:41:LYS:H	1:A:46:THR:H	10	0.02
(1,717) 1:B:41:LYS:H 1:B:45:PHE:HD2 5 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 13 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 13 0.02 (1,614) 1:A:35:THR:H 1:A:83:HIS:HE1 15 0.02 (1,565) 1:B:32:ASN:HA 1:B:32:ASN:HD21 19 0.02		1:B:41:LYS:H	1:B:45:PHE:HD1	5	0.02
(1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 13 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 13 0.02 (1,614) 1:A:35:THR:H 1:A:83:HIS:HE1 15 0.02 (1,565) 1:B:32:ASN:HA 1:B:32:ASN:HD21 19 0.02		1:B:41:LYS:H	1:B:45:PHE:HD2	5	0.02
(1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 11 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 13 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 13 0.02 (1,614) 1:A:35:THR:H 1:A:83:HIS:HE1 15 0.02 (1,565) 1:B:32:ASN:HA 1:B:32:ASN:HD21 19 0.02		1:A:41:LYS:H	1:A:45:PHE:HD1	11	
(1,716) 1:A:41:LYS:H 1:A:45:PHE:HD1 13 0.02 (1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 13 0.02 (1,614) 1:A:35:THR:H 1:A:83:HIS:HE1 15 0.02 (1,565) 1:B:32:ASN:HA 1:B:32:ASN:HD21 19 0.02	, ,	1:A:41:LYS:H	1:A:45:PHE:HD2	11	0.02
(1,716) 1:A:41:LYS:H 1:A:45:PHE:HD2 13 0.02 (1,614) 1:A:35:THR:H 1:A:83:HIS:HE1 15 0.02 (1,565) 1:B:32:ASN:HA 1:B:32:ASN:HD21 19 0.02		1:A:41:LYS:H	1:A:45:PHE:HD1	13	0.02
(1,614) 1:A:35:THR:H 1:A:83:HIS:HE1 15 0.02 (1,565) 1:B:32:ASN:HA 1:B:32:ASN:HD21 19 0.02			1:A:45:PHE:HD2	13	0.02
(1,565) 1:B:32:ASN:HA 1:B:32:ASN:HD21 19 0.02		1:A:35:THR:H	1:A:83:HIS:HE1	15	0.02
	· · /	1:B:32:ASN:HA	1:B:32:ASN:HD21	19	0.02
(1,000) 1.11.02.11011.111021 1.11.00.1111.1110 0.02	(1,563)	1:A:32:ASN:HD21	1:A:33:ILE:HB	7	0.02



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,563)	1:A:32:ASN:HD21	1:A:33:ILE:HB	20	0.02
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD11	10	0.02
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD12	10	0.02
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD13	10	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD11	2	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD12	2	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD13	2	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD11	5	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD12	5	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD13	5	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD11	7	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD12	7	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD13	7	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD11	8	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD12	8	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD13	8	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD11	12	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD12	12	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD13	12	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD11	19	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD12	19	0.02
(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD13	19	0.02
(1,546)	1:B:29:PHE:HD1	1:B:31:THR:H	5	0.02
(1,546)	1:B:29:PHE:HD2	1:B:31:THR:H	5	0.02
(1,545)	1:A:29:PHE:HD1	1:A:31:THR:H	15	0.02
(1,545)	1:A:29:PHE:HD2	1:A:31:THR:H	15	0.02
(1,545)	1:A:29:PHE:HD1	1:A:31:THR:H	19	0.02
(1,545)	1:A:29:PHE:HD2	1:A:31:THR:H	19	0.02
(1,5005)	1:B:77:ARG:H	1:B:77:ARG:HG2	5	0.02
(1,5005)	1:B:77:ARG:H	1:B:77:ARG:HG3	5	0.02
(1,5005)	1:B:77:ARG:H	1:B:77:ARG:HG2	6	0.02
(1,5005)	1:B:77:ARG:H	1:B:77:ARG:HG3	6	0.02
(1,5005)	1:B:77:ARG:H	1:B:77:ARG:HG2	10	0.02
(1,5005)	1:B:77:ARG:H	1:B:77:ARG:HG3	10	0.02
(1,5005)	1:B:77:ARG:H	1:B:77:ARG:HG2	13	0.02
(1,5005)	1:B:77:ARG:H	1:B:77:ARG:HG3	13	0.02
(1,4976)	1:B:63:MET:HE1	1:B:77:ARG:HB2	6	0.02
(1,4976)	1:B:63:MET:HE1	1:B:77:ARG:HB3	6	0.02
(1,4976)	1:B:63:MET:HE2	1:B:77:ARG:HB2	6	0.02
(1,4976)	1:B:63:MET:HE2	1:B:77:ARG:HB3	6	0.02
(1,4976)	1:B:63:MET:HE3	1:B:77:ARG:HB2	6	0.02
(1,4976)	1:B:63:MET:HE3	1:B:77:ARG:HB3	6	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4940)	1:B:55:ASN:HD21	1:B:57:ASP:HB2	2	0.02
(1,4940)	1:B:55:ASN:HD21	1:B:57:ASP:HB3	2	0.02
(1,4940)	1:B:55:ASN:HD22	1:B:57:ASP:HB2	2	0.02
(1,4940)	1:B:55:ASN:HD22	1:B:57:ASP:HB3	2	0.02
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD21	5	0.02
(1,4933)	1:B:54:LYS:HG2	1:B:55:ASN:HD22	5	0.02
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD21	5	0.02
(1,4933)	1:B:54:LYS:HG3	1:B:55:ASN:HD22	5	0.02
(1,4922)	1:B:53:VAL:HA	1:B:54:LYS:HB2	14	0.02
(1,4922)	1:B:53:VAL:HA	1:B:54:LYS:HB3	14	0.02
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE1	13	0.02
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE2	13	0.02
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE3	13	0.02
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE1	13	0.02
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE2	13	0.02
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE3	13	0.02
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE1	19	0.02
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE2	19	0.02
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE3	19	0.02
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE1	19	0.02
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE2	19	0.02
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE3	19	0.02
(1,4899)	1:B:39:ASN:HD21	1:B:46:THR:HB	17	0.02
(1,4899)	1:B:39:ASN:HD22	1:B:46:THR:HB	17	0.02
(1,4898)	1:B:39:ASN:HD21	1:B:41:LYS:HE2	1	0.02
(1,4898)	1:B:39:ASN:HD21	1:B:41:LYS:HE3	1	0.02
(1,4898)	1:B:39:ASN:HD22	1:B:41:LYS:HE2	1	0.02
(1,4898)	1:B:39:ASN:HD22	1:B:41:LYS:HE3	1	0.02
(1,4898)	1:B:39:ASN:HD21	1:B:41:LYS:HE2	10	0.02
(1,4898)	1:B:39:ASN:HD21	1:B:41:LYS:HE3	10	0.02
(1,4898)	1:B:39:ASN:HD22	1:B:41:LYS:HE2	10	0.02
(1,4898)	1:B:39:ASN:HD22	1:B:41:LYS:HE3	10	0.02
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB2	2	0.02
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB3	2	0.02
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB2	2	0.02
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB3	2	0.02
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB2	9	0.02
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB3	9	0.02
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB2	9	0.02
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB3	9	0.02
(1,4887)	1:B:37:VAL:HG11	1:B:48:ASN:HD21	13	0.02
(1,4887)	1:B:37:VAL:HG11	1:B:48:ASN:HD22	13	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4887)	1:B:37:VAL:HG12	1:B:48:ASN:HD21	13	0.02
(1,4887)	1:B:37:VAL:HG12	1:B:48:ASN:HD22	13	0.02
(1,4887)	1:B:37:VAL:HG13	1:B:48:ASN:HD21	13	0.02
(1,4887)	1:B:37:VAL:HG13	1:B:48:ASN:HD22	13	0.02
(1,4883)	1:B:37:VAL:HB	1:B:48:ASN:HB2	19	0.02
(1,4883)	1:B:37:VAL:HB	1:B:48:ASN:HB3	19	0.02
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB2	18	0.02
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB3	18	0.02
(1,4873)	1:B:34:ARG:HG2	1:B:52:PHE:HE1	16	0.02
(1,4873)	1:B:34:ARG:HG2	1:B:52:PHE:HE2	16	0.02
(1,4873)	1:B:34:ARG:HG3	1:B:52:PHE:HE1	16	0.02
(1,4873)	1:B:34:ARG:HG3	1:B:52:PHE:HE2	16	0.02
(1,4872)	1:B:34:ARG:HG2	1:B:52:PHE:HD1	3	0.02
(1,4872)	1:B:34:ARG:HG2	1:B:52:PHE:HD2	3	0.02
(1,4872)	1:B:34:ARG:HG3	1:B:52:PHE:HD1	3	0.02
(1,4872)	1:B:34:ARG:HG3	1:B:52:PHE:HD2	3	0.02
(1,4869)	1:B:34:ARG:HB2	1:B:51:ILE:H	8	0.02
(1,4869)	1:B:34:ARG:HB3	1:B:51:ILE:H	8	0.02
(1,4867)	1:B:34:ARG:HB2	1:B:50:MET:HG2	1	0.02
(1,4867)	1:B:34:ARG:HB3	1:B:50:MET:HG2	1	0.02
(1,4861)	1:B:32:ASN:HD21	1:B:33:ILE:HB	6	0.02
(1,4861)	1:B:32:ASN:HD22	1:B:33:ILE:HB	6	0.02
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD11	10	0.02
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD12	10	0.02
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD13	10	0.02
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD11	10	0.02
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD12	10	0.02
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD13	10	0.02
(1,4854)	1:B:32:ASN:HA	1:B:32:ASN:HD21	4	0.02
(1,4854)	1:B:32:ASN:HA	1:B:32:ASN:HD22	4	0.02
(1,4854)	1:B:32:ASN:HA	1:B:32:ASN:HD21	19	0.02
(1,4854)	1:B:32:ASN:HA	1:B:32:ASN:HD22	19	0.02
(1,4828)	1:B:27:SER:HG	1:B:28:LYS:HD2	13	0.02
(1,4828)	1:B:27:SER:HG	1:B:28:LYS:HD3	13	0.02
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG2	13	0.02
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	13	0.02
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	13	0.02
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG3	13	0.02
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	13	0.02
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	13	0.02
(1,4814)	1:B:25:VAL:HG11	1:B:28:LYS:HD2	9	0.02
(1,4814)	1:B:25:VAL:HG11	1:B:28:LYS:HD3	9	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4814)	1:B:25:VAL:HG12	1:B:28:LYS:HD2	9	0.02
(1,4814)	1:B:25:VAL:HG12	1:B:28:LYS:HD3	9	0.02
(1,4814)	1:B:25:VAL:HG13	1:B:28:LYS:HD2	9	0.02
(1,4814)	1:B:25:VAL:HG13	1:B:28:LYS:HD3	9	0.02
(1,481)	1:A:23:THR:HG21	1:A:28:LYS:H	17	0.02
(1,481)	1:A:23:THR:HG22	1:A:28:LYS:H	17	0.02
(1,481)	1:A:23:THR:HG23	1:A:28:LYS:H	17	0.02
(1,4805)	1:B:24:GLY:HA2	1:B:28:LYS:HE2	16	0.02
(1,4805)	1:B:24:GLY:HA2	1:B:28:LYS:HE3	16	0.02
(1,4805)	1:B:24:GLY:HA3	1:B:28:LYS:HE2	16	0.02
(1,4805)	1:B:24:GLY:HA3	1:B:28:LYS:HE3	16	0.02
(1,4771)	1:B:15:LYS:HD2	1:B:16:ASN:HD21	14	0.02
(1,4771)	1:B:15:LYS:HD2	1:B:16:ASN:HD22	14	0.02
(1,4771)	1:B:15:LYS:HD3	1:B:16:ASN:HD21	14	0.02
(1,4771)	1:B:15:LYS:HD3	1:B:16:ASN:HD22	14	0.02
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG2	15	0.02
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG3	15	0.02
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG2	17	0.02
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG3	17	0.02
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG2	20	0.02
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG3	20	0.02
(1,4690)	1:A:67:ARG:H	1:A:67:ARG:HG2	5	0.02
(1,4690)	1:A:67:ARG:H	1:A:67:ARG:HG3	5	0.02
(1,4660)	1:A:58:LYS:HE2	1:A:62:LEU:H	18	0.02
(1,4660)	1:A:58:LYS:HE3	1:A:62:LEU:H	18	0.02
(1,4643)	1:A:54:LYS:HE2	1:A:55:ASN:HD21	2	0.02
(1,4643)	1:A:54:LYS:HE2	1:A:55:ASN:HD22	2	0.02
(1,4643)	1:A:54:LYS:HE3	1:A:55:ASN:HD21	2	0.02
(1,4643)	1:A:54:LYS:HE3	1:A:55:ASN:HD22	2	0.02
(1,4643)	1:A:54:LYS:HE2	1:A:55:ASN:HD21	14	0.02
(1,4643)	1:A:54:LYS:HE2	1:A:55:ASN:HD22	14	0.02
(1,4643)	1:A:54:LYS:HE3	1:A:55:ASN:HD21	14	0.02
(1,4643)	1:A:54:LYS:HE3	1:A:55:ASN:HD22	14	0.02
(1,4640)	1:A:54:LYS:HG2	1:A:55:ASN:HD21	13	0.02
(1,4640)	1:A:54:LYS:HG2	1:A:55:ASN:HD22	13	0.02
(1,4640)	1:A:54:LYS:HG3	1:A:55:ASN:HD21	13	0.02
(1,4640)	1:A:54:LYS:HG3	1:A:55:ASN:HD22	13	0.02
(1,4638)	1:A:54:LYS:HB2	1:A:55:ASN:HD21	19	0.02
(1,4638)	1:A:54:LYS:HB2	1:A:55:ASN:HD22	19	0.02
(1,4638)	1:A:54:LYS:HB3	1:A:55:ASN:HD21	19	0.02
(1,4638)	1:A:54:LYS:HB3	1:A:55:ASN:HD22	19	0.02
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE1	2	0.02



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(1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 2 0.0 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 2 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 2 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 2 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 2 0.0 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 8 0.0)2)2)2)2)2)2
(1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 2 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 2 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 2 0.0 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 8 0.0 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 8 0.0)2)2)2)2)2
(1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 2 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 2 0.0 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 8 0.0 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 8 0.0)2)2)2)2
(1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 2 0.0 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 8 0.0 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 8 0.0)2)2)2
(1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 8 0.0 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 8 0.0)2
(1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 8 0.0 (1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 8 0.0)2
(1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 8 0.0	
(1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 8 0.0 (1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 8 0.0	
(1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 8 0.0)2
)2
(1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 8 0.0)2
)2
(1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE1 15 0.0)2
(1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE2 15 0.0)2
(1,4623) 1:A:48:ASN:HD21 1:A:50:MET:HE3 15 0.0)2
(1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE1 15 0.0)2
(1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE2 15 0.0)2
(1,4623) 1:A:48:ASN:HD22 1:A:50:MET:HE3 15 0.0)2
(1,4613) 1:A:42:ASP:HB2 1:A:44:ILE:HG12 8 0.0)2
(1,4613) 1:A:42:ASP:HB3 1:A:44:ILE:HG12 8 0.0)2
(1,4607) 1:A:39:ASN:HD21 1:A:48:ASN:HD21 2 0.0)2
(1,4607) 1:A:39:ASN:HD21 1:A:48:ASN:HD22 2 0.0)2
(1,4607) 1:A:39:ASN:HD22 1:A:48:ASN:HD21 2 0.0)2
(1,4607) 1:A:39:ASN:HD22 1:A:48:ASN:HD22 2 0.0)2
(1,4606) 1:A:39:ASN:HD21 1:A:46:THR:HG21 18 0.0)2
(1,4606) 1:A:39:ASN:HD21 1:A:46:THR:HG22 18 0.0)2
(1,4606) 1:A:39:ASN:HD21 1:A:46:THR:HG23 18 0.0)2
(1,4606) 1:A:39:ASN:HD22 1:A:46:THR:HG21 18 0.0)2
(1,4606) 1:A:39:ASN:HD22 1:A:46:THR:HG22 18 0.0)2
(1,4606) 1:A:39:ASN:HD22 1:A:46:THR:HG23 18 0.0)2
(1,4595) 1:A:37:VAL:HG21 1:A:48:ASN:HD21 2 0.0)2
(1,4595) 1:A:37:VAL:HG21 1:A:48:ASN:HD22 2 0.0)2
(1,4595) 1:A:37:VAL:HG22 1:A:48:ASN:HD21 2 0.0)2
(1,4595) 1:A:37:VAL:HG22 1:A:48:ASN:HD22 2 0.0)2
(1,4595) 1:A:37:VAL:HG23 1:A:48:ASN:HD21 2 0.0)2
(1,4595) 1:A:37:VAL:HG23 1:A:48:ASN:HD22 2 0.0)2
(1,4593) 1:A:37:VAL:HG11 1:A:48:ASN:HD21 13 0.0)2
(1,4593) 1:A:37:VAL:HG11 1:A:48:ASN:HD22 13 0.0)2
(1,4593) 1:A:37:VAL:HG12 1:A:48:ASN:HD21 13 0.0)2
(1,4593) 1:A:37:VAL:HG12 1:A:48:ASN:HD22 13 0.0)2
(1,4593) 1:A:37:VAL:HG13 1:A:48:ASN:HD21 13 0.0)2
(1,4593) 1:A:37:VAL:HG13 1:A:48:ASN:HD22 13 0.0)2
(1,4580) 1:A:35:THR:HB 1:A:50:MET:HB2 8 0.0)2



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB3	8	0.02
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB2	13	0.02
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB3	13	0.02
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB2	19	0.02
(1,4580)	1:A:35:THR:HB	1:A:50:MET:HB3	19	0.02
(1,4577)	1:A:34:ARG:HG2	1:A:52:PHE:HD1	7	0.02
(1,4577)	1:A:34:ARG:HG2	1:A:52:PHE:HD2	7	0.02
(1,4577)	1:A:34:ARG:HG3	1:A:52:PHE:HD1	7	0.02
(1,4577)	1:A:34:ARG:HG3	1:A:52:PHE:HD2	7	0.02
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD11	13	0.02
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD12	13	0.02
(1,4564)	1:A:32:ASN:HB2	1:A:33:ILE:HD13	13	0.02
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD11	13	0.02
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD12	13	0.02
(1,4564)	1:A:32:ASN:HB3	1:A:33:ILE:HD13	13	0.02
(1,4538)	1:A:27:SER:HG	1:A:28:LYS:HD2	20	0.02
(1,4538)	1:A:27:SER:HG	1:A:28:LYS:HD3	20	0.02
(1,4534)	1:A:27:SER:HB2	1:A:33:ILE:HD11	7	0.02
(1,4534)	1:A:27:SER:HB2	1:A:33:ILE:HD12	7	0.02
(1,4534)	1:A:27:SER:HB2	1:A:33:ILE:HD13	7	0.02
(1,4534)	1:A:27:SER:HB3	1:A:33:ILE:HD11	7	0.02
(1,4534)	1:A:27:SER:HB3	1:A:33:ILE:HD12	7	0.02
(1,4534)	1:A:27:SER:HB3	1:A:33:ILE:HD13	7	0.02
(1,4514)	1:A:24:GLY:HA2	1:A:28:LYS:HE2	7	0.02
(1,4514)	1:A:24:GLY:HA2	1:A:28:LYS:HE3	7	0.02
(1,4514)	1:A:24:GLY:HA3	1:A:28:LYS:HE2	7	0.02
(1,4514)	1:A:24:GLY:HA3	1:A:28:LYS:HE3	7	0.02
(1,4464)	1:A:15:LYS:HE2	1:A:16:ASN:HD21	12	0.02
(1,4464)	1:A:15:LYS:HE2	1:A:16:ASN:HD22	12	0.02
(1,4464)	1:A:15:LYS:HE3	1:A:16:ASN:HD21	12	0.02
(1,4464)	1:A:15:LYS:HE3	1:A:16:ASN:HD22	12	0.02
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	3	0.02
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	3	0.02
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	3	0.02
(1,4389)	1:B:81:LEU:HB2	1:B:83:HIS:HD2	9	0.02
(1,4389)	1:B:81:LEU:HB3	1:B:83:HIS:HD2	9	0.02
(1,4389)	1:B:81:LEU:HB2	1:B:83:HIS:HD2	10	0.02
(1,4389)	1:B:81:LEU:HB3	1:B:83:HIS:HD2	10	0.02
(1,4388)	1:A:81:LEU:HB2	1:A:83:HIS:HD2	8	0.02
(1,4388)	1:A:81:LEU:HB3	1:A:83:HIS:HD2	8	0.02
(1,4388)	1:A:81:LEU:HB2	1:A:83:HIS:HD2	12	0.02
(1,4388)	1:A:81:LEU:HB3	1:A:83:HIS:HD2	12	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4387)	1:B:5:LEU:HG	1:B:83:HIS:HD2	7	0.02
(1,4387)	1:B:5:LEU:HG	1:B:83:HIS:HD2	17	0.02
(1,4387)	1:B:5:LEU:HG	1:B:83:HIS:HD2	20	0.02
(1,4386)	1:A:5:LEU:HG	1:A:83:HIS:HD2	1	0.02
(1,4386)	1:A:5:LEU:HG	1:A:83:HIS:HD2	6	0.02
(1,4386)	1:A:5:LEU:HG	1:A:83:HIS:HD2	7	0.02
(1,4370)	1:A:13:GLU:H	1:A:73:PHE:HZ	13	0.02
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG21	1	0.02
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG22	1	0.02
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG23	1	0.02
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG21	10	0.02
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG22	10	0.02
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG23	10	0.02
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG21	13	0.02
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG22	13	0.02
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG23	13	0.02
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG21	2	0.02
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG22	2	0.02
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG23	2	0.02
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG21	8	0.02
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG22	8	0.02
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG23	8	0.02
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG21	11	0.02
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG22	11	0.02
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG23	11	0.02
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG21	12	0.02
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG22	12	0.02
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG23	12	0.02
(1,4355)	1:B:44:ILE:HG12	1:B:73:PHE:HE1	11	0.02
(1,4355)	1:B:44:ILE:HG12	1:B:73:PHE:HE2	11	0.02
(1,4353)	1:B:44:ILE:HG13	1:B:73:PHE:HE1	7	0.02
(1,4353)	1:B:44:ILE:HG13	1:B:73:PHE:HE2	7	0.02
(1,4352)	1:A:44:ILE:HG13	1:A:73:PHE:HE1	14	0.02
(1,4352)	1:A:44:ILE:HG13	1:A:73:PHE:HE2	14	0.02
(1,4352)	1:A:44:ILE:HG13	1:A:73:PHE:HE1	16	0.02
(1,4352)	1:A:44:ILE:HG13	1:A:73:PHE:HE2	16	0.02
(1,4343)	1:B:29:PHE:HE1	1:B:65:LYS:HE2	15	0.02
(1,4343)	1:B:29:PHE:HE1	1:B:65:LYS:HE3	15	0.02
(1,4343)	1:B:29:PHE:HE2	1:B:65:LYS:HE2	15	0.02
(1,4343)	1:B:29:PHE:HE2	1:B:65:LYS:HE3	15	0.02
(1,4343)	1:B:29:PHE:HE1	1:B:65:LYS:HE2	20	0.02
(1,4343)	1:B:29:PHE:HE1	1:B:65:LYS:HE3	20	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4343)	1:B:29:PHE:HE2	1:B:65:LYS:HE2	20	0.02
(1,4343)	1:B:29:PHE:HE2	1:B:65:LYS:HE3	20	0.02
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE1	15	0.02
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE2	15	0.02
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE1	15	0.02
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE2	15	0.02
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE1	19	0.02
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE2	19	0.02
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE1	19	0.02
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE2	19	0.02
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE1	12	0.02
(1,4332)	1:A:4:PHE:HB2	1:A:52:PHE:HE2	12	0.02
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE1	12	0.02
(1,4332)	1:A:4:PHE:HB3	1:A:52:PHE:HE2	12	0.02
(1,4329)	1:B:5:LEU:HD21	1:B:52:PHE:HE1	2	0.02
(1,4329)	1:B:5:LEU:HD21	1:B:52:PHE:HE2	2	0.02
(1,4329)	1:B:5:LEU:HD22	1:B:52:PHE:HE1	2	0.02
(1,4329)	1:B:5:LEU:HD22	1:B:52:PHE:HE2	2	0.02
(1,4329)	1:B:5:LEU:HD23	1:B:52:PHE:HE1	2	0.02
(1,4329)	1:B:5:LEU:HD23	1:B:52:PHE:HE2	2	0.02
(1,4329)	1:B:5:LEU:HD21	1:B:52:PHE:HE1	8	0.02
(1,4329)	1:B:5:LEU:HD21	1:B:52:PHE:HE2	8	0.02
(1,4329)	1:B:5:LEU:HD22	1:B:52:PHE:HE1	8	0.02
(1,4329)	1:B:5:LEU:HD22	1:B:52:PHE:HE2	8	0.02
(1,4329)	1:B:5:LEU:HD23	1:B:52:PHE:HE1	8	0.02
(1,4329)	1:B:5:LEU:HD23	1:B:52:PHE:HE2	8	0.02
(1,4329)	1:B:5:LEU:HD21	1:B:52:PHE:HE1	9	0.02
(1,4329)	1:B:5:LEU:HD21	1:B:52:PHE:HE2	9	0.02
(1,4329)	1:B:5:LEU:HD22	1:B:52:PHE:HE1	9	0.02
(1,4329)	1:B:5:LEU:HD22	1:B:52:PHE:HE2	9	0.02
(1,4329)	1:B:5:LEU:HD23	1:B:52:PHE:HE1	9	0.02
(1,4329)	1:B:5:LEU:HD23	1:B:52:PHE:HE2	9	0.02
(1,4328)	1:A:5:LEU:HD21	1:A:52:PHE:HE1	10	0.02
(1,4328)	1:A:5:LEU:HD21	1:A:52:PHE:HE2	10	0.02
(1,4328)	1:A:5:LEU:HD22	1:A:52:PHE:HE1	10	0.02
(1,4328)	1:A:5:LEU:HD22	1:A:52:PHE:HE2	10	0.02
(1,4328)	1:A:5:LEU:HD23	1:A:52:PHE:HE1	10	0.02
(1,4328)	1:A:5:LEU:HD23	1:A:52:PHE:HE2	10	0.02
(1,4328)	1:A:5:LEU:HD21	1:A:52:PHE:HE1	18	0.02
(1,4328)	1:A:5:LEU:HD21	1:A:52:PHE:HE2	18	0.02
(1,4328)	1:A:5:LEU:HD22	1:A:52:PHE:HE1	18	0.02
(1,4328)	1:A:5:LEU:HD22	1:A:52:PHE:HE2	18	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4328)	1:A:5:LEU:HD23	1:A:52:PHE:HE1	18	0.02
(1,4328)	1:A:5:LEU:HD23	1:A:52:PHE:HE2	18	0.02
(1,4328)	1:A:5:LEU:HD21	1:A:52:PHE:HE1	19	0.02
(1,4328)	1:A:5:LEU:HD21	1:A:52:PHE:HE2	19	0.02
(1,4328)	1:A:5:LEU:HD22	1:A:52:PHE:HE1	19	0.02
(1,4328)	1:A:5:LEU:HD22	1:A:52:PHE:HE2	19	0.02
(1,4328)	1:A:5:LEU:HD23	1:A:52:PHE:HE1	19	0.02
(1,4328)	1:A:5:LEU:HD23	1:A:52:PHE:HE2	19	0.02
(1,4323)	1:B:52:PHE:HD1	1:B:53:VAL:H	1	0.02
(1,4323)	1:B:52:PHE:HD2	1:B:53:VAL:H	1	0.02
(1,4323)	1:B:52:PHE:HD1	1:B:53:VAL:H	6	0.02
(1,4323)	1:B:52:PHE:HD2	1:B:53:VAL:H	6	0.02
(1,4322)	1:A:52:PHE:HD1	1:A:53:VAL:H	6	0.02
(1,4322)	1:A:52:PHE:HD2	1:A:53:VAL:H	6	0.02
(1,4322)	1:A:52:PHE:HD1	1:A:53:VAL:H	9	0.02
(1,4322)	1:A:52:PHE:HD2	1:A:53:VAL:H	9	0.02
(1,4322)	1:A:52:PHE:HD1	1:A:53:VAL:H	10	0.02
(1,4322)	1:A:52:PHE:HD2	1:A:53:VAL:H	10	0.02
(1,4311)	1:B:5:LEU:HA	1:B:52:PHE:HD1	12	0.02
(1,4311)	1:B:5:LEU:HA	1:B:52:PHE:HD2	12	0.02
(1,4310)	1:A:5:LEU:HA	1:A:52:PHE:HD1	9	0.02
(1,4310)	1:A:5:LEU:HA	1:A:52:PHE:HD2	9	0.02
(1,4310)	1:A:5:LEU:HA	1:A:52:PHE:HD1	10	0.02
(1,4310)	1:A:5:LEU:HA	1:A:52:PHE:HD2	10	0.02
(1,4310)	1:A:5:LEU:HA	1:A:52:PHE:HD1	14	0.02
(1,4310)	1:A:5:LEU:HA	1:A:52:PHE:HD2	14	0.02
(1,4310)	1:A:5:LEU:HA	1:A:52:PHE:HD1	18	0.02
(1,4310)	1:A:5:LEU:HA	1:A:52:PHE:HD2	18	0.02
(1,4296)	1:A:45:PHE:HZ	1:A:71:GLY:HA3	2	0.02
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	4	0.02
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	7	0.02
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	12	0.02
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	19	0.02
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	2	0.02
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	3	0.02
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	4	0.02
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	5	0.02
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	6	0.02
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	7	0.02
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	8	0.02
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	12	0.02
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	14	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	15	0.02
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	18	0.02
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	20	0.02
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE1	11	0.02
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE2	11	0.02
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE1	11	0.02
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE2	11	0.02
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE1	11	0.02
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE2	11	0.02
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE1	15	0.02
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE2	15	0.02
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE1	15	0.02
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE2	15	0.02
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE1	15	0.02
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE2	15	0.02
(1,4245)	1:B:14:ASP:HA	1:B:45:PHE:HD1	9	0.02
(1,4245)	1:B:14:ASP:HA	1:B:45:PHE:HD2	9	0.02
(1,4234)	1:A:45:PHE:HD1	1:A:47:CYS:HG	16	0.02
(1,4234)	1:A:45:PHE:HD2	1:A:47:CYS:HG	16	0.02
(1,4217)	1:B:26:ILE:HG21	1:B:29:PHE:HZ	3	0.02
(1,4217)	1:B:26:ILE:HG22	1:B:29:PHE:HZ	3	0.02
(1,4217)	1:B:26:ILE:HG23	1:B:29:PHE:HZ	3	0.02
(1,4217)	1:B:26:ILE:HG21	1:B:29:PHE:HZ	4	0.02
(1,4217)	1:B:26:ILE:HG22	1:B:29:PHE:HZ	4	0.02
(1,4217)	1:B:26:ILE:HG23	1:B:29:PHE:HZ	4	0.02
(1,4211)	1:B:29:PHE:H	1:B:29:PHE:HD1	1	0.02
(1,4211)	1:B:29:PHE:H	1:B:29:PHE:HD2	1	0.02
(1,4209)	1:B:29:PHE:HA	1:B:29:PHE:HD1	12	0.02
(1,4209)	1:B:29:PHE:HA	1:B:29:PHE:HD2	12	0.02
(1,4208)	1:A:29:PHE:HA	1:A:29:PHE:HD1	3	0.02
(1,4208)	1:A:29:PHE:HA	1:A:29:PHE:HD2	3	0.02
(1,4205)	1:B:29:PHE:HD1	1:B:65:LYS:HD2	20	0.02
(1,4205)	1:B:29:PHE:HD2	1:B:65:LYS:HD2	20	0.02
(1,4204)	1:A:29:PHE:HD1	1:A:65:LYS:HD2	1	0.02
(1,4204)	1:A:29:PHE:HD2	1:A:65:LYS:HD2	1	0.02
(1,4204)	1:A:29:PHE:HD1	1:A:65:LYS:HD2	13	0.02
(1,4204)	1:A:29:PHE:HD2	1:A:65:LYS:HD2	13	0.02
(1,4204)	1:A:29:PHE:HD1	1:A:65:LYS:HD2	18	0.02
(1,4204)	1:A:29:PHE:HD2	1:A:65:LYS:HD2	18	0.02
(1,4187)	1:B:4:PHE:HZ	1:B:6:ALA:HA	1	0.02
(1,4187)	1:B:4:PHE:HZ	1:B:6:ALA:HA	5	0.02
(1,4187)	1:B:4:PHE:HZ	1:B:6:ALA:HA	7	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4187)	1:B:4:PHE:HZ	1:B:6:ALA:HA	19	0.02
(1,4187)	1:B:4:PHE:HZ	1:B:6:ALA:HA	20	0.02
(1,4186)	1:A:4:PHE:HZ	1:A:6:ALA:HA	7	0.02
(1,4186)	1:A:4:PHE:HZ	1:A:6:ALA:HA	10	0.02
(1,4186)	1:A:4:PHE:HZ	1:A:6:ALA:HA	16	0.02
(1,4182)	1:A:4:PHE:HZ	1:A:56:THR:HA	15	0.02
(1,416)	1:A:24:GLY:H	1:A:27:SER:HG	6	0.02
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD21	4	0.02
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD22	4	0.02
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD23	4	0.02
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD21	4	0.02
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD22	4	0.02
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD23	4	0.02
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD21	6	0.02
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD22	6	0.02
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD23	6	0.02
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD21	6	0.02
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD22	6	0.02
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD23	6	0.02
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD21	11	0.02
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD22	11	0.02
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD23	11	0.02
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD21	11	0.02
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD22	11	0.02
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD23	11	0.02
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD21	17	0.02
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD22	17	0.02
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD23	17	0.02
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD21	17	0.02
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD22	17	0.02
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD23	17	0.02
(1,4145)	1:B:4:PHE:HD1	1:B:5:LEU:H	1	0.02
(1,4145)	1:B:4:PHE:HD2	1:B:5:LEU:H	1	0.02
(1,4145)	1:B:4:PHE:HD1	1:B:5:LEU:H	16	0.02
(1,4145)	1:B:4:PHE:HD2	1:B:5:LEU:H	16	0.02
(1,4145)	1:B:4:PHE:HD1	1:B:5:LEU:H	18	0.02
(1,4145)	1:B:4:PHE:HD2	1:B:5:LEU:H	18	0.02
(1,4144)	1:A:4:PHE:HD1	1:A:5:LEU:H	1	0.02
(1,4144)	1:A:4:PHE:HD2	1:A:5:LEU:H	1	0.02
(1,4144)	1:A:4:PHE:HD1	1:A:5:LEU:H	3	0.02
(1,4144)	1:A:4:PHE:HD2	1:A:5:LEU:H	3	0.02
(1,4144)	1:A:4:PHE:HD1	1:A:5:LEU:H	7	0.02



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Key	$egin{aligned} Atom-1 \end{aligned}$	Atom-2	Model	Violation (Å)
(1,4144)	1:A:4:PHE:HD2	1:A:5:LEU:H	7	0.02
(1,4144)	1:A:4:PHE:HD1	1:A:5:LEU:H	12	0.02
(1,4144)	1:A:4:PHE:HD2	1:A:5:LEU:H	12	0.02
(1,4144)	1:A:4:PHE:HD1	1:A:5:LEU:H	17	0.02
(1,4144)	1:A:4:PHE:HD2	1:A:5:LEU:H	17	0.02
(1,4138)	1:A:4:PHE:HD1	1:A:54:LYS:HA	5	0.02
(1,4138)	1:A:4:PHE:HD2	1:A:54:LYS:HA	5	0.02
(1,4133)	1:B:4:PHE:HD1	1:B:59:LEU:HD21	15	0.02
(1,4133)	1:B:4:PHE:HD1	1:B:59:LEU:HD22	15	0.02
(1,4133)	1:B:4:PHE:HD1	1:B:59:LEU:HD23	15	0.02
(1,4133)	1:B:4:PHE:HD2	1:B:59:LEU:HD21	15	0.02
(1,4133)	1:B:4:PHE:HD2	1:B:59:LEU:HD22	15	0.02
(1,4133)	1:B:4:PHE:HD2	1:B:59:LEU:HD23	15	0.02
(1,4133)	1:B:4:PHE:HD1	1:B:59:LEU:HD21	18	0.02
(1,4133)	1:B:4:PHE:HD1	1:B:59:LEU:HD22	18	0.02
(1,4133)	1:B:4:PHE:HD1	1:B:59:LEU:HD23	18	0.02
(1,4133)	1:B:4:PHE:HD2	1:B:59:LEU:HD21	18	0.02
(1,4133)	1:B:4:PHE:HD2	1:B:59:LEU:HD22	18	0.02
(1,4133)	1:B:4:PHE:HD2	1:B:59:LEU:HD23	18	0.02
(1,4132)	1:A:4:PHE:HD1	1:A:59:LEU:HD21	3	0.02
(1,4132)	1:A:4:PHE:HD1	1:A:59:LEU:HD22	3	0.02
(1,4132)	1:A:4:PHE:HD1	1:A:59:LEU:HD23	3	0.02
(1,4132)	1:A:4:PHE:HD2	1:A:59:LEU:HD21	3	0.02
(1,4132)	1:A:4:PHE:HD2	1:A:59:LEU:HD22	3	0.02
(1,4132)	1:A:4:PHE:HD2	1:A:59:LEU:HD23	3	0.02
(1,4132)	1:A:4:PHE:HD1	1:A:59:LEU:HD21	4	0.02
(1,4132)	1:A:4:PHE:HD1	1:A:59:LEU:HD22	4	0.02
(1,4132)	1:A:4:PHE:HD1	1:A:59:LEU:HD23	4	0.02
(1,4132)	1:A:4:PHE:HD2	1:A:59:LEU:HD21	4	0.02
(1,4132)	1:A:4:PHE:HD2	1:A:59:LEU:HD22	4	0.02
(1,4132)	1:A:4:PHE:HD2	1:A:59:LEU:HD23	4	0.02
(1,4132)	1:A:4:PHE:HD1	1:A:59:LEU:HD21	6	0.02
(1,4132)	1:A:4:PHE:HD1	1:A:59:LEU:HD22	6	0.02
(1,4132)	1:A:4:PHE:HD1	1:A:59:LEU:HD23	6	0.02
(1,4132)	1:A:4:PHE:HD2	1:A:59:LEU:HD21	6	0.02
(1,4132)	1:A:4:PHE:HD2	1:A:59:LEU:HD22	6	0.02
(1,4132)	1:A:4:PHE:HD2	1:A:59:LEU:HD23	6	0.02
(1,4132)	1:A:4:PHE:HD1	1:A:59:LEU:HD21	10	0.02
(1,4132)	1:A:4:PHE:HD1	1:A:59:LEU:HD22	10	0.02
(1,4132)	1:A:4:PHE:HD1	1:A:59:LEU:HD23	10	0.02
(1,4132)	1:A:4:PHE:HD2	1:A:59:LEU:HD21	10	0.02
(1,4132)	1:A:4:PHE:HD2	1:A:59:LEU:HD22	10	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4132)	1:A:4:PHE:HD2	1:A:59:LEU:HD23	10	0.02
(1,4132)	1:A:4:PHE:HD1	1:A:59:LEU:HD21	11	0.02
(1,4132)	1:A:4:PHE:HD1	1:A:59:LEU:HD22	11	0.02
(1,4132)	1:A:4:PHE:HD1	1:A:59:LEU:HD23	11	0.02
(1,4132)	1:A:4:PHE:HD2	1:A:59:LEU:HD21	11	0.02
(1,4132)	1:A:4:PHE:HD2	1:A:59:LEU:HD22	11	0.02
(1,4132)	1:A:4:PHE:HD2	1:A:59:LEU:HD23	11	0.02
(1,4129)	1:B:83:HIS:HA	1:B:83:HIS:HD2	10	0.02
(1,4128)	1:A:83:HIS:HA	1:A:83:HIS:HD2	5	0.02
(1,4119)	1:B:80:ASN:HA	1:B:81:LEU:HG	8	0.02
(1,4119)	1:B:80:ASN:HA	1:B:81:LEU:HG	10	0.02
(1,4119)	1:B:80:ASN:HA	1:B:81:LEU:HG	16	0.02
(1,4118)	1:A:80:ASN:HA	1:A:81:LEU:HG	7	0.02
(1,4118)	1:A:80:ASN:HA	1:A:81:LEU:HG	20	0.02
(1,4115)	1:B:77:ARG:HG2	1:B:79:SER:HA	8	0.02
(1,4112)	1:A:77:ARG:HG3	1:A:79:SER:HA	4	0.02
(1,4112)	1:A:77:ARG:HG3	1:A:79:SER:HA	6	0.02
(1,4111)	1:B:79:SER:HA	1:B:81:LEU:HG	8	0.02
(1,4111)	1:B:79:SER:HA	1:B:81:LEU:HG	18	0.02
(1,4110)	1:A:79:SER:HA	1:A:81:LEU:HG	19	0.02
(1,4109)	1:B:79:SER:HA	1:B:81:LEU:HD21	20	0.02
(1,4109)	1:B:79:SER:HA	1:B:81:LEU:HD22	20	0.02
(1,4109)	1:B:79:SER:HA	1:B:81:LEU:HD23	20	0.02
(1,4091)	1:B:73:PHE:HA	1:B:73:PHE:HD1	3	0.02
(1,4091)	1:B:73:PHE:HA	1:B:73:PHE:HD2	3	0.02
(1,4090)	1:A:73:PHE:HA	1:A:73:PHE:HD1	4	0.02
(1,4090)	1:A:73:PHE:HA	1:A:73:PHE:HD2	4	0.02
(1,4090)	1:A:73:PHE:HA	1:A:73:PHE:HD1	6	0.02
(1,4090)	1:A:73:PHE:HA	1:A:73:PHE:HD2	6	0.02
(1,4090)	1:A:73:PHE:HA	1:A:73:PHE:HD1	13	0.02
(1,4090)	1:A:73:PHE:HA	1:A:73:PHE:HD2	13	0.02
(1,4090)	1:A:73:PHE:HA	1:A:73:PHE:HD1	16	0.02
(1,4090)	1:A:73:PHE:HA	1:A:73:PHE:HD2	16	0.02
(1,4090)	1:A:73:PHE:HA	1:A:73:PHE:HD1	20	0.02
(1,4090)	1:A:73:PHE:HA	1:A:73:PHE:HD2	20	0.02
(1,4053)	1:B:41:LYS:HG2	1:B:42:ASP:HA	9	0.02
(1,4053)	1:B:41:LYS:HG3	1:B:42:ASP:HA	9	0.02
(1,4052)	1:A:41:LYS:HG2	1:A:42:ASP:HA	11	0.02
(1,4052)	1:A:41:LYS:HG3	1:A:42:ASP:HA	11	0.02
(1,4052)	1:A:41:LYS:HG2	1:A:42:ASP:HA	20	0.02
(1,4052)	1:A:41:LYS:HG3	1:A:42:ASP:HA	20	0.02
(1,4049)	1:B:41:LYS:HA	1:B:41:LYS:HD2	9	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4049)	1:B:41:LYS:HA	1:B:41:LYS:HD3	9	0.02
(1,4049)	1:B:41:LYS:HA	1:B:41:LYS:HD2	12	0.02
(1,4049)	1:B:41:LYS:HA	1:B:41:LYS:HD3	12	0.02
(1,4048)	1:A:41:LYS:HA	1:A:41:LYS:HD2	9	0.02
(1,4048)	1:A:41:LYS:HA	1:A:41:LYS:HD3	9	0.02
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG2	6	0.02
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG3	6	0.02
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG2	15	0.02
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG3	15	0.02
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	7	0.02
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	7	0.02
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	3	0.02
(1,4036)	1:A:15:LYS:HA	1:A:17:GLY:H	8	0.02
(1,3994)	1:A:82:GLU:H	1:A:83:HIS:HB3	5	0.02
(1,3994)	1:A:82:GLU:H	1:A:83:HIS:HB3	16	0.02
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD11	10	0.02
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD12	10	0.02
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD13	10	0.02
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD11	10	0.02
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD12	10	0.02
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD13	10	0.02
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD11	10	0.02
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD12	10	0.02
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD13	10	0.02
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD11	18	0.02
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD12	18	0.02
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD13	18	0.02
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD11	18	0.02
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD12	18	0.02
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD13	18	0.02
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD11	18	0.02
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD12	18	0.02
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD13	18	0.02
(1,3984)	1:A:5:LEU:HD11	1:A:81:LEU:HD11	3	0.02
(1,3984)	1:A:5:LEU:HD11	1:A:81:LEU:HD12	3	0.02
(1,3984)	1:A:5:LEU:HD11	1:A:81:LEU:HD13	3	0.02
(1,3984)	1:A:5:LEU:HD12	1:A:81:LEU:HD11	3	0.02
(1,3984)	1:A:5:LEU:HD12	1:A:81:LEU:HD12	3	0.02
(1,3984)	1:A:5:LEU:HD12	1:A:81:LEU:HD13	3	0.02
(1,3984)	1:A:5:LEU:HD13	1:A:81:LEU:HD11	3	0.02
(1,3984)	1:A:5:LEU:HD13	1:A:81:LEU:HD12	3	0.02
(1,3984)	1:A:5:LEU:HD13	1:A:81:LEU:HD13	3	0.02



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3927)	1:B:23:THR:H	1:B:26:ILE:HD11	4	0.02
(1,3927)	1:B:23:THR:H	1:B:26:ILE:HD12	4	0.02
(1,3927)	1:B:23:THR:H	1:B:26:ILE:HD13	4	0.02
(1,3890)	1:B:82:GLU:HA	1:B:83:HIS:HB2	11	0.02
(1,3888)	1:B:8:ILE:H	1:B:81:LEU:HD21	3	0.02
(1,3888)	1:B:8:ILE:H	1:B:81:LEU:HD22	3	0.02
(1,3888)	1:B:8:ILE:H	1:B:81:LEU:HD23	3	0.02
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD21	8	0.02
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD22	8	0.02
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD23	8	0.02
(1,3876)	1:B:50:MET:HG3	1:B:81:LEU:HD21	8	0.02
(1,3876)	1:B:50:MET:HG3	1:B:81:LEU:HD22	8	0.02
(1,3876)	1:B:50:MET:HG3	1:B:81:LEU:HD23	8	0.02
(1,3860)	1:B:50:MET:HG3	1:B:81:LEU:HD11	17	0.02
(1,3860)	1:B:50:MET:HG3	1:B:81:LEU:HD12	17	0.02
(1,3860)	1:B:50:MET:HG3	1:B:81:LEU:HD13	17	0.02
(1,3824)	1:B:9:ARG:HD2	1:B:78:LEU:HD21	5	0.02
(1,3824)	1:B:9:ARG:HD2	1:B:78:LEU:HD22	5	0.02
(1,3824)	1:B:9:ARG:HD2	1:B:78:LEU:HD23	5	0.02
(1,3824)	1:B:9:ARG:HD3	1:B:78:LEU:HD21	5	0.02
(1,3824)	1:B:9:ARG:HD3	1:B:78:LEU:HD22	5	0.02
(1,3824)	1:B:9:ARG:HD3	1:B:78:LEU:HD23	5	0.02
(1,3824)	1:B:9:ARG:HD2	1:B:78:LEU:HD21	6	0.02
(1,3824)	1:B:9:ARG:HD2	1:B:78:LEU:HD22	6	0.02
(1,3824)	1:B:9:ARG:HD2	1:B:78:LEU:HD23	6	0.02
(1,3824)	1:B:9:ARG:HD3	1:B:78:LEU:HD21	6	0.02
(1,3824)	1:B:9:ARG:HD3	1:B:78:LEU:HD22	6	0.02
(1,3824)	1:B:9:ARG:HD3	1:B:78:LEU:HD23	6	0.02
(1,3824)	1:B:9:ARG:HD2	1:B:78:LEU:HD21	19	0.02
(1,3824)	1:B:9:ARG:HD2	1:B:78:LEU:HD22	19	0.02
(1,3824)	1:B:9:ARG:HD2	1:B:78:LEU:HD23	19	0.02
(1,3824)	1:B:9:ARG:HD3	1:B:78:LEU:HD21	19	0.02
(1,3824)	1:B:9:ARG:HD3	1:B:78:LEU:HD22	19	0.02
(1,3824)	1:B:9:ARG:HD3	1:B:78:LEU:HD23	19	0.02
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD21	4	0.02
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD22	4	0.02
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD23	4	0.02
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD21	4	0.02
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD22	4	0.02
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD23	4	0.02
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD21	13	0.02
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD22	13	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD23	13	0.02
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD21	13	0.02
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD22	13	0.02
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD23	13	0.02
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD21	16	0.02
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD22	16	0.02
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD23	16	0.02
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD21	16	0.02
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD22	16	0.02
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD23	16	0.02
(1,3821)	1:A:9:ARG:HB2	1:A:78:LEU:HD21	12	0.02
(1,3821)	1:A:9:ARG:HB2	1:A:78:LEU:HD22	12	0.02
(1,3821)	1:A:9:ARG:HB2	1:A:78:LEU:HD23	12	0.02
(1,3821)	1:A:9:ARG:HB3	1:A:78:LEU:HD21	12	0.02
(1,3821)	1:A:9:ARG:HB3	1:A:78:LEU:HD22	12	0.02
(1,3821)	1:A:9:ARG:HB3	1:A:78:LEU:HD23	12	0.02
(1,3821)	1:A:9:ARG:HB2	1:A:78:LEU:HD21	17	0.02
(1,3821)	1:A:9:ARG:HB2	1:A:78:LEU:HD22	17	0.02
(1,3821)	1:A:9:ARG:HB2	1:A:78:LEU:HD23	17	0.02
(1,3821)	1:A:9:ARG:HB3	1:A:78:LEU:HD21	17	0.02
(1,3821)	1:A:9:ARG:HB3	1:A:78:LEU:HD22	17	0.02
(1,3821)	1:A:9:ARG:HB3	1:A:78:LEU:HD23	17	0.02
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD11	6	0.02
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD12	6	0.02
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD13	6	0.02
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD11	9	0.02
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD12	9	0.02
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD13	9	0.02
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD11	12	0.02
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD12	12	0.02
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD13	12	0.02
(1,381)	1:B:22:ILE:H	1:B:23:THR:HG1	2	0.02
(1,381)	1:B:22:ILE:H	1:B:23:THR:HG1	4	0.02
(1,381)	1:B:22:ILE:H	1:B:23:THR:HG1	5	0.02
(1,381)	1:B:22:ILE:H	1:B:23:THR:HG1	6	0.02
(1,381)	1:B:22:ILE:H	1:B:23:THR:HG1	12	0.02
(1,381)	1:B:22:ILE:H	1:B:23:THR:HG1	13	0.02
(1,381)	1:B:22:ILE:H	1:B:23:THR:HG1	19	0.02
(1,3809)	1:A:48:ASN:HD21	1:A:78:LEU:HD11	12	0.02
(1,3809)	1:A:48:ASN:HD21	1:A:78:LEU:HD12	12	0.02
(1,3809)	1:A:48:ASN:HD21	1:A:78:LEU:HD13	12	0.02
(1,380)	1:A:22:ILE:H	1:A:23:THR:HG1	2	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,380)	1:A:22:ILE:H	1:A:23:THR:HG1	18	0.02
(1,3768)	1:B:77:ARG:HD2	1:B:78:LEU:H	19	0.02
(1,3768)	1:B:77:ARG:HD3	1:B:78:LEU:H	19	0.02
(1,3764)	1:B:4:PHE:HZ	1:B:77:ARG:HD2	18	0.02
(1,3764)	1:B:4:PHE:HZ	1:B:77:ARG:HD3	18	0.02
(1,3755)	1:A:59:LEU:HD21	1:A:77:ARG:HD2	10	0.02
(1,3755)	1:A:59:LEU:HD21	1:A:77:ARG:HD3	10	0.02
(1,3755)	1:A:59:LEU:HD22	1:A:77:ARG:HD2	10	0.02
(1,3755)	1:A:59:LEU:HD22	1:A:77:ARG:HD3	10	0.02
(1,3755)	1:A:59:LEU:HD23	1:A:77:ARG:HD2	10	0.02
(1,3755)	1:A:59:LEU:HD23	1:A:77:ARG:HD3	10	0.02
(1,3754)	1:B:59:LEU:HD11	1:B:77:ARG:HD2	7	0.02
(1,3754)	1:B:59:LEU:HD11	1:B:77:ARG:HD3	7	0.02
(1,3754)	1:B:59:LEU:HD12	1:B:77:ARG:HD2	7	0.02
(1,3754)	1:B:59:LEU:HD12	1:B:77:ARG:HD3	7	0.02
(1,3754)	1:B:59:LEU:HD13	1:B:77:ARG:HD2	7	0.02
(1,3754)	1:B:59:LEU:HD13	1:B:77:ARG:HD3	7	0.02
(1,3753)	1:A:59:LEU:HD11	1:A:77:ARG:HD2	6	0.02
(1,3753)	1:A:59:LEU:HD11	1:A:77:ARG:HD3	6	0.02
(1,3753)	1:A:59:LEU:HD12	1:A:77:ARG:HD2	6	0.02
(1,3753)	1:A:59:LEU:HD12	1:A:77:ARG:HD3	6	0.02
(1,3753)	1:A:59:LEU:HD13	1:A:77:ARG:HD2	6	0.02
(1,3753)	1:A:59:LEU:HD13	1:A:77:ARG:HD3	6	0.02
(1,3753)	1:A:59:LEU:HD11	1:A:77:ARG:HD2	12	0.02
(1,3753)	1:A:59:LEU:HD11	1:A:77:ARG:HD3	12	0.02
(1,3753)	1:A:59:LEU:HD12	1:A:77:ARG:HD2	12	0.02
(1,3753)	1:A:59:LEU:HD12	1:A:77:ARG:HD3	12	0.02
(1,3753)	1:A:59:LEU:HD13	1:A:77:ARG:HD2	12	0.02
(1,3753)	1:A:59:LEU:HD13	1:A:77:ARG:HD3	12	0.02
(1,3753)	1:A:59:LEU:HD11	1:A:77:ARG:HD2	16	0.02
(1,3753)	1:A:59:LEU:HD11	1:A:77:ARG:HD3	16	0.02
(1,3753)	1:A:59:LEU:HD12	1:A:77:ARG:HD2	16	0.02
(1,3753)	1:A:59:LEU:HD12	1:A:77:ARG:HD3	16	0.02
(1,3753)	1:A:59:LEU:HD13	1:A:77:ARG:HD2	16	0.02
(1,3753)	1:A:59:LEU:HD13	1:A:77:ARG:HD3	16	0.02
(1,3734)	1:B:74:THR:HA	1:B:76:GLU:HG2	15	0.02
(1,3734)	1:B:74:THR:HA	1:B:76:GLU:HG3	15	0.02
(1,3732)	1:B:9:ARG:HB2	1:B:76:GLU:HG2	1	0.02
(1,3732)	1:B:9:ARG:HB2	1:B:76:GLU:HG3	1	0.02
(1,3732)	1:B:9:ARG:HB3	1:B:76:GLU:HG2	1	0.02
(1,3732)	1:B:9:ARG:HB3	1:B:76:GLU:HG3	1	0.02
(1,3732)	1:B:9:ARG:HB2	1:B:76:GLU:HG2	15	0.02



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Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,3732)	1:B:9:ARG:HB2	1:B:76:GLU:HG3	15	0.02
(1,3732)	1:B:9:ARG:HB3	1:B:76:GLU:HG2	15	0.02
(1,3732)	1:B:9:ARG:HB3	1:B:76:GLU:HG3	15	0.02
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	8	0.02
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	8	0.02
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	8	0.02
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	17	0.02
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	17	0.02
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	17	0.02
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG21	6	0.02
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG22	6	0.02
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG23	6	0.02
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG21	6	0.02
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG22	6	0.02
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG23	6	0.02
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG21	9	0.02
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG22	9	0.02
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG23	9	0.02
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG21	9	0.02
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG22	9	0.02
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG23	9	0.02
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG21	11	0.02
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG22	11	0.02
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG23	11	0.02
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG21	11	0.02
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG22	11	0.02
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG23	11	0.02
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG21	18	0.02
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG22	18	0.02
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG23	18	0.02
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG21	18	0.02
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG22	18	0.02
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG23	18	0.02
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG21	20	0.02
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG22	20	0.02
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG23	20	0.02
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG21	20	0.02
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG22	20	0.02
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG23	20	0.02
(1,3688)	1:B:74:THR:HB	1:B:75:VAL:H	6	0.02
(1,3686)	1:B:10:ILE:HA	1:B:74:THR:HB	2	0.02
(1,3686)	1:B:10:ILE:HA	1:B:74:THR:HB	17	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3659)	1:A:66:LEU:HA	1:A:72:VAL:HG21	7	0.02
(1,3659)	1:A:66:LEU:HA	1:A:72:VAL:HG22	7	0.02
(1,3659)	1:A:66:LEU:HA	1:A:72:VAL:HG23	7	0.02
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG11	12	0.02
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG12	12	0.02
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG13	12	0.02
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG11	18	0.02
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG12	18	0.02
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG13	18	0.02
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG11	4	0.02
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG12	4	0.02
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG13	4	0.02
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG11	14	0.02
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG12	14	0.02
(1,3637)	1:A:67:ARG:HA	1:A:72:VAL:HG13	14	0.02
(1,3614)	1:B:69:VAL:H	1:B:70:GLN:HB2	6	0.02
(1,3614)	1:B:69:VAL:H	1:B:70:GLN:HB3	6	0.02
(1,3605)	1:A:69:VAL:HG11	1:A:70:GLN:HB2	12	0.02
(1,3605)	1:A:69:VAL:HG11	1:A:70:GLN:HB3	12	0.02
(1,3605)	1:A:69:VAL:HG12	1:A:70:GLN:HB2	12	0.02
(1,3605)	1:A:69:VAL:HG12	1:A:70:GLN:HB3	12	0.02
(1,3605)	1:A:69:VAL:HG13	1:A:70:GLN:HB2	12	0.02
(1,3605)	1:A:69:VAL:HG13	1:A:70:GLN:HB3	12	0.02
(1,3594)	1:B:66:LEU:HA	1:B:69:VAL:HB	12	0.02
(1,3593)	1:A:66:LEU:HA	1:A:69:VAL:HB	5	0.02
(1,3593)	1:A:66:LEU:HA	1:A:69:VAL:HB	9	0.02
(1,3593)	1:A:66:LEU:HA	1:A:69:VAL:HB	13	0.02
(1,3593)	1:A:66:LEU:HA	1:A:69:VAL:HB	14	0.02
(1,3592)	1:B:20:ASN:HA	1:B:22:ILE:HB	10	0.02
(1,3592)	1:B:20:ASN:HA	1:B:22:ILE:HB	11	0.02
(1,3591)	1:A:20:ASN:HA	1:A:22:ILE:HB	1	0.02
(1,3591)	1:A:20:ASN:HA	1:A:22:ILE:HB	6	0.02
(1,3591)	1:A:20:ASN:HA	1:A:22:ILE:HB	15	0.02
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG11	8	0.02
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG12	8	0.02
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG13	8	0.02
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG11	8	0.02
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG12	8	0.02
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG13	8	0.02
(1,3562)	1:B:15:LYS:HE2	1:B:18:MET:H	1	0.02
(1,3562)	1:B:15:LYS:HE3	1:B:18:MET:H	1	0.02
(1,3562)	1:B:15:LYS:HE2	1:B:18:MET:H	10	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3562)	1:B:15:LYS:HE3	1:B:18:MET:H	10	0.02
(1,3561)	1:A:15:LYS:HE2	1:A:18:MET:H	8	0.02
(1,3561)	1:A:15:LYS:HE3	1:A:18:MET:H	8	0.02
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	12	0.02
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	12	0.02
(1,3552)	1:B:68:LYS:HA	1:B:68:LYS:HE2	4	0.02
(1,3552)	1:B:68:LYS:HA	1:B:68:LYS:HE3	4	0.02
(1,3516)	1:B:67:ARG:HD2	1:B:75:VAL:HG11	6	0.02
(1,3516)	1:B:67:ARG:HD2	1:B:75:VAL:HG12	6	0.02
(1,3516)	1:B:67:ARG:HD2	1:B:75:VAL:HG13	6	0.02
(1,3516)	1:B:67:ARG:HD3	1:B:75:VAL:HG11	6	0.02
(1,3516)	1:B:67:ARG:HD3	1:B:75:VAL:HG12	6	0.02
(1,3516)	1:B:67:ARG:HD3	1:B:75:VAL:HG13	6	0.02
(1,3515)	1:A:67:ARG:HD2	1:A:75:VAL:HG11	13	0.02
(1,3515)	1:A:67:ARG:HD2	1:A:75:VAL:HG12	13	0.02
(1,3515)	1:A:67:ARG:HD2	1:A:75:VAL:HG13	13	0.02
(1,3515)	1:A:67:ARG:HD3	1:A:75:VAL:HG11	13	0.02
(1,3515)	1:A:67:ARG:HD3	1:A:75:VAL:HG12	13	0.02
(1,3515)	1:A:67:ARG:HD3	1:A:75:VAL:HG13	13	0.02
(1,3511)	1:A:64:ASP:HA	1:A:67:ARG:HG3	17	0.02
(1,349)	1:B:18:MET:HE1	1:B:21:GLN:HE22	14	0.02
(1,349)	1:B:18:MET:HE2	1:B:21:GLN:HE22	14	0.02
(1,349)	1:B:18:MET:HE3	1:B:21:GLN:HE22	14	0.02
(1,348)	1:A:18:MET:HE1	1:A:21:GLN:HE22	20	0.02
(1,348)	1:A:18:MET:HE2	1:A:21:GLN:HE22	20	0.02
(1,348)	1:A:18:MET:HE3	1:A:21:GLN:HE22	20	0.02
(1,3423)	1:B:9:ARG:H	1:B:63:MET:HE1	20	0.02
(1,3423)	1:B:9:ARG:H	1:B:63:MET:HE2	20	0.02
(1,3423)	1:B:9:ARG:H	1:B:63:MET:HE3	20	0.02
(1,3422)	1:A:9:ARG:H	1:A:63:MET:HE1	4	0.02
(1,3422)	1:A:9:ARG:H	1:A:63:MET:HE2	4	0.02
(1,3422)	1:A:9:ARG:H	1:A:63:MET:HE3	4	0.02
(1,3421)	1:B:63:MET:HE1	1:B:77:ARG:H	12	0.02
(1,3421)	1:B:63:MET:HE2	1:B:77:ARG:H	12	0.02
(1,3421)	1:B:63:MET:HE3	1:B:77:ARG:H	12	0.02
(1,3421)	1:B:63:MET:HE1	1:B:77:ARG:H	15	0.02
(1,3421)	1:B:63:MET:HE2	1:B:77:ARG:H	15	0.02
(1,3421)	1:B:63:MET:HE3	1:B:77:ARG:H	15	0.02
(1,3421)	1:B:63:MET:HE1	1:B:77:ARG:H	19	0.02
(1,3421)	1:B:63:MET:HE2	1:B:77:ARG:H	19	0.02
(1,3421)	1:B:63:MET:HE3	1:B:77:ARG:H	19	0.02
(1,3420)	1:A:63:MET:HE1	1:A:77:ARG:H	11	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3420)	1:A:63:MET:HE2	1:A:77:ARG:H	11	0.02
(1,3420)	1:A:63:MET:HE3	1:A:77:ARG:H	11	0.02
(1,3420)	1:A:63:MET:HE1	1:A:77:ARG:H	17	0.02
(1,3420)	1:A:63:MET:HE2	1:A:77:ARG:H	17	0.02
(1,3420)	1:A:63:MET:HE3	1:A:77:ARG:H	17	0.02
(1,3413)	1:B:63:MET:HE1	1:B:76:GLU:HA	15	0.02
(1,3413)	1:B:63:MET:HE2	1:B:76:GLU:HA	15	0.02
(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	15	0.02
(1,3413)	1:B:63:MET:HE1	1:B:76:GLU:HA	16	0.02
(1,3413)	1:B:63:MET:HE2	1:B:76:GLU:HA	16	0.02
(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	16	0.02
(1,3412)	1:A:63:MET:HE1	1:A:76:GLU:HA	13	0.02
(1,3412)	1:A:63:MET:HE2	1:A:76:GLU:HA	13	0.02
(1,3412)	1:A:63:MET:HE3	1:A:76:GLU:HA	13	0.02
(1,3343)	1:B:62:LEU:HD11	1:B:63:MET:HA	3	0.02
(1,3343)	1:B:62:LEU:HD12	1:B:63:MET:HA	3	0.02
(1,3343)	1:B:62:LEU:HD13	1:B:63:MET:HA	3	0.02
(1,3335)	1:B:58:LYS:HE2	1:B:62:LEU:HD11	3	0.02
(1,3335)	1:B:58:LYS:HE2	1:B:62:LEU:HD12	3	0.02
(1,3335)	1:B:58:LYS:HE2	1:B:62:LEU:HD13	3	0.02
(1,3335)	1:B:58:LYS:HE2	1:B:62:LEU:HD11	18	0.02
(1,3335)	1:B:58:LYS:HE2	1:B:62:LEU:HD12	18	0.02
(1,3335)	1:B:58:LYS:HE2	1:B:62:LEU:HD13	18	0.02
(1,3334)	1:A:58:LYS:HE2	1:A:62:LEU:HD11	12	0.02
(1,3334)	1:A:58:LYS:HE2	1:A:62:LEU:HD12	12	0.02
(1,3334)	1:A:58:LYS:HE2	1:A:62:LEU:HD13	12	0.02
(1,3331)	1:B:62:LEU:HD11	1:B:66:LEU:HG	11	0.02
(1,3331)	1:B:62:LEU:HD12	1:B:66:LEU:HG	11	0.02
(1,3331)	1:B:62:LEU:HD13	1:B:66:LEU:HG	11	0.02
(1,3330)	1:A:62:LEU:HD11	1:A:66:LEU:HG	4	0.02
(1,3330)	1:A:62:LEU:HD12	1:A:66:LEU:HG	4	0.02
(1,3330)	1:A:62:LEU:HD13	1:A:66:LEU:HG	4	0.02
(1,3293)	1:A:58:LYS:HZ1	1:A:61:THR:HG21	1	0.02
(1,3293)	1:A:58:LYS:HZ1	1:A:61:THR:HG22	1	0.02
(1,3293)	1:A:58:LYS:HZ1	1:A:61:THR:HG23	1	0.02
(1,3293)	1:A:58:LYS:HZ2	1:A:61:THR:HG21	1	0.02
(1,3293)	1:A:58:LYS:HZ2	1:A:61:THR:HG22	1	0.02
(1,3293)	1:A:58:LYS:HZ2	1:A:61:THR:HG23	1	0.02
(1,3293)	1:A:58:LYS:HZ3	1:A:61:THR:HG21	1	0.02
(1,3293)	1:A:58:LYS:HZ3	1:A:61:THR:HG22	1	0.02
(1,3293)	1:A:58:LYS:HZ3	1:A:61:THR:HG23	1	0.02
(1,3288)	1:B:61:THR:HG21	1:B:65:LYS:HE2	3	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3288)	1:B:61:THR:HG21	1:B:65:LYS:HE3	3	0.02
(1,3288)	1:B:61:THR:HG22	1:B:65:LYS:HE2	3	0.02
(1,3288)	1:B:61:THR:HG22	1:B:65:LYS:HE3	3	0.02
(1,3288)	1:B:61:THR:HG23	1:B:65:LYS:HE2	3	0.02
(1,3288)	1:B:61:THR:HG23	1:B:65:LYS:HE3	3	0.02
(1,3288)	1:B:61:THR:HG21	1:B:65:LYS:HE2	10	0.02
(1,3288)	1:B:61:THR:HG21	1:B:65:LYS:HE3	10	0.02
(1,3288)	1:B:61:THR:HG22	1:B:65:LYS:HE2	10	0.02
(1,3288)	1:B:61:THR:HG22	1:B:65:LYS:HE3	10	0.02
(1,3288)	1:B:61:THR:HG23	1:B:65:LYS:HE2	10	0.02
(1,3288)	1:B:61:THR:HG23	1:B:65:LYS:HE3	10	0.02
(1,3224)	1:B:6:ALA:HB1	1:B:59:LEU:HD21	4	0.02
(1,3224)	1:B:6:ALA:HB1	1:B:59:LEU:HD22	4	0.02
(1,3224)	1:B:6:ALA:HB1	1:B:59:LEU:HD23	4	0.02
(1,3224)	1:B:6:ALA:HB2	1:B:59:LEU:HD21	4	0.02
(1,3224)	1:B:6:ALA:HB2	1:B:59:LEU:HD22	4	0.02
(1,3224)	1:B:6:ALA:HB2	1:B:59:LEU:HD23	4	0.02
(1,3224)	1:B:6:ALA:HB3	1:B:59:LEU:HD21	4	0.02
(1,3224)	1:B:6:ALA:HB3	1:B:59:LEU:HD22	4	0.02
(1,3224)	1:B:6:ALA:HB3	1:B:59:LEU:HD23	4	0.02
(1,3224)	1:B:6:ALA:HB1	1:B:59:LEU:HD21	13	0.02
(1,3224)	1:B:6:ALA:HB1	1:B:59:LEU:HD22	13	0.02
(1,3224)	1:B:6:ALA:HB1	1:B:59:LEU:HD23	13	0.02
(1,3224)	1:B:6:ALA:HB2	1:B:59:LEU:HD21	13	0.02
(1,3224)	1:B:6:ALA:HB2	1:B:59:LEU:HD22	13	0.02
(1,3224)	1:B:6:ALA:HB2	1:B:59:LEU:HD23	13	0.02
(1,3224)	1:B:6:ALA:HB3	1:B:59:LEU:HD21	13	0.02
(1,3224)	1:B:6:ALA:HB3	1:B:59:LEU:HD22	13	0.02
(1,3224)	1:B:6:ALA:HB3	1:B:59:LEU:HD23	13	0.02
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD21	9	0.02
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD22	9	0.02
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD23	9	0.02
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD21	9	0.02
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD22	9	0.02
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD23	9	0.02
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD21	9	0.02
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD22	9	0.02
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD23	9	0.02
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD21	15	0.02
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD22	15	0.02
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD23	15	0.02
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD21	15	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD22	15	0.02
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD23	15	0.02
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD21	15	0.02
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD22	15	0.02
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD23	15	0.02
(1,3212)	1:B:6:ALA:HB1	1:B:59:LEU:HD11	13	0.02
(1,3212)	1:B:6:ALA:HB1	1:B:59:LEU:HD12	13	0.02
(1,3212)	1:B:6:ALA:HB1	1:B:59:LEU:HD13	13	0.02
(1,3212)	1:B:6:ALA:HB2	1:B:59:LEU:HD11	13	0.02
(1,3212)	1:B:6:ALA:HB2	1:B:59:LEU:HD12	13	0.02
(1,3212)	1:B:6:ALA:HB2	1:B:59:LEU:HD13	13	0.02
(1,3212)	1:B:6:ALA:HB3	1:B:59:LEU:HD11	13	0.02
(1,3212)	1:B:6:ALA:HB3	1:B:59:LEU:HD12	13	0.02
(1,3212)	1:B:6:ALA:HB3	1:B:59:LEU:HD13	13	0.02
(1,3212)	1:B:6:ALA:HB1	1:B:59:LEU:HD11	18	0.02
(1,3212)	1:B:6:ALA:HB1	1:B:59:LEU:HD12	18	0.02
(1,3212)	1:B:6:ALA:HB1	1:B:59:LEU:HD13	18	0.02
(1,3212)	1:B:6:ALA:HB2	1:B:59:LEU:HD11	18	0.02
(1,3212)	1:B:6:ALA:HB2	1:B:59:LEU:HD12	18	0.02
(1,3212)	1:B:6:ALA:HB2	1:B:59:LEU:HD13	18	0.02
(1,3212)	1:B:6:ALA:HB3	1:B:59:LEU:HD11	18	0.02
(1,3212)	1:B:6:ALA:HB3	1:B:59:LEU:HD12	18	0.02
(1,3212)	1:B:6:ALA:HB3	1:B:59:LEU:HD13	18	0.02
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD11	2	0.02
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD12	2	0.02
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD13	2	0.02
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD11	2	0.02
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD12	2	0.02
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD13	2	0.02
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD11	2	0.02
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD12	2	0.02
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD13	2	0.02
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD11	7	0.02
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD12	7	0.02
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD13	7	0.02
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD11	7	0.02
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD12	7	0.02
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD13	7	0.02
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD11	7	0.02
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD12	7	0.02
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD13	7	0.02
(1,3185)	1:A:58:LYS:H	1:A:58:LYS:HD2	6	0.02



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3185)	1:A:58:LYS:H	1:A:58:LYS:HD3	6	0.02
(1,3176)	1:B:30:ASP:HB2	1:B:58:LYS:HD2	9	0.02
(1,3176)	1:B:30:ASP:HB2	1:B:58:LYS:HD3	9	0.02
(1,3176)	1:B:30:ASP:HB3	1:B:58:LYS:HD2	9	0.02
(1,3176)	1:B:30:ASP:HB3	1:B:58:LYS:HD3	9	0.02
(1,3175)	1:A:30:ASP:HB2	1:A:58:LYS:HD2	18	0.02
(1,3175)	1:A:30:ASP:HB2	1:A:58:LYS:HD3	18	0.02
(1,3175)	1:A:30:ASP:HB3	1:A:58:LYS:HD2	18	0.02
(1,3175)	1:A:30:ASP:HB3	1:A:58:LYS:HD3	18	0.02
(1,3130)	1:B:4:PHE:HD1	1:B:56:THR:HG21	11	0.02
(1,3130)	1:B:4:PHE:HD1	1:B:56:THR:HG22	11	0.02
(1,3130)	1:B:4:PHE:HD1	1:B:56:THR:HG23	11	0.02
(1,3130)	1:B:4:PHE:HD2	1:B:56:THR:HG21	11	0.02
(1,3130)	1:B:4:PHE:HD2	1:B:56:THR:HG22	11	0.02
(1,3130)	1:B:4:PHE:HD2	1:B:56:THR:HG23	11	0.02
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG21	10	0.02
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG22	10	0.02
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG23	10	0.02
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG21	10	0.02
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG22	10	0.02
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG23	10	0.02
(1,3099)	1:A:54:LYS:H	1:A:54:LYS:HD2	9	0.02
(1,3099)	1:A:54:LYS:H	1:A:54:LYS:HD3	9	0.02
(1,3093)	1:A:15:LYS:HD2	1:A:16:ASN:HD22	15	0.02
(1,3093)	1:A:15:LYS:HD3	1:A:16:ASN:HD22	15	0.02
(1,3091)	1:A:54:LYS:HA	1:A:54:LYS:HD2	7	0.02
(1,3091)	1:A:54:LYS:HA	1:A:54:LYS:HD3	7	0.02
(1,3091)	1:A:54:LYS:HA	1:A:54:LYS:HD2	12	0.02
(1,3091)	1:A:54:LYS:HA	1:A:54:LYS:HD3	12	0.02
(1,3041)	1:A:5:LEU:HA	1:A:53:VAL:HG21	9	0.02
(1,3041)	1:A:5:LEU:HA	1:A:53:VAL:HG22	9	0.02
(1,3041)	1:A:5:LEU:HA	1:A:53:VAL:HG23	9	0.02
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG11	5	0.02
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG12	5	0.02
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG13	5	0.02
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG11	3	0.02
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG12	3	0.02
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG13	3	0.02
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG11	15	0.02
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG12	15	0.02
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG13	15	0.02
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	6	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	6	0.02
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	6	0.02
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	6	0.02
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	6	0.02
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	6	0.02
(1,2972)	1:B:53:VAL:HG11	1:B:62:LEU:HD21	4	0.02
(1,2972)	1:B:53:VAL:HG11	1:B:62:LEU:HD22	4	0.02
(1,2972)	1:B:53:VAL:HG11	1:B:62:LEU:HD23	4	0.02
(1,2972)	1:B:53:VAL:HG12	1:B:62:LEU:HD21	4	0.02
(1,2972)	1:B:53:VAL:HG12	1:B:62:LEU:HD22	4	0.02
(1,2972)	1:B:53:VAL:HG12	1:B:62:LEU:HD23	4	0.02
(1,2972)	1:B:53:VAL:HG13	1:B:62:LEU:HD21	4	0.02
(1,2972)	1:B:53:VAL:HG13	1:B:62:LEU:HD22	4	0.02
(1,2972)	1:B:53:VAL:HG13	1:B:62:LEU:HD23	4	0.02
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD11	17	0.02
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD12	17	0.02
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD13	17	0.02
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	8	0.02
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	8	0.02
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	8	0.02
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	8	0.02
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	8	0.02
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	8	0.02
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	8	0.02
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	8	0.02
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	8	0.02
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD11	16	0.02
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD12	16	0.02
(1,2946)	1:B:29:PHE:HD1	1:B:51:ILE:HD13	16	0.02
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD11	16	0.02
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD12	16	0.02
(1,2946)	1:B:29:PHE:HD2	1:B:51:ILE:HD13	16	0.02
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD11	3	0.02
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD12	3	0.02
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD13	3	0.02
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD11	3	0.02
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD12	3	0.02
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD13	3	0.02
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD11	11	0.02
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD12	11	0.02
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD13	11	0.02
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD11	11	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD12	11	0.02
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD13	11	0.02
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD21	9	0.02
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD22	9	0.02
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD23	9	0.02
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD21	9	0.02
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD22	9	0.02
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD23	9	0.02
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD21	9	0.02
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD22	9	0.02
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD23	9	0.02
(1,2902)	1:A:51:ILE:HG21	1:B:20:ASN:HD22	18	0.02
(1,2902)	1:A:51:ILE:HG22	1:B:20:ASN:HD22	18	0.02
(1,2902)	1:A:51:ILE:HG23	1:B:20:ASN:HD22	18	0.02
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG21	2	0.02
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG22	2	0.02
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG23	2	0.02
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG21	4	0.02
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG22	4	0.02
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG23	4	0.02
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG21	6	0.02
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG22	6	0.02
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG23	6	0.02
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG21	11	0.02
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG22	11	0.02
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG23	11	0.02
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG21	17	0.02
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG22	17	0.02
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG23	17	0.02
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG21	1	0.02
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG22	1	0.02
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG23	1	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG21	2	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG22	2	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG23	2	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG21	3	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG22	3	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG23	3	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG21	4	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG22	4	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG23	4	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG21	5	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG22	5	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG23	5	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG21	10	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG22	10	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG23	10	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG21	15	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG22	15	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG23	15	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG21	16	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG22	16	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG23	16	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG21	18	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG22	18	0.02
(1,2888)	1:B:33:ILE:HA	1:B:51:ILE:HG23	18	0.02
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG21	4	0.02
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG22	4	0.02
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG23	4	0.02
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG21	7	0.02
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG22	7	0.02
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG23	7	0.02
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG21	16	0.02
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG22	16	0.02
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG23	16	0.02
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG21	19	0.02
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG22	19	0.02
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG23	19	0.02
(1,2882)	1:B:8:ILE:HG21	1:B:62:LEU:HD11	4	0.02
(1,2882)	1:B:8:ILE:HG21	1:B:62:LEU:HD12	4	0.02
(1,2882)	1:B:8:ILE:HG21	1:B:62:LEU:HD13	4	0.02
(1,2882)	1:B:8:ILE:HG22	1:B:62:LEU:HD11	4	0.02
(1,2882)	1:B:8:ILE:HG22	1:B:62:LEU:HD12	4	0.02
(1,2882)	1:B:8:ILE:HG22	1:B:62:LEU:HD13	4	0.02
(1,2882)	1:B:8:ILE:HG23	1:B:62:LEU:HD11	4	0.02
(1,2882)	1:B:8:ILE:HG23	1:B:62:LEU:HD12	4	0.02
(1,2882)	1:B:8:ILE:HG23	1:B:62:LEU:HD13	4	0.02
(1,2833)	1:A:6:ALA:HA	1:A:50:MET:HE1	1	0.02
(1,2833)	1:A:6:ALA:HA	1:A:50:MET:HE2	1	0.02
(1,2833)	1:A:6:ALA:HA	1:A:50:MET:HE3	1	0.02
(1,2830)	1:B:50:MET:HE1	1:B:81:LEU:HA	9	0.02
(1,2830)	1:B:50:MET:HE2	1:B:81:LEU:HA	9	0.02
(1,2830)	1:B:50:MET:HE3	1:B:81:LEU:HA	9	0.02
(1,2816)	1:B:50:MET:HE1	1:B:51:ILE:HG13	9	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2816)	1:B:50:MET:HE2	1:B:51:ILE:HG13	9	0.02
(1,2816)	1:B:50:MET:HE3	1:B:51:ILE:HG13	9	0.02
(1,2816)	1:B:50:MET:HE1	1:B:51:ILE:HG13	20	0.02
(1,2816)	1:B:50:MET:HE2	1:B:51:ILE:HG13	20	0.02
(1,2816)	1:B:50:MET:HE3	1:B:51:ILE:HG13	20	0.02
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	2	0.02
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	2	0.02
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	2	0.02
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	6	0.02
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	6	0.02
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	6	0.02
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	7	0.02
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	7	0.02
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	7	0.02
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	16	0.02
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	16	0.02
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	16	0.02
(1,2812)	1:B:50:MET:HE1	1:B:81:LEU:HD21	8	0.02
(1,2812)	1:B:50:MET:HE1	1:B:81:LEU:HD22	8	0.02
(1,2812)	1:B:50:MET:HE1	1:B:81:LEU:HD23	8	0.02
(1,2812)	1:B:50:MET:HE2	1:B:81:LEU:HD21	8	0.02
(1,2812)	1:B:50:MET:HE2	1:B:81:LEU:HD22	8	0.02
(1,2812)	1:B:50:MET:HE2	1:B:81:LEU:HD23	8	0.02
(1,2812)	1:B:50:MET:HE3	1:B:81:LEU:HD21	8	0.02
(1,2812)	1:B:50:MET:HE3	1:B:81:LEU:HD22	8	0.02
(1,2812)	1:B:50:MET:HE3	1:B:81:LEU:HD23	8	0.02
(1,2792)	1:B:8:ILE:H	1:B:50:MET:HG3	13	0.02
(1,2792)	1:B:8:ILE:H	1:B:50:MET:HG3	19	0.02
(1,2791)	1:A:8:ILE:H	1:A:50:MET:HG3	9	0.02
(1,2791)	1:A:8:ILE:H	1:A:50:MET:HG3	19	0.02
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	1	0.02
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	4	0.02
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	11	0.02
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	12	0.02
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	13	0.02
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD11	1	0.02
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD12	1	0.02
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD13	1	0.02
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD11	1	0.02
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD12	1	0.02
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD13	1	0.02
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD11	1	0.02



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD12	1	0.02
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD13	1	0.02
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD11	3	0.02
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD12	3	0.02
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD13	3	0.02
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD11	3	0.02
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD12	3	0.02
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD13	3	0.02
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD11	3	0.02
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD12	3	0.02
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD13	3	0.02
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD11	13	0.02
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD12	13	0.02
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD13	13	0.02
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD11	13	0.02
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD12	13	0.02
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD13	13	0.02
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD11	13	0.02
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD12	13	0.02
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD13	13	0.02
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD11	14	0.02
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD12	14	0.02
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD13	14	0.02
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD11	14	0.02
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD12	14	0.02
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD13	14	0.02
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD11	14	0.02
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD12	14	0.02
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD13	14	0.02
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD11	6	0.02
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD12	6	0.02
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD13	6	0.02
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD11	6	0.02
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD12	6	0.02
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD13	6	0.02
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD11	6	0.02
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD12	6	0.02
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD13	6	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD21	2	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD22	2	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD23	2	0.02
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD21	2	0.02



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD22	2	0.02
	1:B:49:LEU:HD12		2	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD21	2	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD22	2	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD23	2	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD21	7	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD22	7	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD23	7	0.02
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD21	7	0.02
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD22	7	0.02
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD23	7	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD21	7	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD22	7	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD23	7	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD21	8	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD22	8	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD23	8	0.02
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD21	8	0.02
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD22	8	0.02
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD23	8	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD21	8	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD22	8	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD23	8	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD21	13	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD22	13	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD23	13	0.02
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD21	13	0.02
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD22	13	0.02
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD23	13	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD21	13	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD22	13	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD23	13	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD21	16	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD22	16	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD23	16	0.02
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD21	16	0.02
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD22	16	0.02
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD23	16	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD21	16	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD22	16	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD23	16	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD21	20	0.02



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD22	20	0.02
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD23	20	0.02
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD21	20	0.02
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD22	20	0.02
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD23	20	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD21	20	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD22	20	0.02
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD23	20	0.02
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD21	12	0.02
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD22	12	0.02
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD23	12	0.02
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD21	12	0.02
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD22	12	0.02
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD23	12	0.02
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD21	12	0.02
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD22	12	0.02
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD23	12	0.02
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD21	13	0.02
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD22	13	0.02
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD23	13	0.02
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD21	13	0.02
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD22	13	0.02
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD23	13	0.02
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD21	13	0.02
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD22	13	0.02
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD23	13	0.02
(1,2668)	1:B:23:THR:HG1	1:B:47:CYS:HB3	3	0.02
(1,2668)	1:B:23:THR:HG1	1:B:47:CYS:HB3	9	0.02
(1,2667)	1:A:23:THR:HG1	1:A:47:CYS:HB3	1	0.02
(1,2667)	1:A:23:THR:HG1	1:A:47:CYS:HB3	5	0.02
(1,2640)	1:B:46:THR:HG21	1:B:47:CYS:H	5	0.02
(1,2640)	1:B:46:THR:HG22	1:B:47:CYS:H	5	0.02
(1,2640)	1:B:46:THR:HG23	1:B:47:CYS:H	5	0.02
(1,2640)	1:B:46:THR:HG21	1:B:47:CYS:H	8	0.02
(1,2640)	1:B:46:THR:HG22	1:B:47:CYS:H	8	0.02
(1,2640)	1:B:46:THR:HG23	1:B:47:CYS:H	8	0.02
(1,2640)	1:B:46:THR:HG21	1:B:47:CYS:H	17	0.02
(1,2640)	1:B:46:THR:HG22	1:B:47:CYS:H	17	0.02
(1,2640)	1:B:46:THR:HG23	1:B:47:CYS:H	17	0.02
(1,2639)	1:A:46:THR:HG21	1:A:47:CYS:H	4	0.02
(1,2639)	1:A:46:THR:HG22	1:A:47:CYS:H	4	0.02
(1,2639)	1:A:46:THR:HG23	1:A:47:CYS:H	4	0.02



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2639)	1:A:46:THR:HG21	1:A:47:CYS:H	6	0.02
(1,2639)	1:A:46:THR:HG22	1:A:47:CYS:H	6	0.02
(1,2639)	1:A:46:THR:HG23	1:A:47:CYS:H	6	0.02
(1,2639)	1:A:46:THR:HG21	1:A:47:CYS:H	11	0.02
(1,2639)	1:A:46:THR:HG22	1:A:47:CYS:H	11	0.02
(1,2639)	1:A:46:THR:HG23	1:A:47:CYS:H	11	0.02
(1,2638)	1:B:10:ILE:H	1:B:46:THR:HG21	17	0.02
(1,2638)	1:B:10:ILE:H	1:B:46:THR:HG22	17	0.02
(1,2638)	1:B:10:ILE:H	1:B:46:THR:HG23	17	0.02
(1,2637)	1:A:10:ILE:H	1:A:46:THR:HG21	9	0.02
(1,2637)	1:A:10:ILE:H	1:A:46:THR:HG22	9	0.02
(1,2637)	1:A:10:ILE:H	1:A:46:THR:HG23	9	0.02
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG21	8	0.02
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG22	8	0.02
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG23	8	0.02
(1,2618)	1:B:9:ARG:HD2	1:B:46:THR:HG21	3	0.02
(1,2618)	1:B:9:ARG:HD2	1:B:46:THR:HG22	3	0.02
(1,2618)	1:B:9:ARG:HD2	1:B:46:THR:HG23	3	0.02
(1,2618)	1:B:9:ARG:HD3	1:B:46:THR:HG21	3	0.02
(1,2618)	1:B:9:ARG:HD3	1:B:46:THR:HG22	3	0.02
(1,2618)	1:B:9:ARG:HD3	1:B:46:THR:HG23	3	0.02
(1,2617)	1:A:9:ARG:HD2	1:A:46:THR:HG21	8	0.02
(1,2617)	1:A:9:ARG:HD2	1:A:46:THR:HG22	8	0.02
(1,2617)	1:A:9:ARG:HD2	1:A:46:THR:HG23	8	0.02
(1,2617)	1:A:9:ARG:HD3	1:A:46:THR:HG21	8	0.02
(1,2617)	1:A:9:ARG:HD3	1:A:46:THR:HG22	8	0.02
(1,2617)	1:A:9:ARG:HD3	1:A:46:THR:HG23	8	0.02
(1,2617)	1:A:9:ARG:HD2	1:A:46:THR:HG21	17	0.02
(1,2617)	1:A:9:ARG:HD2	1:A:46:THR:HG22	17	0.02
(1,2617)	1:A:9:ARG:HD2	1:A:46:THR:HG23	17	0.02
(1,2617)	1:A:9:ARG:HD3	1:A:46:THR:HG21	17	0.02
(1,2617)	1:A:9:ARG:HD3	1:A:46:THR:HG22	17	0.02
(1,2617)	1:A:9:ARG:HD3	1:A:46:THR:HG23	17	0.02
(1,2615)	1:A:41:LYS:HE2	1:A:46:THR:HG21	10	0.02
(1,2615)	1:A:41:LYS:HE2	1:A:46:THR:HG22	10	0.02
(1,2615)	1:A:41:LYS:HE2	1:A:46:THR:HG23	10	0.02
(1,2615)	1:A:41:LYS:HE3	1:A:46:THR:HG21	10	0.02
(1,2615)	1:A:41:LYS:HE3	1:A:46:THR:HG22	10	0.02
(1,2615)	1:A:41:LYS:HE3	1:A:46:THR:HG23	10	0.02
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG21	9	0.02
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG22	9	0.02
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG23	9	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG21	10	0.02
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG22	10	0.02
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG23	10	0.02
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG21	20	0.02
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG22	20	0.02
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG23	20	0.02
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG21	4	0.02
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG22	4	0.02
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG23	4	0.02
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG21	7	0.02
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG22	7	0.02
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG23	7	0.02
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG21	11	0.02
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG22	11	0.02
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG23	11	0.02
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG21	13	0.02
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG22	13	0.02
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG23	13	0.02
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD11	6	0.02
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD12	6	0.02
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD13	6	0.02
(1,2590)	1:B:44:ILE:HD11	1:B:73:PHE:HD1	14	0.02
(1,2590)	1:B:44:ILE:HD11	1:B:73:PHE:HD2	14	0.02
(1,2590)	1:B:44:ILE:HD12	1:B:73:PHE:HD1	14	0.02
(1,2590)	1:B:44:ILE:HD12	1:B:73:PHE:HD2	14	0.02
(1,2590)	1:B:44:ILE:HD13	1:B:73:PHE:HD1	14	0.02
(1,2590)	1:B:44:ILE:HD13	1:B:73:PHE:HD2	14	0.02
(1,2589)	1:A:44:ILE:HD11	1:A:73:PHE:HD1	20	0.02
(1,2589)	1:A:44:ILE:HD11	1:A:73:PHE:HD2	20	0.02
(1,2589)	1:A:44:ILE:HD12	1:A:73:PHE:HD1	20	0.02
(1,2589)	1:A:44:ILE:HD12	1:A:73:PHE:HD2	20	0.02
(1,2589)	1:A:44:ILE:HD13	1:A:73:PHE:HD1	20	0.02
(1,2589)	1:A:44:ILE:HD13	1:A:73:PHE:HD2	20	0.02
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD11	5	0.02
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD12	5	0.02
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD13	5	0.02
(1,2584)	1:B:44:ILE:HD11	1:B:46:THR:HB	6	0.02
(1,2584)	1:B:44:ILE:HD12	1:B:46:THR:HB	6	0.02
(1,2584)	1:B:44:ILE:HD13	1:B:46:THR:HB	6	0.02
(1,2583)	1:A:44:ILE:HD11	1:A:46:THR:HB	19	0.02
(1,2583)	1:A:44:ILE:HD12	1:A:46:THR:HB	19	0.02
(1,2583)	1:A:44:ILE:HD13	1:A:46:THR:HB	19	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2576)	1:B:44:ILE:HG21	1:B:45:PHE:H	14	0.02
(1,2576)	1:B:44:ILE:HG22	1:B:45:PHE:H	14	0.02
(1,2576)	1:B:44:ILE:HG23	1:B:45:PHE:H	14	0.02
(1,2572)	1:B:14:ASP:H	1:B:44:ILE:HG21	17	0.02
(1,2572)	1:B:14:ASP:H	1:B:44:ILE:HG22	17	0.02
(1,2572)	1:B:14:ASP:H	1:B:44:ILE:HG23	17	0.02
(1,2552)	1:B:44:ILE:HG13	1:B:45:PHE:H	13	0.02
(1,2526)	1:B:13:GLU:HA	1:B:44:ILE:HB	16	0.02
(1,2525)	1:A:13:GLU:HA	1:A:44:ILE:HB	5	0.02
(1,2486)	1:B:40:ALA:HA	1:B:45:PHE:HA	8	0.02
(1,2486)	1:B:40:ALA:HA	1:B:45:PHE:HA	18	0.02
(1,2485)	1:A:40:ALA:HA	1:A:45:PHE:HA	2	0.02
(1,2485)	1:A:40:ALA:HA	1:A:45:PHE:HA	4	0.02
(1,2485)	1:A:40:ALA:HA	1:A:45:PHE:HA	7	0.02
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD21	2	0.02
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD22	2	0.02
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD23	2	0.02
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD21	6	0.02
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD22	6	0.02
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD23	6	0.02
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD21	9	0.02
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD22	9	0.02
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD23	9	0.02
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD21	18	0.02
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD22	18	0.02
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD23	18	0.02
(1,2424)	1:B:38:LEU:HD11	1:B:39:ASN:H	4	0.02
(1,2424)	1:B:38:LEU:HD12	1:B:39:ASN:H	4	0.02
(1,2424)	1:B:38:LEU:HD13	1:B:39:ASN:H	4	0.02
(1,2423)	1:A:38:LEU:HD11	1:A:39:ASN:H	6	0.02
(1,2423)	1:A:38:LEU:HD12	1:A:39:ASN:H	6	0.02
(1,2423)	1:A:38:LEU:HD13	1:A:39:ASN:H	6	0.02
(1,2418)	1:B:38:LEU:HD11	1:B:45:PHE:HZ	12	0.02
(1,2418)	1:B:38:LEU:HD12	1:B:45:PHE:HZ	12	0.02
(1,2418)	1:B:38:LEU:HD13	1:B:45:PHE:HZ	12	0.02
(1,2417)	1:A:38:LEU:HD11	1:A:45:PHE:HZ	11	0.02
(1,2417)	1:A:38:LEU:HD12	1:A:45:PHE:HZ	11	0.02
(1,2417)	1:A:38:LEU:HD13	1:A:45:PHE:HZ	11	0.02
(1,2388)	1:B:37:VAL:HG21	1:B:38:LEU:H	1	0.02
(1,2388)	1:B:37:VAL:HG22	1:B:38:LEU:H	1	0.02
(1,2388)	1:B:37:VAL:HG23	1:B:38:LEU:H	1	0.02
(1,2388)	1:B:37:VAL:HG21	1:B:38:LEU:H	20	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2388)	1:B:37:VAL:HG22	1:B:38:LEU:H	20	0.02
(1,2388)	1:B:37:VAL:HG23	1:B:38:LEU:H	20	0.02
(1,2387)	1:A:37:VAL:HG21	1:A:38:LEU:H	4	0.02
(1,2387)	1:A:37:VAL:HG22	1:A:38:LEU:H	4	0.02
(1,2387)	1:A:37:VAL:HG23	1:A:38:LEU:H	4	0.02
(1,2387)	1:A:37:VAL:HG21	1:A:38:LEU:H	5	0.02
(1,2387)	1:A:37:VAL:HG22	1:A:38:LEU:H	5	0.02
(1,2387)	1:A:37:VAL:HG23	1:A:38:LEU:H	5	0.02
(1,2387)	1:A:37:VAL:HG21	1:A:38:LEU:H	15	0.02
(1,2387)	1:A:37:VAL:HG22	1:A:38:LEU:H	15	0.02
(1,2387)	1:A:37:VAL:HG23	1:A:38:LEU:H	15	0.02
(1,2387)	1:A:37:VAL:HG21	1:A:38:LEU:H	17	0.02
(1,2387)	1:A:37:VAL:HG22	1:A:38:LEU:H	17	0.02
(1,2387)	1:A:37:VAL:HG23	1:A:38:LEU:H	17	0.02
(1,2385)	1:A:37:VAL:HG21	1:A:48:ASN:H	15	0.02
(1,2385)	1:A:37:VAL:HG22	1:A:48:ASN:H	15	0.02
(1,2385)	1:A:37:VAL:HG23	1:A:48:ASN:H	15	0.02
(1,2380)	1:B:37:VAL:HG21	1:B:48:ASN:HD22	7	0.02
(1,2380)	1:B:37:VAL:HG22	1:B:48:ASN:HD22	7	0.02
(1,2380)	1:B:37:VAL:HG23	1:B:48:ASN:HD22	7	0.02
(1,2379)	1:A:37:VAL:HG21	1:A:48:ASN:HD22	4	0.02
(1,2379)	1:A:37:VAL:HG22	1:A:48:ASN:HD22	4	0.02
(1,2379)	1:A:37:VAL:HG23	1:A:48:ASN:HD22	4	0.02
(1,2379)	1:A:37:VAL:HG21	1:A:48:ASN:HD22	5	0.02
(1,2379)	1:A:37:VAL:HG22	1:A:48:ASN:HD22	5	0.02
(1,2379)	1:A:37:VAL:HG23	1:A:48:ASN:HD22	5	0.02
(1,2379)	1:A:37:VAL:HG21	1:A:48:ASN:HD22	7	0.02
(1,2379)	1:A:37:VAL:HG22	1:A:48:ASN:HD22	7	0.02
(1,2379)	1:A:37:VAL:HG23	1:A:48:ASN:HD22	7	0.02
(1,2379)	1:A:37:VAL:HG21	1:A:48:ASN:HD22	12	0.02
(1,2379)	1:A:37:VAL:HG22	1:A:48:ASN:HD22	12	0.02
(1,2379)	1:A:37:VAL:HG23	1:A:48:ASN:HD22	12	0.02
(1,237)	1:B:19:THR:H	1:B:40:ALA:HB1	9	0.02
(1,237)	1:B:19:THR:H	1:B:40:ALA:HB2	9	0.02
(1,237)	1:B:19:THR:H	1:B:40:ALA:HB3	9	0.02
(1,2329)	1:A:36:ILE:HD11	1:A:38:LEU:H	12	0.02
(1,2329)	1:A:36:ILE:HD12	1:A:38:LEU:H	12	0.02
(1,2329)	1:A:36:ILE:HD13	1:A:38:LEU:H	12	0.02
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD11	5	0.02
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD12	5	0.02
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD13	5	0.02
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	4	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	4	0.02
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	4	0.02
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	15	0.02
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	15	0.02
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	15	0.02
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	6	0.02
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	6	0.02
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	6	0.02
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	10	0.02
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	10	0.02
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	10	0.02
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	15	0.02
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	15	0.02
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	15	0.02
(1,2288)	1:B:35:THR:HB	1:B:36:ILE:HG21	12	0.02
(1,2288)	1:B:35:THR:HB	1:B:36:ILE:HG22	12	0.02
(1,2288)	1:B:35:THR:HB	1:B:36:ILE:HG23	12	0.02
(1,2282)	1:B:36:ILE:HG21	1:B:37:VAL:HB	3	0.02
(1,2282)	1:B:36:ILE:HG22	1:B:37:VAL:HB	3	0.02
(1,2282)	1:B:36:ILE:HG23	1:B:37:VAL:HB	3	0.02
(1,2282)	1:B:36:ILE:HG21	1:B:37:VAL:HB	5	0.02
(1,2282)	1:B:36:ILE:HG22	1:B:37:VAL:HB	5	0.02
(1,2282)	1:B:36:ILE:HG23	1:B:37:VAL:HB	5	0.02
(1,2281)	1:A:36:ILE:HG21	1:A:37:VAL:HB	1	0.02
(1,2281)	1:A:36:ILE:HG22	1:A:37:VAL:HB	1	0.02
(1,2281)	1:A:36:ILE:HG23	1:A:37:VAL:HB	1	0.02
(1,2258)	1:B:35:THR:HB	1:B:50:MET:HB2	12	0.02
(1,2258)	1:B:35:THR:HB	1:B:50:MET:HB2	20	0.02
(1,2257)	1:A:35:THR:HB	1:A:50:MET:HB2	16	0.02
(1,2247)	1:A:33:ILE:HD11	1:A:34:ARG:H	7	0.02
(1,2247)	1:A:33:ILE:HD12	1:A:34:ARG:H	7	0.02
(1,2247)	1:A:33:ILE:HD13	1:A:34:ARG:H	7	0.02
(1,2242)	1:A:33:ILE:HD11	1:B:20:ASN:HD22	3	0.02
(1,2242)	1:A:33:ILE:HD12	1:B:20:ASN:HD22	3	0.02
(1,2242)	1:A:33:ILE:HD13	1:B:20:ASN:HD22	3	0.02
(1,2241)	1:A:20:ASN:HD22	1:B:33:ILE:HD11	13	0.02
(1,2241)	1:A:20:ASN:HD22	1:B:33:ILE:HD12	13	0.02
(1,2241)	1:A:20:ASN:HD22	1:B:33:ILE:HD13	13	0.02
(1,2237)	1:A:20:ASN:HA	1:B:33:ILE:HD11	16	0.02
(1,2237)	1:A:20:ASN:HA	1:B:33:ILE:HD12	16	0.02
(1,2237)	1:A:20:ASN:HA	1:B:33:ILE:HD13	16	0.02
(1,2237)	1:A:20:ASN:HA	1:B:33:ILE:HD11	20	4



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2237)	1:A:20:ASN:HA	1:B:33:ILE:HD12	20	0.02
(1,2237)	1:A:20:ASN:HA	1:B:33:ILE:HD13	20	0.02
(1,2182)	1:B:29:PHE:HD1	1:B:31:THR:HB	13	0.02
(1,2182)	1:B:29:PHE:HD2	1:B:31:THR:HB	13	0.02
(1,2181)	1:A:29:PHE:HD1	1:A:31:THR:HB	8	0.02
(1,2181)	1:A:29:PHE:HD2	1:A:31:THR:HB	8	0.02
(1,2175)	1:A:25:VAL:HA	1:A:28:LYS:HE2	2	0.02
(1,2175)	1:A:25:VAL:HA	1:A:28:LYS:HE3	2	0.02
(1,217)	1:B:18:MET:H	1:B:18:MET:HG3	15	0.02
(1,217)	1:B:18:MET:H	1:B:18:MET:HG3	17	0.02
(1,2143)	1:A:20:ASN:HD22	1:B:27:SER:HA	12	0.02
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	7	0.02
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	7	0.02
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	7	0.02
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	10	0.02
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	10	0.02
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	10	0.02
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	12	0.02
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	12	0.02
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	12	0.02
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	14	0.02
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	14	0.02
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	14	0.02
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	18	0.02
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	18	0.02
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	18	0.02
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	11	0.02
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	11	0.02
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	11	0.02
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	13	0.02
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	13	0.02
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	13	0.02
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	16	0.02
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	16	0.02
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	16	0.02
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	18	0.02
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	18	0.02
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	18	0.02
(1,2100)	1:B:25:VAL:HG21	1:B:29:PHE:HD1	2	0.02
(1,2100)	1:B:25:VAL:HG21	1:B:29:PHE:HD2	2	0.02
(1,2100)	1:B:25:VAL:HG22	1:B:29:PHE:HD1	2	0.02
(1,2100)	1:B:25:VAL:HG22	1:B:29:PHE:HD2	2	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2100)	1:B:25:VAL:HG23	1:B:29:PHE:HD1	2	0.02
	1:B:25:VAL:HG23	1:B:29:PHE:HD2	2	0.02
(1,2094)	1:B:22:ILE:HA	1:B:25:VAL:HG21	19	0.02
(1,2094)	1:B:22:ILE:HA	1:B:25:VAL:HG22	19	0.02
(1,2094)	1:B:22:ILE:HA	1:B:25:VAL:HG23	19	0.02
(1,2088)	1:B:25:VAL:HG11	1:B:27:SER:H	4	0.02
(1,2088)	1:B:25:VAL:HG12	1:B:27:SER:H	4	0.02
(1,2088)	1:B:25:VAL:HG13	1:B:27:SER:H	4	0.02
(1,2088)	1:B:25:VAL:HG11	1:B:27:SER:H	12	0.02
(1,2088)	1:B:25:VAL:HG12	1:B:27:SER:H	12	0.02
(1,2088)	1:B:25:VAL:HG13	1:B:27:SER:H	12	0.02
(1,2088)	1:B:25:VAL:HG11	1:B:27:SER:H	16	0.02
(1,2088)	1:B:25:VAL:HG12	1:B:27:SER:H	16	0.02
(1,2088)	1:B:25:VAL:HG13	1:B:27:SER:H	16	0.02
(1,2088)	1:B:25:VAL:HG11	1:B:27:SER:H	20	0.02
(1,2088)	1:B:25:VAL:HG12	1:B:27:SER:H	20	0.02
(1,2088)	1:B:25:VAL:HG13	1:B:27:SER:H	20	0.02
(1,2087)	1:A:25:VAL:HG11	1:A:27:SER:H	8	0.02
(1,2087)	1:A:25:VAL:HG12	1:A:27:SER:H	8	0.02
(1,2087)	1:A:25:VAL:HG13	1:A:27:SER:H	8	0.02
(1,2087)	1:A:25:VAL:HG11	1:A:27:SER:H	11	0.02
(1,2087)	1:A:25:VAL:HG12	1:A:27:SER:H	11	0.02
(1,2087)	1:A:25:VAL:HG13	1:A:27:SER:H	11	0.02
(1,2087)	1:A:25:VAL:HG11	1:A:27:SER:H	12	0.02
(1,2087)	1:A:25:VAL:HG12	1:A:27:SER:H	12	0.02
(1,2087)	1:A:25:VAL:HG13	1:A:27:SER:H	12	0.02
(1,2067)	1:A:25:VAL:HG11	1:A:28:LYS:HD3	8	0.02
(1,2067)	1:A:25:VAL:HG12	1:A:28:LYS:HD3	8	0.02
(1,2067)	1:A:25:VAL:HG13	1:A:28:LYS:HD3	8	0.02
(1,2051)	1:A:67:ARG:HE	1:A:75:VAL:HG11	19	0.02
(1,2051)	1:A:67:ARG:HE	1:A:75:VAL:HG12	19	0.02
(1,2051)	1:A:67:ARG:HE	1:A:75:VAL:HG13	19	0.02
(1,200)	1:B:15:LYS:HE2	1:B:16:ASN:HD22	5	0.02
(1,200)	1:B:15:LYS:HE3	1:B:16:ASN:HD22	5	0.02
(1,200)	1:B:15:LYS:HE2	1:B:16:ASN:HD22	10	0.02
(1,200)	1:B:15:LYS:HE3	1:B:16:ASN:HD22	10	0.02
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG21	4	0.02
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG22	4	0.02
(1,1988)	1:B:19:THR:HA	1:B:22:ILE:HG23	4	0.02
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	4	0.02
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	4	0.02
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	4	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG21	17	0.02
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG22	17	0.02
(1,1987)	1:A:19:THR:HA	1:A:22:ILE:HG23	17	0.02
(1,1941)	1:B:22:ILE:HB	1:B:47:CYS:HG	2	0.02
(1,1941)	1:B:22:ILE:HB	1:B:47:CYS:HG	13	0.02
(1,1937)	1:B:19:THR:HG21	1:B:22:ILE:HB	11	0.02
(1,1937)	1:B:19:THR:HG22	1:B:22:ILE:HB	11	0.02
(1,1937)	1:B:19:THR:HG23	1:B:22:ILE:HB	11	0.02
(1,1933)	1:B:21:GLN:HE21	1:B:22:ILE:HA	3	0.02
(1,1932)	1:A:21:GLN:HE21	1:A:22:ILE:HA	2	0.02
(1,1932)	1:A:21:GLN:HE21	1:A:22:ILE:HA	4	0.02
(1,1932)	1:A:21:GLN:HE21	1:A:22:ILE:HA	7	0.02
(1,1932)	1:A:21:GLN:HE21	1:A:22:ILE:HA	14	0.02
(1,1873)	1:B:18:MET:HE1	1:B:70:GLN:H	14	0.02
(1,1873)	1:B:18:MET:HE2	1:B:70:GLN:H	14	0.02
(1,1873)	1:B:18:MET:HE3	1:B:70:GLN:H	14	0.02
(1,1861)	1:B:18:MET:HE1	1:B:71:GLY:HA2	4	0.02
(1,1861)	1:B:18:MET:HE2	1:B:71:GLY:HA2	4	0.02
(1,1861)	1:B:18:MET:HE3	1:B:71:GLY:HA2	4	0.02
(1,1860)	1:A:18:MET:HE1	1:A:71:GLY:HA2	9	0.02
(1,1860)	1:A:18:MET:HE2	1:A:71:GLY:HA2	9	0.02
(1,1860)	1:A:18:MET:HE3	1:A:71:GLY:HA2	9	0.02
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	14	0.02
(1,1837)	1:A:18:MET:HA	1:A:21:GLN:HG2	20	0.02
(1,1837)	1:A:18:MET:HA	1:A:21:GLN:HG3	20	0.02
(1,1832)	1:B:16:ASN:HB3	1:B:17:GLY:H	1	0.02
(1,1831)	1:A:16:ASN:HB3	1:A:17:GLY:H	1	0.02
(1,1816)	1:A:15:LYS:HG2	1:A:15:LYS:HE2	2	0.02
(1,1816)	1:A:15:LYS:HG2	1:A:15:LYS:HE3	2	0.02
(1,1816)	1:A:15:LYS:HG3	1:A:15:LYS:HE2	2	0.02
(1,1816)	1:A:15:LYS:HG3	1:A:15:LYS:HE3	2	0.02
(1,1813)	1:B:25:VAL:HG21	1:B:65:LYS:HE2	19	0.02
(1,1813)	1:B:25:VAL:HG21	1:B:65:LYS:HE3	19	0.02
(1,1813)	1:B:25:VAL:HG22	1:B:65:LYS:HE2	19	0.02
(1,1813)	1:B:25:VAL:HG22	1:B:65:LYS:HE3	19	0.02
(1,1813)	1:B:25:VAL:HG23	1:B:65:LYS:HE2	19	0.02
(1,1813)	1:B:25:VAL:HG23	1:B:65:LYS:HE3	19	0.02
(1,1812)	1:A:25:VAL:HG21	1:A:65:LYS:HE2	3	0.02
(1,1812)	1:A:25:VAL:HG21	1:A:65:LYS:HE3	3	0.02
(1,1812)	1:A:25:VAL:HG22	1:A:65:LYS:HE2	3	0.02
(1,1812)	1:A:25:VAL:HG22	1:A:65:LYS:HE3	3	0.02
(1,1812)	1:A:25:VAL:HG23	1:A:65:LYS:HE2	3	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1812)	1:A:25:VAL:HG23	1:A:65:LYS:HE3	3	0.02
(1,181)	1:A:15:LYS:H	1:A:44:ILE:HA	4	0.02
(1,181)	1:A:15:LYS:H	1:A:44:ILE:HA	6	0.02
(1,1809)	1:B:11:VAL:HG21	1:B:41:LYS:HE2	14	0.02
(1,1809)	1:B:11:VAL:HG21	1:B:41:LYS:HE3	14	0.02
(1,1809)	1:B:11:VAL:HG22	1:B:41:LYS:HE2	14	0.02
(1,1809)	1:B:11:VAL:HG22	1:B:41:LYS:HE3	14	0.02
(1,1809)	1:B:11:VAL:HG23	1:B:41:LYS:HE2	14	0.02
(1,1809)	1:B:11:VAL:HG23	1:B:41:LYS:HE3	14	0.02
(1,1807)	1:B:15:LYS:HD2	1:B:71:GLY:HA2	15	0.02
(1,1807)	1:B:15:LYS:HD3	1:B:71:GLY:HA2	15	0.02
(1,1792)	1:B:13:GLU:HG2	1:B:15:LYS:HB3	5	0.02
(1,1792)	1:B:13:GLU:HG3	1:B:15:LYS:HB3	5	0.02
(1,1792)	1:B:13:GLU:HG2	1:B:15:LYS:HB3	16	0.02
(1,1792)	1:B:13:GLU:HG3	1:B:15:LYS:HB3	16	0.02
(1,1791)	1:A:13:GLU:HG2	1:A:15:LYS:HB3	11	0.02
(1,1791)	1:A:13:GLU:HG3	1:A:15:LYS:HB3	11	0.02
(1,1791)	1:A:13:GLU:HG2	1:A:15:LYS:HB3	12	0.02
(1,1791)	1:A:13:GLU:HG3	1:A:15:LYS:HB3	12	0.02
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG11	10	0.02
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG12	10	0.02
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG13	10	0.02
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG11	10	0.02
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG12	10	0.02
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG13	10	0.02
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG11	11	0.02
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG12	11	0.02
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG13	11	0.02
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG11	11	0.02
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG12	11	0.02
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG13	11	0.02
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG11	19	0.02
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG12	19	0.02
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG13	19	0.02
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG11	19	0.02
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG12	19	0.02
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG13	19	0.02
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG11	7	0.02
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG12	7	0.02
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG13	7	0.02
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG11	7	0.02
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG12	7	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG13	7	0.02
(1,175)	1:A:15:LYS:H	1:A:18:MET:HG2	17	0.02
(1,172)	1:B:13:GLU:HG2	1:B:15:LYS:H	9	0.02
(1,172)	1:B:13:GLU:HG3	1:B:15:LYS:H	9	0.02
(1,171)	1:A:13:GLU:HG2	1:A:15:LYS:H	12	0.02
(1,171)	1:A:13:GLU:HG3	1:A:15:LYS:H	12	0.02
(1,171)	1:A:13:GLU:HG2	1:A:15:LYS:H	19	0.02
(1,171)	1:A:13:GLU:HG3	1:A:15:LYS:H	19	0.02
(1,1707)	1:B:11:VAL:HG11	1:B:41:LYS:HE2	1	0.02
(1,1707)	1:B:11:VAL:HG11	1:B:41:LYS:HE3	1	0.02
(1,1707)	1:B:11:VAL:HG12	1:B:41:LYS:HE2	1	0.02
(1,1707)	1:B:11:VAL:HG12	1:B:41:LYS:HE3	1	0.02
(1,1707)	1:B:11:VAL:HG13	1:B:41:LYS:HE2	1	0.02
(1,1707)	1:B:11:VAL:HG13	1:B:41:LYS:HE3	1	0.02
(1,170)	1:B:15:LYS:H	1:B:18:MET:HB2	7	0.02
(1,170)	1:B:15:LYS:H	1:B:18:MET:HB3	7	0.02
(1,1699)	1:B:11:VAL:HG21	1:B:45:PHE:HE1	9	0.02
(1,1699)	1:B:11:VAL:HG21	1:B:45:PHE:HE2	9	0.02
(1,1699)	1:B:11:VAL:HG22	1:B:45:PHE:HE1	9	0.02
(1,1699)	1:B:11:VAL:HG22	1:B:45:PHE:HE2	9	0.02
(1,1699)	1:B:11:VAL:HG23	1:B:45:PHE:HE1	9	0.02
(1,1699)	1:B:11:VAL:HG23	1:B:45:PHE:HE2	9	0.02
(1,1699)	1:B:11:VAL:HG21	1:B:45:PHE:HE1	19	0.02
(1,1699)	1:B:11:VAL:HG21	1:B:45:PHE:HE2	19	0.02
(1,1699)	1:B:11:VAL:HG22	1:B:45:PHE:HE1	19	0.02
(1,1699)	1:B:11:VAL:HG22	1:B:45:PHE:HE2	19	0.02
(1,1699)	1:B:11:VAL:HG23	1:B:45:PHE:HE1	19	0.02
(1,1699)	1:B:11:VAL:HG23	1:B:45:PHE:HE2	19	0.02
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	15	0.02
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	15	0.02
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	15	0.02
(1,1690)	1:A:11:VAL:HG21	1:A:46:THR:HB	1	0.02
(1,1690)	1:A:11:VAL:HG22	1:A:46:THR:HB	1	0.02
(1,1690)	1:A:11:VAL:HG23	1:A:46:THR:HB	1	0.02
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	6	0.02
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	6	0.02
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	6	0.02
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	6	0.02
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	6	0.02
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG23	6	0.02
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	6	0.02
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	6	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	6	0.02
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	9	0.02
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	9	0.02
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	9	0.02
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	9	0.02
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	9	0.02
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG23	9	0.02
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	9	0.02
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	9	0.02
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	9	0.02
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	18	0.02
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	18	0.02
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	18	0.02
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	18	0.02
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	18	0.02
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG23	18	0.02
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	18	0.02
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	18	0.02
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	18	0.02
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG21	8	0.02
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG22	8	0.02
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG23	8	0.02
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG21	8	0.02
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG22	8	0.02
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG23	8	0.02
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG21	8	0.02
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG22	8	0.02
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG23	8	0.02
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG21	10	0.02
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG22	10	0.02
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG23	10	0.02
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG21	10	0.02
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG22	10	0.02
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG23	10	0.02
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG21	10	0.02
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG22	10	0.02
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG23	10	0.02
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG21	15	0.02
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG22	15	0.02
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG23	15	0.02
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG21	15	0.02
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG22	15	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG23	15	0.02
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG21	15	0.02
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG22	15	0.02
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG23	15	0.02
(1,167)	1:A:15:LYS:H	1:A:18:MET:HE1	16	0.02
(1,167)	1:A:15:LYS:H	1:A:18:MET:HE2	16	0.02
(1,167)	1:A:15:LYS:H	1:A:18:MET:HE3	16	0.02
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD11	3	0.02
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD12	3	0.02
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD13	3	0.02
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD11	18	0.02
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD12	18	0.02
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD13	18	0.02
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD11	5	0.02
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD12	5	0.02
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD13	5	0.02
(1,1631)	1:B:9:ARG:HA	1:B:10:ILE:HG21	8	0.02
(1,1631)	1:B:9:ARG:HA	1:B:10:ILE:HG22	8	0.02
(1,1631)	1:B:9:ARG:HA	1:B:10:ILE:HG23	8	0.02
(1,1577)	1:B:9:ARG:HD2	1:B:11:VAL:HB	9	0.02
(1,1577)	1:B:9:ARG:HD3	1:B:11:VAL:HB	9	0.02
(1,1577)	1:B:9:ARG:HD2	1:B:11:VAL:HB	20	0.02
(1,1577)	1:B:9:ARG:HD3	1:B:11:VAL:HB	20	0.02
(1,1576)	1:A:9:ARG:HD2	1:A:11:VAL:HB	11	0.02
(1,1576)	1:A:9:ARG:HD3	1:A:11:VAL:HB	11	0.02
(1,1558)	1:B:24:GLY:H	1:B:26:ILE:HD11	20	0.02
(1,1558)	1:B:24:GLY:H	1:B:26:ILE:HD12	20	0.02
(1,1558)	1:B:24:GLY:H	1:B:26:ILE:HD13	20	0.02
(1,1557)	1:A:24:GLY:H	1:A:26:ILE:HD11	17	0.02
(1,1557)	1:A:24:GLY:H	1:A:26:ILE:HD12	17	0.02
(1,1557)	1:A:24:GLY:H	1:A:26:ILE:HD13	17	0.02
(1,1552)	1:B:8:ILE:HD11	1:B:77:ARG:HA	2	0.02
(1,1552)	1:B:8:ILE:HD12	1:B:77:ARG:HA	2	0.02
(1,1552)	1:B:8:ILE:HD13	1:B:77:ARG:HA	2	0.02
(1,1552)	1:B:8:ILE:HD11	1:B:77:ARG:HA	6	0.02
(1,1552)	1:B:8:ILE:HD12	1:B:77:ARG:HA	6	0.02
(1,1552)	1:B:8:ILE:HD13	1:B:77:ARG:HA	6	0.02
(1,1552)	1:B:8:ILE:HD11	1:B:77:ARG:HA	15	0.02
(1,1552)	1:B:8:ILE:HD12	1:B:77:ARG:HA	15	0.02
(1,1552)	1:B:8:ILE:HD13	1:B:77:ARG:HA	15	0.02
(1,1552)	1:B:8:ILE:HD11	1:B:77:ARG:HA	20	0.02
(1,1552)	1:B:8:ILE:HD12	1:B:77:ARG:HA	20	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1552)	1:B:8:ILE:HD13	1:B:77:ARG:HA	20	0.02
(1,1551)	1:A:8:ILE:HD11	1:A:77:ARG:HA	13	0.02
(1,1551)	1:A:8:ILE:HD12	1:A:77:ARG:HA	13	0.02
(1,1551)	1:A:8:ILE:HD13	1:A:77:ARG:HA	13	0.02
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	6	0.02
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	6	0.02
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	6	0.02
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	6	0.02
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	6	0.02
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	6	0.02
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	6	0.02
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	6	0.02
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	6	0.02
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	14	0.02
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	14	0.02
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	14	0.02
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	14	0.02
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	14	0.02
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	14	0.02
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	14	0.02
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	14	0.02
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	14	0.02
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	11	0.02
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	11	0.02
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	11	0.02
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	11	0.02
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	11	0.02
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	11	0.02
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	18	0.02
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	18	0.02
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	18	0.02
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	18	0.02
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	18	0.02
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	18	0.02
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	8	0.02
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	8	0.02
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	8	0.02
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	8	0.02
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	8	0.02
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	8	0.02
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	10	0.02
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	10	0.02



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	10	0.02
	1:A:8:ILE:HG22	1:A:77:ARG:HD3	10	0.02
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	10	0.02
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	10	0.02
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	2	0.02
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	2	0.02
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	2	0.02
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	8	0.02
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	8	0.02
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	8	0.02
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	3	0.02
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	3	0.02
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	3	0.02
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	6	0.02
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	6	0.02
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	6	0.02
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	11	0.02
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	11	0.02
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	11	0.02
(1,1479)	1:A:5:LEU:HD21	1:A:52:PHE:HA	18	0.02
(1,1479)	1:A:5:LEU:HD22	1:A:52:PHE:HA	18	0.02
(1,1479)	1:A:5:LEU:HD23	1:A:52:PHE:HA	18	0.02
(1,1414)	1:B:3:ASP:HB2	1:B:53:VAL:H	8	0.02
(1,1356)	1:B:82:GLU:H	1:B:82:GLU:HG2	10	0.02
(1,1356)	1:B:82:GLU:H	1:B:82:GLU:HG3	10	0.02
(1,1339)	1:A:81:LEU:H	1:A:81:LEU:HD11	2	0.02
(1,1339)	1:A:81:LEU:H	1:A:81:LEU:HD12	2	0.02
(1,1339)	1:A:81:LEU:H	1:A:81:LEU:HD13	2	0.02
(1,1310)	1:B:77:ARG:H	1:B:77:ARG:HD2	2	0.02
(1,1310)	1:B:77:ARG:H	1:B:77:ARG:HD3	2	0.02
(1,1266)	1:B:74:THR:HG21	1:B:75:VAL:H	6	0.02
(1,1266)	1:B:74:THR:HG22	1:B:75:VAL:H	6	0.02
(1,1266)	1:B:74:THR:HG23	1:B:75:VAL:H	6	0.02
(1,1227)	1:A:70:GLN:HA	1:A:72:VAL:H	9	0.02
(1,1227)	1:A:70:GLN:HA	1:A:72:VAL:H	11	0.02
(1,1223)	1:A:69:VAL:HG21	1:A:72:VAL:H	8	0.02
(1,1223)	1:A:69:VAL:HG22	1:A:72:VAL:H	8	0.02
(1,1223)	1:A:69:VAL:HG23	1:A:72:VAL:H	8	0.02
(1,1212)	1:B:69:VAL:HG11	1:B:71:GLY:H	3	0.02
(1,1212)	1:B:69:VAL:HG12	1:B:71:GLY:H	3	0.02
(1,1212)	1:B:69:VAL:HG13	1:B:71:GLY:H	3	0.02
(1,1212)	1:B:69:VAL:HG11	1:B:71:GLY:H	4	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1212)	1:B:69:VAL:HG12	1:B:71:GLY:H	4	0.02
(1,1212)	1:B:69:VAL:HG13	1:B:71:GLY:H	4	0.02
(1,1212)	1:B:69:VAL:HG11	1:B:71:GLY:H	6	0.02
(1,1212)	1:B:69:VAL:HG12	1:B:71:GLY:H	6	0.02
(1,1212)	1:B:69:VAL:HG13	1:B:71:GLY:H	6	0.02
(1,1211)	1:A:69:VAL:HG11	1:A:71:GLY:H	10	0.02
(1,1211)	1:A:69:VAL:HG12	1:A:71:GLY:H	10	0.02
(1,1211)	1:A:69:VAL:HG13	1:A:71:GLY:H	10	0.02
(1,1196)	1:B:69:VAL:H	1:B:70:GLN:H	3	0.02
(1,1196)	1:B:69:VAL:H	1:B:70:GLN:H	15	0.02
(1,1195)	1:A:69:VAL:H	1:A:70:GLN:H	17	0.02
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	5	0.02
(1,1124)	1:B:67:ARG:H	1:B:69:VAL:HG21	9	0.02
(1,1124)	1:B:67:ARG:H	1:B:69:VAL:HG22	9	0.02
(1,1124)	1:B:67:ARG:H	1:B:69:VAL:HG23	9	0.02
(1,1124)	1:B:67:ARG:H	1:B:69:VAL:HG21	14	0.02
(1,1124)	1:B:67:ARG:H	1:B:69:VAL:HG22	14	0.02
(1,1124)	1:B:67:ARG:H	1:B:69:VAL:HG23	14	0.02
(1,1123)	1:A:67:ARG:H	1:A:69:VAL:HG21	19	0.02
(1,1123)	1:A:67:ARG:H	1:A:69:VAL:HG22	19	0.02
(1,1123)	1:A:67:ARG:H	1:A:69:VAL:HG23	19	0.02
(1,1106)	1:B:62:LEU:HD11	1:B:66:LEU:H	15	0.02
(1,1106)	1:B:62:LEU:HD12	1:B:66:LEU:H	15	0.02
(1,1106)	1:B:62:LEU:HD13	1:B:66:LEU:H	15	0.02
(1,1106)	1:B:62:LEU:HD11	1:B:66:LEU:H	18	0.02
(1,1106)	1:B:62:LEU:HD12	1:B:66:LEU:H	18	0.02
(1,1106)	1:B:62:LEU:HD13	1:B:66:LEU:H	18	0.02
(1,1105)	1:A:62:LEU:HD11	1:A:66:LEU:H	1	0.02
(1,1105)	1:A:62:LEU:HD12	1:A:66:LEU:H	1	0.02
(1,1105)	1:A:62:LEU:HD13	1:A:66:LEU:H	1	0.02
(1,1105)	1:A:62:LEU:HD11	1:A:66:LEU:H	8	0.02
(1,1105)	1:A:62:LEU:HD12	1:A:66:LEU:H	8	0.02
(1,1105)	1:A:62:LEU:HD13	1:A:66:LEU:H	8	0.02
(1,1105)	1:A:62:LEU:HD11	1:A:66:LEU:H	17	0.02
(1,1105)	1:A:62:LEU:HD12	1:A:66:LEU:H	17	0.02
(1,1105)	1:A:62:LEU:HD13	1:A:66:LEU:H	17	0.02
(1,1104)	1:B:62:LEU:HD11	1:B:65:LYS:H	13	0.02
(1,1104)	1:B:62:LEU:HD12	1:B:65:LYS:H	13	0.02
(1,1104)	1:B:62:LEU:HD13	1:B:65:LYS:H	13	0.02
(1,1104)	1:B:62:LEU:HD11	1:B:65:LYS:H	19	0.02
(1,1104)	1:B:62:LEU:HD12	1:B:65:LYS:H	19	0.02
(1,1104)	1:B:62:LEU:HD13	1:B:65:LYS:H	19	0.02



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1103)	1:A:62:LEU:HD11	1:A:65:LYS:H	5	0.02
(1,1103)	1:A:62:LEU:HD12	1:A:65:LYS:H	5	0.02
(1,1103)	1:A:62:LEU:HD13	1:A:65:LYS:H	5	0.02
(1,1103)	1:A:62:LEU:HD11	1:A:65:LYS:H	8	0.02
(1,1103)	1:A:62:LEU:HD12	1:A:65:LYS:H	8	0.02
(1,1103)	1:A:62:LEU:HD13	1:A:65:LYS:H	8	0.02
(1,1103)	1:A:62:LEU:HD11	1:A:65:LYS:H	10	0.02
(1,1103)	1:A:62:LEU:HD12	1:A:65:LYS:H	10	0.02
(1,1103)	1:A:62:LEU:HD13	1:A:65:LYS:H	10	0.02
(1,1103)	1:A:62:LEU:HD11	1:A:65:LYS:H	12	0.02
(1,1103)	1:A:62:LEU:HD12	1:A:65:LYS:H	12	0.02
(1,1103)	1:A:62:LEU:HD13	1:A:65:LYS:H	12	0.02
(1,1103)	1:A:62:LEU:HD11	1:A:65:LYS:H	14	0.02
(1,1103)	1:A:62:LEU:HD12	1:A:65:LYS:H	14	0.02
(1,1103)	1:A:62:LEU:HD13	1:A:65:LYS:H	14	0.02
(1,1103)	1:A:62:LEU:HD11	1:A:65:LYS:H	17	0.02
(1,1103)	1:A:62:LEU:HD12	1:A:65:LYS:H	17	0.02
(1,1103)	1:A:62:LEU:HD13	1:A:65:LYS:H	17	0.02
(1,1067)	1:B:64:ASP:H	1:B:75:VAL:HG11	9	0.02
(1,1067)	1:B:64:ASP:H	1:B:75:VAL:HG12	9	0.02
(1,1067)	1:B:64:ASP:H	1:B:75:VAL:HG13	9	0.02
(1,1046)	1:A:58:LYS:HZ1	1:A:62:LEU:H	20	0.02
(1,1046)	1:A:58:LYS:HZ2	1:A:62:LEU:H	20	0.02
(1,1046)	1:A:58:LYS:HZ3	1:A:62:LEU:H	20	0.02
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	7	0.02
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	7	0.02
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	7	0.02
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	12	0.02
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	12	0.02
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	12	0.02
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	16	0.02
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	16	0.02
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	16	0.02
(1,1020)	1:A:58:LYS:HZ1	1:A:61:THR:H	2	0.02
(1,1020)	1:A:58:LYS:HZ2	1:A:61:THR:H	2	0.02
(1,1020)	1:A:58:LYS:HZ3	1:A:61:THR:H	2	0.02
(1,1020)	1:A:58:LYS:HZ1	1:A:61:THR:H	8	0.02
(1,1020)	1:A:58:LYS:HZ2	1:A:61:THR:H	8	0.02
(1,1020)	1:A:58:LYS:HZ3	1:A:61:THR:H	8	0.02
(1,956)	1:A:53:VAL:HG21	1:A:58:LYS:H	13	0.01
(1,956)	1:A:53:VAL:HG22	1:A:58:LYS:H	13	0.01
(1,956)	1:A:53:VAL:HG23	1:A:58:LYS:H	13	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,899)	1:B:51:ILE:HG12	1:B:52:PHE:H	2	0.01
(1,898)	1:A:51:ILE:HG12	1:A:52:PHE:H	7	0.01
(1,898)	1:A:51:ILE:HG12	1:A:52:PHE:H	10	0.01
(1,898)	1:A:51:ILE:HG12	1:A:52:PHE:H	14	0.01
(1,833)	1:B:47:CYS:HG	1:B:48:ASN:H	14	0.01
(1,833)	1:B:47:CYS:HG	1:B:48:ASN:H	17	0.01
(1,832)	1:A:47:CYS:HG	1:A:48:ASN:H	5	0.01
(1,83)	1:B:9:ARG:HE	1:B:11:VAL:HG21	8	0.01
(1,83)	1:B:9:ARG:HE	1:B:11:VAL:HG22	8	0.01
(1,83)	1:B:9:ARG:HE	1:B:11:VAL:HG23	8	0.01
(1,829)	1:B:36:ILE:HD11	1:B:48:ASN:H	8	0.01
(1,829)	1:B:36:ILE:HD12	1:B:48:ASN:H	8	0.01
(1,829)	1:B:36:ILE:HD13	1:B:48:ASN:H	8	0.01
(1,829)	1:B:36:ILE:HD11	1:B:48:ASN:H	20	0.01
(1,829)	1:B:36:ILE:HD12	1:B:48:ASN:H	20	0.01
(1,829)	1:B:36:ILE:HD13	1:B:48:ASN:H	20	0.01
(1,823)	1:B:45:PHE:HZ	1:B:47:CYS:H	6	0.01
(1,760)	1:A:43:GLY:H	1:A:44:ILE:H	11	0.01
(1,745)	1:B:44:ILE:H	1:B:44:ILE:HG21	15	0.01
(1,745)	1:B:44:ILE:H	1:B:44:ILE:HG22	15	0.01
(1,745)	1:B:44:ILE:H	1:B:44:ILE:HG23	15	0.01
(1,744)	1:A:44:ILE:H	1:A:44:ILE:HG21	10	0.01
(1,744)	1:A:44:ILE:H	1:A:44:ILE:HG22	10	0.01
(1,744)	1:A:44:ILE:H	1:A:44:ILE:HG23	10	0.01
(1,723)	1:B:41:LYS:H	1:B:43:GLY:H	14	0.01
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD1	15	0.01
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD2	15	0.01
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD1	20	0.01
(1,717)	1:B:41:LYS:H	1:B:45:PHE:HD2	20	0.01
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD1	6	0.01
(1,716)	1:A:41:LYS:H	1:A:45:PHE:HD2	6	0.01
(1,695)	1:B:41:LYS:H	1:B:44:ILE:HG21	1	0.01
(1,695)	1:B:41:LYS:H	1:B:44:ILE:HG22	1	0.01
(1,695)	1:B:41:LYS:H	1:B:44:ILE:HG23	1	0.01
(1,615)	1:B:35:THR:H	1:B:83:HIS:HE1	20	0.01
(1,577)	1:A:32:ASN:HD22	1:B:17:GLY:H	3	0.01
(1,565)	1:B:32:ASN:HA	1:B:32:ASN:HD21	4	0.01
(1,565)	1:B:32:ASN:HA	1:B:32:ASN:HD21	6	0.01
(1,563)	1:A:32:ASN:HD21	1:A:33:ILE:HB	6	0.01
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD11	1	0.01
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD12	1	0.01
(1,552)	1:B:32:ASN:H	1:B:51:ILE:HD13	1	0.01



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(1,551) 1:A:32:ASN:H 1:A:51:ILE:HD11 6 0.01 (1,551) 1:A:32:ASN:H 1:A:51:ILE:HD12 6 0.01 (1,551) 1:A:32:ASN:H 1:A:51:ILE:HD13 6 0.01 (1,551) 1:A:32:ASN:H 1:A:51:ILE:HD12 16 0.01 (1,551) 1:A:32:ASN:H 1:A:51:ILE:HD13 16 0.01 (1,546) 1:B:29:PHE:HD1 1:B:31:THR:H 2 0.01 (1,546) 1:B:29:PHE:HD2 1:B:31:THR:H 2 0.01 (1,546) 1:B:29:PHE:HD2 1:B:31:THR:H 7 0.01 (1,546) 1:B:29:PHE:HD2 1:B:31:THR:H 7 0.01 (1,546) 1:B:29:PHE:HD2 1:B:31:THR:H 7 0.01 (1,546) 1:B:29:PHE:HD2 1:B:31:THR:H 13 0.01 (1,546) 1:B:29:PHE:HD2 1:B:31:THR:H 13 0.01 (1,546) 1:B:29:PHE:HD2 1:B:31:THR:H 14 0.01 (1,546) 1:B:29:PHE:HD2 1:B:31:THR:H 17	Key	Atom-1	Atom-2	Model	Violation (Å)
(1,551) 1:A:32:ASN:H 1:A:51:ILE:HD13 6 0.01 (1,551) 1:A:32:ASN:H 1:A:51:ILE:HD11 16 0.01 (1,551) 1:A:32:ASN:H 1:A:51:ILE:HD13 16 0.01 (1,551) 1:A:32:ASN:H 1:A:51:ILE:HD13 16 0.01 (1,546) 1:B:29:PHE:HD1 1:B:31:THR:H 2 0.01 (1,546) 1:B:29:PHE:HD2 1:B:31:THR:H 7 0.01 (1,546) 1:B:29:PHE:HD1 1:B:31:THR:H 7 0.01 (1,546) 1:B:29:PHE:HD2 1:B:31:THR:H 7 0.01 (1,546) 1:B:29:PHE:HD1 1:B:31:THR:H 13 0.01 (1,546) 1:B:29:PHE:HD2 1:B:31:THR:H 14 0.01 (1,546) 1:B:29:PHE:HD1 1:B:31:THR:H 14 0.01 (1,546) 1:B:29:PHE:HD2 1:B:31:THR:H 17 0.01 (1,546) 1:B:29:PHE:HD1 1:B:31:THR:H 17 0.01 (1,545) 1:A:29:PHE:HD2 1:B:31:THR:H 17	(1,551)	1:A:32:ASN:H	1:A:51:ILE:HD11	6	0.01
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(1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB3 1 0.01 (1,4976) 1:B:63:MET:HE2 1:B:77:ARG:HB2 1 0.01 (1,4976) 1:B:63:MET:HE2 1:B:77:ARG:HB3 1 0.01 (1,4976) 1:B:63:MET:HE3 1:B:77:ARG:HB2 1 0.01 (1,4976) 1:B:63:MET:HE3 1:B:77:ARG:HB3 1 0.01 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB2 5 0.01 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB3 5 0.01	· · /	1:B:63:MET:HE1	1:B:77:ARG:HB2	1	0.01
(1,4976) 1:B:63:MET:HE2 1:B:77:ARG:HB2 1 0.01 (1,4976) 1:B:63:MET:HE2 1:B:77:ARG:HB3 1 0.01 (1,4976) 1:B:63:MET:HE3 1:B:77:ARG:HB2 1 0.01 (1,4976) 1:B:63:MET:HE3 1:B:77:ARG:HB3 1 0.01 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB2 5 0.01 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB3 5 0.01		1:B:63:MET:HE1	1:B:77:ARG:HB3	1	0.01
(1,4976) 1:B:63:MET:HE3 1:B:77:ARG:HB2 1 0.01 (1,4976) 1:B:63:MET:HE3 1:B:77:ARG:HB3 1 0.01 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB2 5 0.01 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB3 5 0.01		1:B:63:MET:HE2	1:B:77:ARG:HB2	1	0.01
(1,4976) 1:B:63:MET:HE3 1:B:77:ARG:HB2 1 0.01 (1,4976) 1:B:63:MET:HE3 1:B:77:ARG:HB3 1 0.01 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB2 5 0.01 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB3 5 0.01	(1,4976)	1:B:63:MET:HE2	1:B:77:ARG:HB3	1	0.01
(1,4976) 1:B:63:MET:HE3 1:B:77:ARG:HB3 1 0.01 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB2 5 0.01 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB3 5 0.01	(1,4976)	1:B:63:MET:HE3	1:B:77:ARG:HB2	1	0.01
(1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB2 5 0.01 (1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB3 5 0.01	· · /	1:B:63:MET:HE3	1:B:77:ARG:HB3	1	0.01
(1,4976) 1:B:63:MET:HE1 1:B:77:ARG:HB3 5 0.01	, ,	1:B:63:MET:HE1	1:B:77:ARG:HB2	5	0.01
	· · /	1:B:63:MET:HE1	1:B:77:ARG:HB3	5	0.01
	· '	1:B:63:MET:HE2	1:B:77:ARG:HB2	5	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4976)	1:B:63:MET:HE2	1:B:77:ARG:HB3	5	0.01
(1,4976)	1:B:63:MET:HE3	1:B:77:ARG:HB2	5	0.01
(1,4976)	1:B:63:MET:HE3	1:B:77:ARG:HB3	5	0.01
(1,4976)	1:B:63:MET:HE1	1:B:77:ARG:HB2	19	0.01
(1,4976)	1:B:63:MET:HE1	1:B:77:ARG:HB3	19	0.01
(1,4976)	1:B:63:MET:HE2	1:B:77:ARG:HB2	19	0.01
(1,4976)	1:B:63:MET:HE2	1:B:77:ARG:HB3	19	0.01
(1,4976)	1:B:63:MET:HE3	1:B:77:ARG:HB2	19	0.01
(1,4976)	1:B:63:MET:HE3	1:B:77:ARG:HB3	19	0.01
(1,4961)	1:B:59:LEU:HD21	1:B:77:ARG:HG2	4	0.01
(1,4961)	1:B:59:LEU:HD21	1:B:77:ARG:HG3	4	0.01
(1,4961)	1:B:59:LEU:HD22	1:B:77:ARG:HG2	4	0.01
(1,4961)	1:B:59:LEU:HD22	1:B:77:ARG:HG3	4	0.01
(1,4961)	1:B:59:LEU:HD23	1:B:77:ARG:HG2	4	0.01
(1,4961)	1:B:59:LEU:HD23	1:B:77:ARG:HG3	4	0.01
(1,4936)	1:B:54:LYS:HE2	1:B:55:ASN:HD21	5	0.01
(1,4936)	1:B:54:LYS:HE2	1:B:55:ASN:HD22	5	0.01
(1,4936)	1:B:54:LYS:HE3	1:B:55:ASN:HD21	5	0.01
(1,4936)	1:B:54:LYS:HE3	1:B:55:ASN:HD22	5	0.01
(1,4935)	1:B:54:LYS:HD2	1:B:55:ASN:HD21	3	0.01
(1,4935)	1:B:54:LYS:HD2	1:B:55:ASN:HD22	3	0.01
(1,4935)	1:B:54:LYS:HD3	1:B:55:ASN:HD21	3	0.01
(1,4935)	1:B:54:LYS:HD3	1:B:55:ASN:HD22	3	0.01
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE1	2	0.01
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE2	2	0.01
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE3	2	0.01
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE1	2	0.01
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE2	2	0.01
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE3	2	0.01
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE1	9	0.01
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE2	9	0.01
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE3	9	0.01
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE1	9	0.01
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE2	9	0.01
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE3	9	0.01
(1,4899)	1:B:39:ASN:HD21	1:B:46:THR:HB	5	0.01
(1,4899)	1:B:39:ASN:HD22	1:B:46:THR:HB	5	0.01
(1,4899)	1:B:39:ASN:HD21	1:B:46:THR:HB	16	0.01
(1,4899)	1:B:39:ASN:HD22	1:B:46:THR:HB	16	0.01
(1,4898)	1:B:39:ASN:HD21	1:B:41:LYS:HE2	4	0.01
(1,4898)	1:B:39:ASN:HD21	1:B:41:LYS:HE3	4	0.01
(1,4898)	1:B:39:ASN:HD22	1:B:41:LYS:HE2	4	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4898)	1:B:39:ASN:HD22	1:B:41:LYS:HE3	4	0.01
(1,4889)	1:B:37:VAL:HG21	1:B:48:ASN:HD21	13	0.01
(1,4889)	1:B:37:VAL:HG21	1:B:48:ASN:HD22	13	0.01
(1,4889)	1:B:37:VAL:HG22	1:B:48:ASN:HD21	13	0.01
(1,4889)	1:B:37:VAL:HG22	1:B:48:ASN:HD22	13	0.01
(1,4889)	1:B:37:VAL:HG23	1:B:48:ASN:HD21	13	0.01
(1,4889)	1:B:37:VAL:HG23	1:B:48:ASN:HD22	13	0.01
(1,4889)	1:B:37:VAL:HG21	1:B:48:ASN:HD21	20	0.01
(1,4889)	1:B:37:VAL:HG21	1:B:48:ASN:HD22	20	0.01
(1,4889)	1:B:37:VAL:HG22	1:B:48:ASN:HD21	20	0.01
(1,4889)	1:B:37:VAL:HG22	1:B:48:ASN:HD22	20	0.01
(1,4889)	1:B:37:VAL:HG23	1:B:48:ASN:HD21	20	0.01
(1,4889)	1:B:37:VAL:HG23	1:B:48:ASN:HD22	20	0.01
(1,4887)	1:B:37:VAL:HG11	1:B:48:ASN:HD21	6	0.01
(1,4887)	1:B:37:VAL:HG11	1:B:48:ASN:HD22	6	0.01
(1,4887)	1:B:37:VAL:HG12	1:B:48:ASN:HD21	6	0.01
(1,4887)	1:B:37:VAL:HG12	1:B:48:ASN:HD22	6	0.01
(1,4887)	1:B:37:VAL:HG13	1:B:48:ASN:HD21	6	0.01
(1,4887)	1:B:37:VAL:HG13	1:B:48:ASN:HD22	6	0.01
(1,4887)	1:B:37:VAL:HG11	1:B:48:ASN:HD21	7	0.01
(1,4887)	1:B:37:VAL:HG11	1:B:48:ASN:HD22	7	0.01
(1,4887)	1:B:37:VAL:HG12	1:B:48:ASN:HD21	7	0.01
(1,4887)	1:B:37:VAL:HG12	1:B:48:ASN:HD22	7	0.01
(1,4887)	1:B:37:VAL:HG13	1:B:48:ASN:HD21	7	0.01
(1,4887)	1:B:37:VAL:HG13	1:B:48:ASN:HD22	7	0.01
(1,4887)	1:B:37:VAL:HG11	1:B:48:ASN:HD21	19	0.01
(1,4887)	1:B:37:VAL:HG11	1:B:48:ASN:HD22	19	0.01
(1,4887)	1:B:37:VAL:HG12	1:B:48:ASN:HD21	19	0.01
(1,4887)	1:B:37:VAL:HG12	1:B:48:ASN:HD22	19	0.01
(1,4887)	1:B:37:VAL:HG13	1:B:48:ASN:HD21	19	0.01
(1,4887)	1:B:37:VAL:HG13	1:B:48:ASN:HD22	19	0.01
(1,4883)	1:B:37:VAL:HB	1:B:48:ASN:HB2	5	0.01
(1,4883)	1:B:37:VAL:HB	1:B:48:ASN:HB3	5	0.01
(1,4883)	1:B:37:VAL:HB	1:B:48:ASN:HB2	10	0.01
(1,4883)	1:B:37:VAL:HB	1:B:48:ASN:HB3	10	0.01
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB2	3	0.01
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB3	3	0.01
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB2	4	0.01
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB3	4	0.01
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB2	7	0.01
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB3	7	0.01
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB2	13	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB3	13	0.01
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB2	14	0.01
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB3	14	0.01
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB2	15	0.01
(1,4875)	1:B:35:THR:HB	1:B:50:MET:HB3	15	0.01
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD11	20	0.01
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD12	20	0.01
(1,4858)	1:B:32:ASN:HB2	1:B:33:ILE:HD13	20	0.01
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD11	20	0.01
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD12	20	0.01
(1,4858)	1:B:32:ASN:HB3	1:B:33:ILE:HD13	20	0.01
(1,4857)	1:B:32:ASN:HB2	1:B:33:ILE:HG12	18	0.01
(1,4857)	1:B:32:ASN:HB2	1:B:33:ILE:HG13	18	0.01
(1,4857)	1:B:32:ASN:HB3	1:B:33:ILE:HG12	18	0.01
(1,4857)	1:B:32:ASN:HB3	1:B:33:ILE:HG13	18	0.01
(1,4854)	1:B:32:ASN:HA	1:B:32:ASN:HD21	6	0.01
(1,4854)	1:B:32:ASN:HA	1:B:32:ASN:HD22	6	0.01
(1,4828)	1:B:27:SER:HG	1:B:28:LYS:HD2	5	0.01
(1,4828)	1:B:27:SER:HG	1:B:28:LYS:HD3	5	0.01
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG2	5	0.01
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	5	0.01
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	5	0.01
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG3	5	0.01
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	5	0.01
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	5	0.01
(1,4792)	1:B:20:ASN:HB2	1:B:21:GLN:HE21	15	0.01
(1,4792)	1:B:20:ASN:HB3	1:B:21:GLN:HE21	15	0.01
(1,4731)	1:B:7:GLY:H	1:B:77:ARG:HG2	8	0.01
(1,4731)	1:B:7:GLY:H	1:B:77:ARG:HG3	8	0.01
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG2	2	0.01
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG3	2	0.01
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG2	5	0.01
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG3	5	0.01
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG2	12	0.01
(1,4706)	1:A:77:ARG:H	1:A:77:ARG:HG3	12	0.01
(1,4690)	1:A:67:ARG:H	1:A:67:ARG:HG2	7	0.01
(1,4690)	1:A:67:ARG:H	1:A:67:ARG:HG3	7	0.01
(1,4690)	1:A:67:ARG:H	1:A:67:ARG:HG2	9	0.01
(1,4690)	1:A:67:ARG:H	1:A:67:ARG:HG3	9	0.01
(1,4690)	1:A:67:ARG:H	1:A:67:ARG:HG2	13	0.01
(1,4690)	1:A:67:ARG:H	1:A:67:ARG:HG3	13	0.01
(1,4690)	1:A:67:ARG:H	1:A:67:ARG:HG2	16	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4690)	1:A:67:ARG:H	1:A:67:ARG:HG3	16	0.01
(1,4690)	1:A:67:ARG:H	1:A:67:ARG:HG2	18	0.01
(1,4690)	1:A:67:ARG:H	1:A:67:ARG:HG3	18	0.01
(1,4660)	1:A:58:LYS:HE2	1:A:62:LEU:H	14	0.01
(1,4660)	1:A:58:LYS:HE3	1:A:62:LEU:H	14	0.01
(1,4640)	1:A:54:LYS:HG2	1:A:55:ASN:HD21	11	0.01
(1,4640)	1:A:54:LYS:HG2	1:A:55:ASN:HD22	11	0.01
(1,4640)	1:A:54:LYS:HG3	1:A:55:ASN:HD21	11	0.01
(1,4640)	1:A:54:LYS:HG3	1:A:55:ASN:HD22	11	0.01
(1,4640)	1:A:54:LYS:HG2	1:A:55:ASN:HD21	16	0.01
(1,4640)	1:A:54:LYS:HG2	1:A:55:ASN:HD22	16	0.01
(1,4640)	1:A:54:LYS:HG3	1:A:55:ASN:HD21	16	0.01
(1,4640)	1:A:54:LYS:HG3	1:A:55:ASN:HD22	16	0.01
(1,4635)	1:A:54:LYS:H	1:A:54:LYS:HG2	4	0.01
(1,4635)	1:A:54:LYS:H	1:A:54:LYS:HG3	4	0.01
(1,4635)	1:A:54:LYS:H	1:A:54:LYS:HG2	13	0.01
(1,4635)	1:A:54:LYS:H	1:A:54:LYS:HG3	13	0.01
(1,4633)	1:A:53:VAL:HG21	1:A:54:LYS:HG2	4	0.01
(1,4633)	1:A:53:VAL:HG21	1:A:54:LYS:HG3	4	0.01
(1,4633)	1:A:53:VAL:HG22	1:A:54:LYS:HG2	4	0.01
(1,4633)	1:A:53:VAL:HG22	1:A:54:LYS:HG3	4	0.01
(1,4633)	1:A:53:VAL:HG23	1:A:54:LYS:HG2	4	0.01
(1,4633)	1:A:53:VAL:HG23	1:A:54:LYS:HG3	4	0.01
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE1	16	0.01
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE2	16	0.01
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE3	16	0.01
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE1	16	0.01
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE2	16	0.01
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE3	16	0.01
(1,462)	1:B:25:VAL:HB	1:B:27:SER:H	9	0.01
(1,462)	1:B:25:VAL:HB	1:B:27:SER:H	20	0.01
(1,4613)	1:A:42:ASP:HB2	1:A:44:ILE:HG12	3	0.01
(1,4613)	1:A:42:ASP:HB3	1:A:44:ILE:HG12	3	0.01
(1,4613)	1:A:42:ASP:HB2	1:A:44:ILE:HG12	18	0.01
(1,4613)	1:A:42:ASP:HB3	1:A:44:ILE:HG12	18	0.01
(1,461)	1:A:25:VAL:HB	1:A:27:SER:H	4	0.01
(1,4605)	1:A:39:ASN:HD21	1:A:46:THR:HB	6	0.01
(1,4605)	1:A:39:ASN:HD22	1:A:46:THR:HB	6	0.01
(1,4595)	1:A:37:VAL:HG21	1:A:48:ASN:HD21	12	0.01
(1,4595)	1:A:37:VAL:HG21	1:A:48:ASN:HD22	12	0.01
(1,4595)	1:A:37:VAL:HG22	1:A:48:ASN:HD21	12	0.01
(1,4595)	1:A:37:VAL:HG22	1:A:48:ASN:HD22	12	0.01



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(1,4595) 1:A:37:VAL:HG23 1:A:48:ASN:HD21 12 0.01 (1,4595) 1:A:37:VAL:HG23 1:A:48:ASN:HD22 12 0.01 (1,4593) 1:A:37:VAL:HG11 1:A:48:ASN:HD21 3 0.01 (1,4593) 1:A:37:VAL:HG12 1:A:48:ASN:HD22 3 0.01 (1,4593) 1:A:37:VAL:HG12 1:A:48:ASN:HD22 3 0.01 (1,4593) 1:A:37:VAL:HG13 1:A:48:ASN:HD22 3 0.01 (1,4593) 1:A:37:VAL:HG13 1:A:48:ASN:HD22 3 0.01 (1,4593) 1:A:35:THR:HB 1:A:50:MET:HB2 2 0.01 (1,4580) 1:A:35:THR:HB 1:A:50:MET:HB2 2 0.01 (1,4580) 1:A:35:THR:HB 1:A:50:MET:HB3 3 0.01 (1,4580) 1:A:35:THR:HB 1:A:50:MET:HB2 5 0.01 (1,4580) 1:A:35:THR:HB 1:A:50:MET:HB3 5 0.01 (1,4580) 1:A:35:THR:HB 1:A:50:MET:HB3 7 0.01 (1,4580) 1:A:33:THR:HB 1:A:50	Key	Atom-1	Atom-2	Model	Violation (Å)
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(1.4510) 1.4.95.VAI.IIA 1.4.90.IVC.IID2 20 0.01	(1,4518)	1:A:25:VAL:HA	1:A:28:LYS:HB2	20	0.01
(1,4010) 1:A:20:VAL:HA 1:A:28:LY5:HB3 20 0.01	(1,4518)	1:A:25:VAL:HA	1:A:28:LYS:HB3	20	0.01
(1,4504) 1:A:23:THR:HG21 1:A:27:SER:HB2 17 0.01	(1,4504)	1:A:23:THR:HG21	1:A:27:SER:HB2	17	0.01
(1,4504) 1:A:23:THR:HG21 1:A:27:SER:HB3 17 0.01	(1,4504)	1:A:23:THR:HG21	1:A:27:SER:HB3	17	0.01



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4504)	1:A:23:THR:HG22	1:A:27:SER:HB2	17	0.01
(1,4504)	1:A:23:THR:HG22	1:A:27:SER:HB3	17	0.01
(1,4504)	1:A:23:THR:HG23	1:A:27:SER:HB2	17	0.01
(1,4504)	1:A:23:THR:HG23	1:A:27:SER:HB3	17	0.01
(1,4496)	1:A:20:ASN:HB2	1:A:21:GLN:HE21	12	0.01
(1,4496)	1:A:20:ASN:HB3	1:A:21:GLN:HE21	12	0.01
(1,4496)	1:A:20:ASN:HB2	1:A:21:GLN:HE21	14	0.01
(1,4496)	1:A:20:ASN:HB3	1:A:21:GLN:HE21	14	0.01
(1,4496)	1:A:20:ASN:HB2	1:A:21:GLN:HE21	16	0.01
(1,4496)	1:A:20:ASN:HB3	1:A:21:GLN:HE21	16	0.01
(1,4478)	1:A:18:MET:HB2	1:A:18:MET:HE1	2	0.01
(1,4478)	1:A:18:MET:HB2	1:A:18:MET:HE2	2	0.01
(1,4478)	1:A:18:MET:HB2	1:A:18:MET:HE3	2	0.01
(1,4478)	1:A:18:MET:HB3	1:A:18:MET:HE1	2	0.01
(1,4478)	1:A:18:MET:HB3	1:A:18:MET:HE2	2	0.01
(1,4478)	1:A:18:MET:HB3	1:A:18:MET:HE3	2	0.01
(1,4478)	1:A:18:MET:HB2	1:A:18:MET:HE1	17	0.01
(1,4478)	1:A:18:MET:HB2	1:A:18:MET:HE2	17	0.01
(1,4478)	1:A:18:MET:HB2	1:A:18:MET:HE3	17	0.01
(1,4478)	1:A:18:MET:HB3	1:A:18:MET:HE1	17	0.01
(1,4478)	1:A:18:MET:HB3	1:A:18:MET:HE2	17	0.01
(1,4478)	1:A:18:MET:HB3	1:A:18:MET:HE3	17	0.01
(1,4458)	1:A:15:LYS:HB2	1:A:18:MET:HG2	14	0.01
(1,4458)	1:A:15:LYS:HB2	1:A:18:MET:HG3	14	0.01
(1,4458)	1:A:15:LYS:HB3	1:A:18:MET:HG2	14	0.01
(1,4458)	1:A:15:LYS:HB3	1:A:18:MET:HG3	14	0.01
(1,4406)	1:A:3:ASP:HB2	1:A:52:PHE:HB2	10	0.01
(1,4406)	1:A:3:ASP:HB2	1:A:52:PHE:HB3	10	0.01
(1,4406)	1:A:3:ASP:HB3	1:A:52:PHE:HB2	10	0.01
(1,4406)	1:A:3:ASP:HB3	1:A:52:PHE:HB3	10	0.01
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	19	0.01
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	19	0.01
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	19	0.01
(1,4387)	1:B:5:LEU:HG	1:B:83:HIS:HD2	6	0.01
(1,4386)	1:A:5:LEU:HG	1:A:83:HIS:HD2	14	0.01
(1,4386)	1:A:5:LEU:HG	1:A:83:HIS:HD2	18	0.01
(1,4386)	1:A:5:LEU:HG	1:A:83:HIS:HD2	20	0.01
(1,4385)	1:B:81:LEU:HD11	1:B:83:HIS:HD2	5	0.01
(1,4385)	1:B:81:LEU:HD12	1:B:83:HIS:HD2	5	0.01
(1,4385)	1:B:81:LEU:HD13	1:B:83:HIS:HD2	5	0.01
(1,4380)	1:A:5:LEU:HD21	1:A:83:HIS:HD2	2	0.01
(1,4380)	1:A:5:LEU:HD22	1:A:83:HIS:HD2	2	0.01



 $Continued\ from\ previous\ page...$

Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,4380)	1:A:5:LEU:HD23	1:A:83:HIS:HD2	2	0.01
(1,4380)	1:A:5:LEU:HD21	1:A:83:HIS:HD2	5	0.01
(1,4380)	1:A:5:LEU:HD22	1:A:83:HIS:HD2	5	0.01
(1,4380)	1:A:5:LEU:HD23	1:A:83:HIS:HD2	5	0.01
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG21	11	0.01
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG22	11	0.01
(1,4365)	1:B:73:PHE:HZ	1:B:74:THR:HG23	11	0.01
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG21	5	0.01
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG22	5	0.01
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG23	5	0.01
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG21	18	0.01
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG22	18	0.01
(1,4364)	1:A:73:PHE:HZ	1:A:74:THR:HG23	18	0.01
(1,4354)	1:A:44:ILE:HG12	1:A:73:PHE:HE1	15	0.01
(1,4354)	1:A:44:ILE:HG12	1:A:73:PHE:HE2	15	0.01
(1,4342)	1:A:29:PHE:HE1	1:A:65:LYS:HE2	5	0.01
(1,4342)	1:A:29:PHE:HE1	1:A:65:LYS:HE3	5	0.01
(1,4342)	1:A:29:PHE:HE2	1:A:65:LYS:HE2	5	0.01
(1,4342)	1:A:29:PHE:HE2	1:A:65:LYS:HE3	5	0.01
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE1	11	0.01
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE2	11	0.01
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE1	11	0.01
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE2	11	0.01
(1,4329)	1:B:5:LEU:HD21	1:B:52:PHE:HE1	5	0.01
(1,4329)	1:B:5:LEU:HD21	1:B:52:PHE:HE2	5	0.01
(1,4329)	1:B:5:LEU:HD22	1:B:52:PHE:HE1	5	0.01
(1,4329)	1:B:5:LEU:HD22	1:B:52:PHE:HE2	5	0.01
(1,4329)	1:B:5:LEU:HD23	1:B:52:PHE:HE1	5	0.01
(1,4329)	1:B:5:LEU:HD23	1:B:52:PHE:HE2	5	0.01
(1,4329)	1:B:5:LEU:HD21	1:B:52:PHE:HE1	14	0.01
(1,4329)	1:B:5:LEU:HD21	1:B:52:PHE:HE2	14	0.01
(1,4329)	1:B:5:LEU:HD22	1:B:52:PHE:HE1	14	0.01
(1,4329)	1:B:5:LEU:HD22	1:B:52:PHE:HE2	14	0.01
(1,4329)	1:B:5:LEU:HD23	1:B:52:PHE:HE1	14	0.01
(1,4329)	1:B:5:LEU:HD23	1:B:52:PHE:HE2	14	0.01
(1,4328)	1:A:5:LEU:HD21	1:A:52:PHE:HE1	3	0.01
(1,4328)	1:A:5:LEU:HD21	1:A:52:PHE:HE2	3	0.01
(1,4328)	1:A:5:LEU:HD22	1:A:52:PHE:HE1	3	0.01
(1,4328)	1:A:5:LEU:HD22	1:A:52:PHE:HE2	3	0.01
(1,4328)	1:A:5:LEU:HD23	1:A:52:PHE:HE1	3	0.01
(1,4328)	1:A:5:LEU:HD23	1:A:52:PHE:HE2	3	0.01
(1,4328)	1:A:5:LEU:HD21	1:A:52:PHE:HE1	4	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4328)	1:A:5:LEU:HD21	1:A:52:PHE:HE2	4	0.01
(1,4328)	1:A:5:LEU:HD22	1:A:52:PHE:HE1	4	0.01
(1,4328)	1:A:5:LEU:HD22	1:A:52:PHE:HE2	4	0.01
(1,4328)	1:A:5:LEU:HD23	1:A:52:PHE:HE1	4	0.01
(1,4328)	1:A:5:LEU:HD23	1:A:52:PHE:HE2	4	0.01
(1,4325)	1:B:6:ALA:H	1:B:52:PHE:HD1	2	0.01
(1,4325)	1:B:6:ALA:H	1:B:52:PHE:HD2	2	0.01
(1,4324)	1:A:6:ALA:H	1:A:52:PHE:HD1	7	0.01
(1,4324)	1:A:6:ALA:H	1:A:52:PHE:HD2	7	0.01
(1,4323)	1:B:52:PHE:HD1	1:B:53:VAL:H	17	0.01
(1,4323)	1:B:52:PHE:HD2	1:B:53:VAL:H	17	0.01
(1,4322)	1:A:52:PHE:HD1	1:A:53:VAL:H	3	0.01
(1,4322)	1:A:52:PHE:HD2	1:A:53:VAL:H	3	0.01
(1,4322)	1:A:52:PHE:HD1	1:A:53:VAL:H	14	0.01
(1,4322)	1:A:52:PHE:HD2	1:A:53:VAL:H	14	0.01
(1,4311)	1:B:5:LEU:HA	1:B:52:PHE:HD1	11	0.01
(1,4311)	1:B:5:LEU:HA	1:B:52:PHE:HD2	11	0.01
(1,4310)	1:A:5:LEU:HA	1:A:52:PHE:HD1	8	0.01
(1,4310)	1:A:5:LEU:HA	1:A:52:PHE:HD2	8	0.01
(1,4310)	1:A:5:LEU:HA	1:A:52:PHE:HD1	19	0.01
(1,4310)	1:A:5:LEU:HA	1:A:52:PHE:HD2	19	0.01
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	3	0.01
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	5	0.01
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	6	0.01
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	11	0.01
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	15	0.01
(1,4295)	1:B:22:ILE:HG13	1:B:45:PHE:HZ	18	0.01
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	16	0.01
(1,4294)	1:A:22:ILE:HG13	1:A:45:PHE:HZ	19	0.01
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE1	7	0.01
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE2	7	0.01
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE1	7	0.01
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE2	7	0.01
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE1	7	0.01
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE2	7	0.01
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE1	9	0.01
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE2	9	0.01
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE1	9	0.01
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE2	9	0.01
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE1	9	0.01
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE2	9	0.01
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE1	16	0.01



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE2	16	0.01
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE1	16	0.01
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE2	16	0.01
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE1	16	0.01
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE2	16	0.01
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE1	19	0.01
(1,4265)	1:B:22:ILE:HD11	1:B:45:PHE:HE2	19	0.01
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE1	19	0.01
(1,4265)	1:B:22:ILE:HD12	1:B:45:PHE:HE2	19	0.01
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE1	19	0.01
(1,4265)	1:B:22:ILE:HD13	1:B:45:PHE:HE2	19	0.01
(1,4264)	1:A:22:ILE:HD11	1:A:45:PHE:HE1	8	0.01
(1,4264)	1:A:22:ILE:HD11	1:A:45:PHE:HE2	8	0.01
(1,4264)	1:A:22:ILE:HD12	1:A:45:PHE:HE1	8	0.01
(1,4264)	1:A:22:ILE:HD12	1:A:45:PHE:HE2	8	0.01
(1,4264)	1:A:22:ILE:HD13	1:A:45:PHE:HE1	8	0.01
(1,4264)	1:A:22:ILE:HD13	1:A:45:PHE:HE2	8	0.01
(1,4264)	1:A:22:ILE:HD11	1:A:45:PHE:HE1	10	0.01
(1,4264)	1:A:22:ILE:HD11	1:A:45:PHE:HE2	10	0.01
(1,4264)	1:A:22:ILE:HD12	1:A:45:PHE:HE1	10	0.01
(1,4264)	1:A:22:ILE:HD12	1:A:45:PHE:HE2	10	0.01
(1,4264)	1:A:22:ILE:HD13	1:A:45:PHE:HE1	10	0.01
(1,4264)	1:A:22:ILE:HD13	1:A:45:PHE:HE2	10	0.01
(1,4264)	1:A:22:ILE:HD11	1:A:45:PHE:HE1	16	0.01
(1,4264)	1:A:22:ILE:HD11	1:A:45:PHE:HE2	16	0.01
(1,4264)	1:A:22:ILE:HD12	1:A:45:PHE:HE1	16	0.01
(1,4264)	1:A:22:ILE:HD12	1:A:45:PHE:HE2	16	0.01
(1,4264)	1:A:22:ILE:HD13	1:A:45:PHE:HE1	16	0.01
(1,4264)	1:A:22:ILE:HD13	1:A:45:PHE:HE2	16	0.01
(1,4241)	1:B:18:MET:HE1	1:B:45:PHE:HD1	16	0.01
(1,4241)	1:B:18:MET:HE1	1:B:45:PHE:HD2	16	0.01
(1,4241)	1:B:18:MET:HE2	1:B:45:PHE:HD1	16	0.01
(1,4241)	1:B:18:MET:HE2	1:B:45:PHE:HD2	16	0.01
(1,4241)	1:B:18:MET:HE3	1:B:45:PHE:HD1	16	0.01
(1,4241)	1:B:18:MET:HE3	1:B:45:PHE:HD2	16	0.01
(1,4237)	1:B:40:ALA:HB1	1:B:45:PHE:HD1	13	0.01
(1,4237)	1:B:40:ALA:HB1	1:B:45:PHE:HD2	13	0.01
(1,4237)	1:B:40:ALA:HB2	1:B:45:PHE:HD1	13	0.01
(1,4237)	1:B:40:ALA:HB2	1:B:45:PHE:HD2	13	0.01
(1,4237)	1:B:40:ALA:HB3	1:B:45:PHE:HD1	13	0.01
(1,4237)	1:B:40:ALA:HB3	1:B:45:PHE:HD2	13	0.01
(1,4211)	1:B:29:PHE:H	1:B:29:PHE:HD1	12	0.01



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Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,4211)	1:B:29:PHE:H	1:B:29:PHE:HD2	12	0.01
(1,4210)	1:A:29:PHE:H	1:A:29:PHE:HD1	20	0.01
(1,4210)	1:A:29:PHE:H	1:A:29:PHE:HD2	20	0.01
(1,4208)	1:A:29:PHE:HA	1:A:29:PHE:HD1	12	0.01
(1,4208)	1:A:29:PHE:HA	1:A:29:PHE:HD2	12	0.01
(1,4205)	1:B:29:PHE:HD1	1:B:65:LYS:HD2	17	0.01
(1,4205)	1:B:29:PHE:HD2	1:B:65:LYS:HD2	17	0.01
(1,4204)	1:A:29:PHE:HD1	1:A:65:LYS:HD2	20	0.01
(1,4204)	1:A:29:PHE:HD2	1:A:65:LYS:HD2	20	0.01
(1,4187)	1:B:4:PHE:HZ	1:B:6:ALA:HA	6	0.01
(1,4187)	1:B:4:PHE:HZ	1:B:6:ALA:HA	17	0.01
(1,4187)	1:B:4:PHE:HZ	1:B:6:ALA:HA	18	0.01
(1,4186)	1:A:4:PHE:HZ	1:A:6:ALA:HA	1	0.01
(1,4186)	1:A:4:PHE:HZ	1:A:6:ALA:HA	8	0.01
(1,4186)	1:A:4:PHE:HZ	1:A:6:ALA:HA	9	0.01
(1,4186)	1:A:4:PHE:HZ	1:A:6:ALA:HA	17	0.01
(1,4179)	1:B:4:PHE:HZ	1:B:59:LEU:HD21	4	0.01
(1,4179)	1:B:4:PHE:HZ	1:B:59:LEU:HD22	4	0.01
(1,4179)	1:B:4:PHE:HZ	1:B:59:LEU:HD23	4	0.01
(1,416)	1:A:24:GLY:H	1:A:27:SER:HG	4	0.01
(1,416)	1:A:24:GLY:H	1:A:27:SER:HG	12	0.01
(1,416)	1:A:24:GLY:H	1:A:27:SER:HG	15	0.01
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD21	1	0.01
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD22	1	0.01
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD23	1	0.01
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD21	1	0.01
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD22	1	0.01
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD23	1	0.01
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD21	15	0.01
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD22	15	0.01
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD23	15	0.01
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD21	15	0.01
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD22	15	0.01
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD23	15	0.01
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD21	18	0.01
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD22	18	0.01
(1,4151)	1:B:4:PHE:HE1	1:B:59:LEU:HD23	18	0.01
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD21	18	0.01
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD22	18	0.01
(1,4151)	1:B:4:PHE:HE2	1:B:59:LEU:HD23	18	0.01
(1,4150)	1:A:4:PHE:HE1	1:A:59:LEU:HD21	3	0.01
(1,4150)	1:A:4:PHE:HE1	1:A:59:LEU:HD22	3	0.01



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4150)	1:A:4:PHE:HE1	1:A:59:LEU:HD23	3	0.01
(1,4150)	1:A:4:PHE:HE2	1:A:59:LEU:HD21	3	0.01
(1,4150)	1:A:4:PHE:HE2	1:A:59:LEU:HD22	3	0.01
(1,4150)	1:A:4:PHE:HE2	1:A:59:LEU:HD23	3	0.01
(1,4150)	1:A:4:PHE:HE1	1:A:59:LEU:HD21	6	0.01
(1,4150)	1:A:4:PHE:HE1	1:A:59:LEU:HD22	6	0.01
(1,4150)	1:A:4:PHE:HE1	1:A:59:LEU:HD23	6	0.01
(1,4150)	1:A:4:PHE:HE2	1:A:59:LEU:HD21	6	0.01
(1,4150)	1:A:4:PHE:HE2	1:A:59:LEU:HD22	6	0.01
(1,4150)	1:A:4:PHE:HE2	1:A:59:LEU:HD23	6	0.01
(1,4150)	1:A:4:PHE:HE1	1:A:59:LEU:HD21	10	0.01
(1,4150)	1:A:4:PHE:HE1	1:A:59:LEU:HD22	10	0.01
(1,4150)	1:A:4:PHE:HE1	1:A:59:LEU:HD23	10	0.01
(1,4150)	1:A:4:PHE:HE2	1:A:59:LEU:HD21	10	0.01
(1,4150)	1:A:4:PHE:HE2	1:A:59:LEU:HD22	10	0.01
(1,4150)	1:A:4:PHE:HE2	1:A:59:LEU:HD23	10	0.01
(1,4150)	1:A:4:PHE:HE1	1:A:59:LEU:HD21	11	0.01
(1,4150)	1:A:4:PHE:HE1	1:A:59:LEU:HD22	11	0.01
(1,4150)	1:A:4:PHE:HE1	1:A:59:LEU:HD23	11	0.01
(1,4150)	1:A:4:PHE:HE2	1:A:59:LEU:HD21	11	0.01
(1,4150)	1:A:4:PHE:HE2	1:A:59:LEU:HD22	11	0.01
(1,4150)	1:A:4:PHE:HE2	1:A:59:LEU:HD23	11	0.01
(1,4145)	1:B:4:PHE:HD1	1:B:5:LEU:H	3	0.01
(1,4145)	1:B:4:PHE:HD2	1:B:5:LEU:H	3	0.01
(1,4145)	1:B:4:PHE:HD1	1:B:5:LEU:H	4	0.01
(1,4145)	1:B:4:PHE:HD2	1:B:5:LEU:H	4	0.01
(1,4145)	1:B:4:PHE:HD1	1:B:5:LEU:H	5	0.01
(1,4145)	1:B:4:PHE:HD2	1:B:5:LEU:H	5	0.01
(1,4145)	1:B:4:PHE:HD1	1:B:5:LEU:H	8	0.01
(1,4145)	1:B:4:PHE:HD2	1:B:5:LEU:H	8	0.01
(1,4145)	1:B:4:PHE:HD1	1:B:5:LEU:H	10	0.01
(1,4145)	1:B:4:PHE:HD2	1:B:5:LEU:H	10	0.01
(1,4145)	1:B:4:PHE:HD1	1:B:5:LEU:H	17	0.01
(1,4145)	1:B:4:PHE:HD2	1:B:5:LEU:H	17	0.01
(1,4145)	1:B:4:PHE:HD1	1:B:5:LEU:H	20	0.01
(1,4145)	1:B:4:PHE:HD2	1:B:5:LEU:H	20	0.01
(1,4144)	1:A:4:PHE:HD1	1:A:5:LEU:H	2	0.01
(1,4144)	1:A:4:PHE:HD2	1:A:5:LEU:H	2	0.01
(1,4144)	1:A:4:PHE:HD1	1:A:5:LEU:H	5	0.01
(1,4144)	1:A:4:PHE:HD2	1:A:5:LEU:H	5	0.01
(1,4144)	1:A:4:PHE:HD1	1:A:5:LEU:H	8	0.01
(1,4144)	1:A:4:PHE:HD2	1:A:5:LEU:H	8	0.01



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Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,4144)	1:A:4:PHE:HD1	1:A:5:LEU:H	18	0.01
(1,4144)	1:A:4:PHE:HD2	1:A:5:LEU:H	18	0.01
(1,4139)	1:B:4:PHE:HD1	1:B:54:LYS:HA	9	0.01
(1,4139)	1:B:4:PHE:HD2	1:B:54:LYS:HA	9	0.01
(1,4138)	1:A:4:PHE:HD1	1:A:54:LYS:HA	2	0.01
(1,4138)	1:A:4:PHE:HD2	1:A:54:LYS:HA	2	0.01
(1,4138)	1:A:4:PHE:HD1	1:A:54:LYS:HA	7	0.01
(1,4138)	1:A:4:PHE:HD2	1:A:54:LYS:HA	7	0.01
(1,4138)	1:A:4:PHE:HD1	1:A:54:LYS:HA	16	0.01
(1,4138)	1:A:4:PHE:HD2	1:A:54:LYS:HA	16	0.01
(1,4138)	1:A:4:PHE:HD1	1:A:54:LYS:HA	19	0.01
(1,4138)	1:A:4:PHE:HD2	1:A:54:LYS:HA	19	0.01
(1,4129)	1:B:83:HIS:HA	1:B:83:HIS:HD2	7	0.01
(1,4129)	1:B:83:HIS:HA	1:B:83:HIS:HD2	20	0.01
(1,4128)	1:A:83:HIS:HA	1:A:83:HIS:HD2	3	0.01
(1,4128)	1:A:83:HIS:HA	1:A:83:HIS:HD2	14	0.01
(1,4119)	1:B:80:ASN:HA	1:B:81:LEU:HG	14	0.01
(1,4118)	1:A:80:ASN:HA	1:A:81:LEU:HG	2	0.01
(1,4113)	1:B:77:ARG:HG3	1:B:79:SER:HA	5	0.01
(1,4113)	1:B:77:ARG:HG3	1:B:79:SER:HA	11	0.01
(1,4112)	1:A:77:ARG:HG3	1:A:79:SER:HA	8	0.01
(1,4112)	1:A:77:ARG:HG3	1:A:79:SER:HA	17	0.01
(1,4108)	1:A:79:SER:HA	1:A:81:LEU:HD21	2	0.01
(1,4108)	1:A:79:SER:HA	1:A:81:LEU:HD22	2	0.01
(1,4108)	1:A:79:SER:HA	1:A:81:LEU:HD23	2	0.01
(1,4093)	1:B:74:THR:HA	1:B:75:VAL:HG21	4	0.01
(1,4093)	1:B:74:THR:HA	1:B:75:VAL:HG22	4	0.01
(1,4093)	1:B:74:THR:HA	1:B:75:VAL:HG23	4	0.01
(1,4091)	1:B:73:PHE:HA	1:B:73:PHE:HD1	5	0.01
(1,4091)	1:B:73:PHE:HA	1:B:73:PHE:HD2	5	0.01
(1,4090)	1:A:73:PHE:HA	1:A:73:PHE:HD1	18	0.01
(1,4090)	1:A:73:PHE:HA	1:A:73:PHE:HD2	18	0.01
(1,4086)	1:A:73:PHE:HA	1:A:75:VAL:HG21	2	0.01
(1,4086)	1:A:73:PHE:HA	1:A:75:VAL:HG22	2	0.01
(1,4086)	1:A:73:PHE:HA	1:A:75:VAL:HG23	2	0.01
(1,4052)	1:A:41:LYS:HG2	1:A:42:ASP:HA	2	0.01
(1,4052)	1:A:41:LYS:HG3	1:A:42:ASP:HA	2	0.01
(1,4049)	1:B:41:LYS:HA	1:B:41:LYS:HD2	1	0.01
(1,4049)	1:B:41:LYS:HA	1:B:41:LYS:HD3	1	0.01
(1,4049)	1:B:41:LYS:HA	1:B:41:LYS:HD2	10	0.01
(1,4049)	1:B:41:LYS:HA	1:B:41:LYS:HD3	10	0.01
(1,4048)	1:A:41:LYS:HA	1:A:41:LYS:HD2	20	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,4048)	1:A:41:LYS:HA	1:A:41:LYS:HD3	20	0.01
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG2	8	0.01
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG3	8	0.01
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG2	11	0.01
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG3	11	0.01
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG2	14	0.01
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG3	14	0.01
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG2	20	0.01
(1,4047)	1:B:41:LYS:HA	1:B:41:LYS:HG3	20	0.01
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG2	4	0.01
(1,4046)	1:A:41:LYS:HA	1:A:41:LYS:HG3	4	0.01
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	5	0.01
(1,4036)	1:A:15:LYS:HA	1:A:17:GLY:H	14	0.01
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	7	0.01
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	9	0.01
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	17	0.01
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	19	0.01
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD11	1	0.01
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD12	1	0.01
(1,3985)	1:B:5:LEU:HD11	1:B:81:LEU:HD13	1	0.01
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD11	1	0.01
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD12	1	0.01
(1,3985)	1:B:5:LEU:HD12	1:B:81:LEU:HD13	1	0.01
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD11	1	0.01
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD12	1	0.01
(1,3985)	1:B:5:LEU:HD13	1:B:81:LEU:HD13	1	0.01
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD11	7	0.01
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD12	7	0.01
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD13	7	0.01
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD11	20	0.01
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD12	20	0.01
(1,3939)	1:B:11:VAL:HA	1:B:44:ILE:HD13	20	0.01
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD11	2	0.01
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD12	2	0.01
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD13	2	0.01
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD11	5	0.01
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD12	5	0.01
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD13	5	0.01
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD11	11	0.01
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD12	11	0.01
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD13	11	0.01
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD11	17	0.01



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD12	17	0.01
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD13	17	0.01
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD11	19	0.01
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD12	19	0.01
(1,3938)	1:A:11:VAL:HA	1:A:44:ILE:HD13	19	0.01
(1,3928)	1:A:23:THR:H	1:B:33:ILE:HD11	18	0.01
(1,3928)	1:A:23:THR:H	1:B:33:ILE:HD12	18	0.01
(1,3928)	1:A:23:THR:H	1:B:33:ILE:HD13	18	0.01
(1,3917)	1:A:18:MET:HE1	1:A:21:GLN:HE21	10	0.01
(1,3917)	1:A:18:MET:HE2	1:A:21:GLN:HE21	10	0.01
(1,3917)	1:A:18:MET:HE3	1:A:21:GLN:HE21	10	0.01
(1,3916)	1:B:18:MET:HE1	1:B:72:VAL:HG21	4	0.01
(1,3916)	1:B:18:MET:HE1	1:B:72:VAL:HG22	4	0.01
(1,3916)	1:B:18:MET:HE1	1:B:72:VAL:HG23	4	0.01
(1,3916)	1:B:18:MET:HE2	1:B:72:VAL:HG21	4	0.01
(1,3916)	1:B:18:MET:HE2	1:B:72:VAL:HG22	4	0.01
(1,3916)	1:B:18:MET:HE2	1:B:72:VAL:HG23	4	0.01
(1,3916)	1:B:18:MET:HE3	1:B:72:VAL:HG21	4	0.01
(1,3916)	1:B:18:MET:HE3	1:B:72:VAL:HG22	4	0.01
(1,3916)	1:B:18:MET:HE3	1:B:72:VAL:HG23	4	0.01
(1,3913)	1:A:18:MET:HE1	1:A:69:VAL:HG11	10	0.01
(1,3913)	1:A:18:MET:HE1	1:A:69:VAL:HG12	10	0.01
(1,3913)	1:A:18:MET:HE1	1:A:69:VAL:HG13	10	0.01
(1,3913)	1:A:18:MET:HE2	1:A:69:VAL:HG11	10	0.01
(1,3913)	1:A:18:MET:HE2	1:A:69:VAL:HG12	10	0.01
(1,3913)	1:A:18:MET:HE2	1:A:69:VAL:HG13	10	0.01
(1,3913)	1:A:18:MET:HE3	1:A:69:VAL:HG11	10	0.01
(1,3913)	1:A:18:MET:HE3	1:A:69:VAL:HG12	10	0.01
(1,3913)	1:A:18:MET:HE3	1:A:69:VAL:HG13	10	0.01
(1,3913)	1:A:18:MET:HE1	1:A:69:VAL:HG11	17	0.01
(1,3913)	1:A:18:MET:HE1	1:A:69:VAL:HG12	17	0.01
(1,3913)	1:A:18:MET:HE1	1:A:69:VAL:HG13	17	0.01
(1,3913)	1:A:18:MET:HE2	1:A:69:VAL:HG11	17	0.01
(1,3913)	1:A:18:MET:HE2	1:A:69:VAL:HG12	17	0.01
(1,3913)	1:A:18:MET:HE2	1:A:69:VAL:HG13	17	0.01
(1,3913)	1:A:18:MET:HE3	1:A:69:VAL:HG11	17	0.01
(1,3913)	1:A:18:MET:HE3	1:A:69:VAL:HG12	17	0.01
(1,3913)	1:A:18:MET:HE3	1:A:69:VAL:HG13	17	0.01
(1,3890)	1:B:82:GLU:HA	1:B:83:HIS:HB2	1	0.01
(1,3890)	1:B:82:GLU:HA	1:B:83:HIS:HB2	17	0.01
(1,3889)	1:A:82:GLU:HA	1:A:83:HIS:HB2	2	0.01
(1,3889)	1:A:82:GLU:HA	1:A:83:HIS:HB2	10	0.01



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(Atom-1	Atom-2	Model	Violation (Å)
(1,3889)	1:A:82:GLU:HA	1:A:83:HIS:HB2	15	0.01
(1,3888)	1:B:8:ILE:H	1:B:81:LEU:HD21	9	0.01
(1,3888)	1:B:8:ILE:H	1:B:81:LEU:HD22	9	0.01
(1,3888)	1:B:8:ILE:H	1:B:81:LEU:HD23	9	0.01
(1,3888)	1:B:8:ILE:H	1:B:81:LEU:HD21	10	0.01
(1,3888)	1:B:8:ILE:H	1:B:81:LEU:HD22	10	0.01
(1,3888)	1:B:8:ILE:H	1:B:81:LEU:HD23	10	0.01
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD21	12	0.01
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD22	12	0.01
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD23	12	0.01
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD21	17	0.01
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD22	17	0.01
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD23	17	0.01
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD21	19	0.01
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD22	19	0.01
(1,3887)	1:A:8:ILE:H	1:A:81:LEU:HD23	19	0.01
(1,3886)	1:B:79:SER:H	1:B:81:LEU:HD21	6	0.01
(1,3886)	1:B:79:SER:H	1:B:81:LEU:HD22	6	0.01
(1,3886)	1:B:79:SER:H	1:B:81:LEU:HD23	6	0.01
(1,3876)	1:B:50:MET:HG3	1:B:81:LEU:HD21	18	0.01
(1,3876)	1:B:50:MET:HG3	1:B:81:LEU:HD22	18	0.01
(1,3876)	1:B:50:MET:HG3	1:B:81:LEU:HD23	18	0.01
(1,3857)	1:A:50:MET:HG2	1:A:81:LEU:HD11	10	0.01
(1,3857)	1:A:50:MET:HG2	1:A:81:LEU:HD12	10	0.01
(1,3857)	1:A:50:MET:HG2	1:A:81:LEU:HD13	10	0.01
(1,3846)	1:B:80:ASN:HB3	1:B:81:LEU:HD21	1	0.01
(1,3846)	1:B:80:ASN:HB3	1:B:81:LEU:HD22	1	0.01
(1,3846)	1:B:80:ASN:HB3	1:B:81:LEU:HD23	1	0.01
(1,3842)	1:B:80:ASN:HB2	1:B:81:LEU:HD21	9	0.01
(1,3842)	1:B:80:ASN:HB2	1:B:81:LEU:HD22	9	0.01
(1,3842)	1:B:80:ASN:HB2	1:B:81:LEU:HD23	9	0.01
(1,3842)	1:B:80:ASN:HB2	1:B:81:LEU:HD21	16	0.01
(1,3842)	1:B:80:ASN:HB2	1:B:81:LEU:HD22	16	0.01
(1,3842)	1:B:80:ASN:HB2	1:B:81:LEU:HD23	16	0.01
(1,3836)	1:B:9:ARG:H	1:B:78:LEU:HD21	6	0.01
(1,3836)	1:B:9:ARG:H	1:B:78:LEU:HD22	6	0.01
(1,3836)	1:B:9:ARG:H	1:B:78:LEU:HD23	6	0.01
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD21	8	0.01
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD22	8	0.01
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD23	8	0.01
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD21	8	0.01
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD22	8	0.01



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD23	8	0.01
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD21	12	0.01
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD22	12	0.01
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD23	12	0.01
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD21	12	0.01
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD22	12	0.01
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD23	12	0.01
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD21	18	0.01
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD22	18	0.01
(1,3822)	1:B:9:ARG:HB2	1:B:78:LEU:HD23	18	0.01
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD21	18	0.01
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD22	18	0.01
(1,3822)	1:B:9:ARG:HB3	1:B:78:LEU:HD23	18	0.01
(1,3821)	1:A:9:ARG:HB2	1:A:78:LEU:HD21	6	0.01
(1,3821)	1:A:9:ARG:HB2	1:A:78:LEU:HD22	6	0.01
(1,3821)	1:A:9:ARG:HB2	1:A:78:LEU:HD23	6	0.01
(1,3821)	1:A:9:ARG:HB3	1:A:78:LEU:HD21	6	0.01
(1,3821)	1:A:9:ARG:HB3	1:A:78:LEU:HD22	6	0.01
(1,3821)	1:A:9:ARG:HB3	1:A:78:LEU:HD23	6	0.01
(1,3821)	1:A:9:ARG:HB2	1:A:78:LEU:HD21	16	0.01
(1,3821)	1:A:9:ARG:HB2	1:A:78:LEU:HD22	16	0.01
(1,3821)	1:A:9:ARG:HB2	1:A:78:LEU:HD23	16	0.01
(1,3821)	1:A:9:ARG:HB3	1:A:78:LEU:HD21	16	0.01
(1,3821)	1:A:9:ARG:HB3	1:A:78:LEU:HD22	16	0.01
(1,3821)	1:A:9:ARG:HB3	1:A:78:LEU:HD23	16	0.01
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD11	1	0.01
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD12	1	0.01
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD13	1	0.01
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD11	5	0.01
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD12	5	0.01
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD13	5	0.01
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD11	11	0.01
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD12	11	0.01
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD13	11	0.01
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD11	17	0.01
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD12	17	0.01
(1,3818)	1:B:76:GLU:H	1:B:78:LEU:HD13	17	0.01
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD11	3	0.01
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD12	3	0.01
(1,3817)	1:A:76:GLU:H	1:A:78:LEU:HD13	3	0.01
(1,381)	1:B:22:ILE:H	1:B:23:THR:HG1	9	0.01
(1,381)	1:B:22:ILE:H	1:B:23:THR:HG1	10	0.01



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Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,381)	1:B:22:ILE:H	1:B:23:THR:HG1	15	0.01
(1,380)	1:A:22:ILE:H	1:A:23:THR:HG1	1	0.01
(1,380)	1:A:22:ILE:H	1:A:23:THR:HG1	7	0.01
(1,380)	1:A:22:ILE:H	1:A:23:THR:HG1	9	0.01
(1,380)	1:A:22:ILE:H	1:A:23:THR:HG1	17	0.01
(1,3798)	1:B:9:ARG:HD2	1:B:78:LEU:HD11	12	0.01
(1,3798)	1:B:9:ARG:HD2	1:B:78:LEU:HD12	12	0.01
(1,3798)	1:B:9:ARG:HD2	1:B:78:LEU:HD13	12	0.01
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD11	12	0.01
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD12	12	0.01
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD13	12	0.01
(1,3798)	1:B:9:ARG:HD2	1:B:78:LEU:HD11	18	0.01
(1,3798)	1:B:9:ARG:HD2	1:B:78:LEU:HD12	18	0.01
(1,3798)	1:B:9:ARG:HD2	1:B:78:LEU:HD13	18	0.01
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD11	18	0.01
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD12	18	0.01
(1,3798)	1:B:9:ARG:HD3	1:B:78:LEU:HD13	18	0.01
(1,3797)	1:A:9:ARG:HD2	1:A:78:LEU:HD11	2	0.01
(1,3797)	1:A:9:ARG:HD2	1:A:78:LEU:HD12	2	0.01
(1,3797)	1:A:9:ARG:HD2	1:A:78:LEU:HD13	2	0.01
(1,3797)	1:A:9:ARG:HD3	1:A:78:LEU:HD11	2	0.01
(1,3797)	1:A:9:ARG:HD3	1:A:78:LEU:HD12	2	0.01
(1,3797)	1:A:9:ARG:HD3	1:A:78:LEU:HD13	2	0.01
(1,3768)	1:B:77:ARG:HD2	1:B:78:LEU:H	17	0.01
(1,3768)	1:B:77:ARG:HD3	1:B:78:LEU:H	17	0.01
(1,3758)	1:B:6:ALA:HB1	1:B:77:ARG:HD2	7	0.01
(1,3758)	1:B:6:ALA:HB1	1:B:77:ARG:HD3	7	0.01
(1,3758)	1:B:6:ALA:HB2	1:B:77:ARG:HD2	7	0.01
(1,3758)	1:B:6:ALA:HB2	1:B:77:ARG:HD3	7	0.01
(1,3758)	1:B:6:ALA:HB3	1:B:77:ARG:HD2	7	0.01
(1,3758)	1:B:6:ALA:HB3	1:B:77:ARG:HD3	7	0.01
(1,3758)	1:B:6:ALA:HB1	1:B:77:ARG:HD2	8	0.01
(1,3758)	1:B:6:ALA:HB1	1:B:77:ARG:HD3	8	0.01
(1,3758)	1:B:6:ALA:HB2	1:B:77:ARG:HD2	8	0.01
(1,3758)	1:B:6:ALA:HB2	1:B:77:ARG:HD3	8	0.01
(1,3758)	1:B:6:ALA:HB3	1:B:77:ARG:HD2	8	0.01
(1,3758)	1:B:6:ALA:HB3	1:B:77:ARG:HD3	8	0.01
(1,3758)	1:B:6:ALA:HB1	1:B:77:ARG:HD2	19	0.01
(1,3758)	1:B:6:ALA:HB1	1:B:77:ARG:HD3	19	0.01
(1,3758)	1:B:6:ALA:HB2	1:B:77:ARG:HD2	19	0.01
(1,3758)	1:B:6:ALA:HB2	1:B:77:ARG:HD3	19	0.01
(1,3758)	1:B:6:ALA:HB3	1:B:77:ARG:HD2	19	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3758)	1:B:6:ALA:HB3	1:B:77:ARG:HD3	19	0.01
(1,3757)	1:A:6:ALA:HB1	1:A:77:ARG:HD2	18	0.01
(1,3757)	1:A:6:ALA:HB1	1:A:77:ARG:HD3	18	0.01
(1,3757)	1:A:6:ALA:HB2	1:A:77:ARG:HD2	18	0.01
(1,3757)	1:A:6:ALA:HB2	1:A:77:ARG:HD3	18	0.01
(1,3757)	1:A:6:ALA:HB3	1:A:77:ARG:HD2	18	0.01
(1,3757)	1:A:6:ALA:HB3	1:A:77:ARG:HD3	18	0.01
(1,3753)	1:A:59:LEU:HD11	1:A:77:ARG:HD2	15	0.01
(1,3753)	1:A:59:LEU:HD11	1:A:77:ARG:HD3	15	0.01
(1,3753)	1:A:59:LEU:HD12	1:A:77:ARG:HD2	15	0.01
(1,3753)	1:A:59:LEU:HD12	1:A:77:ARG:HD3	15	0.01
(1,3753)	1:A:59:LEU:HD13	1:A:77:ARG:HD2	15	0.01
(1,3753)	1:A:59:LEU:HD13	1:A:77:ARG:HD3	15	0.01
(1,3738)	1:B:59:LEU:HD11	1:B:77:ARG:HG2	16	0.01
(1,3738)	1:B:59:LEU:HD12	1:B:77:ARG:HG2	16	0.01
(1,3738)	1:B:59:LEU:HD13	1:B:77:ARG:HG2	16	0.01
(1,3737)	1:A:59:LEU:HD11	1:A:77:ARG:HG2	1	0.01
(1,3737)	1:A:59:LEU:HD12	1:A:77:ARG:HG2	1	0.01
(1,3737)	1:A:59:LEU:HD13	1:A:77:ARG:HG2	1	0.01
(1,3734)	1:B:74:THR:HA	1:B:76:GLU:HG2	1	0.01
(1,3734)	1:B:74:THR:HA	1:B:76:GLU:HG3	1	0.01
(1,3734)	1:B:74:THR:HA	1:B:76:GLU:HG2	3	0.01
(1,3734)	1:B:74:THR:HA	1:B:76:GLU:HG3	3	0.01
(1,3731)	1:A:9:ARG:HB2	1:A:76:GLU:HG2	17	0.01
(1,3731)	1:A:9:ARG:HB2	1:A:76:GLU:HG3	17	0.01
(1,3731)	1:A:9:ARG:HB3	1:A:76:GLU:HG2	17	0.01
(1,3731)	1:A:9:ARG:HB3	1:A:76:GLU:HG3	17	0.01
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG21	19	0.01
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG22	19	0.01
(1,3698)	1:B:73:PHE:HD1	1:B:74:THR:HG23	19	0.01
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG21	19	0.01
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG22	19	0.01
(1,3698)	1:B:73:PHE:HD2	1:B:74:THR:HG23	19	0.01
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG21	6	0.01
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG22	6	0.01
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG23	6	0.01
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG21	6	0.01
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG22	6	0.01
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG23	6	0.01
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG21	14	0.01
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG22	14	0.01
(1,3697)	1:A:73:PHE:HD1	1:A:74:THR:HG23	14	0.01



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG21	14	0.01
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG22	14	0.01
(1,3697)	1:A:73:PHE:HD2	1:A:74:THR:HG23	14	0.01
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG21	7	0.01
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG22	7	0.01
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG23	7	0.01
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG21	9	0.01
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG22	9	0.01
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG23	9	0.01
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG21	18	0.01
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG22	18	0.01
(1,3696)	1:B:73:PHE:HA	1:B:74:THR:HG23	18	0.01
(1,3686)	1:B:10:ILE:HA	1:B:74:THR:HB	9	0.01
(1,3685)	1:A:10:ILE:HA	1:A:74:THR:HB	12	0.01
(1,3660)	1:B:66:LEU:HA	1:B:72:VAL:HG21	13	0.01
(1,3660)	1:B:66:LEU:HA	1:B:72:VAL:HG22	13	0.01
(1,3660)	1:B:66:LEU:HA	1:B:72:VAL:HG23	13	0.01
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG11	11	0.01
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG12	11	0.01
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG13	11	0.01
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG11	13	0.01
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG12	13	0.01
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG13	13	0.01
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG11	14	0.01
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG12	14	0.01
(1,3638)	1:B:67:ARG:HA	1:B:72:VAL:HG13	14	0.01
(1,3614)	1:B:69:VAL:H	1:B:70:GLN:HB2	3	0.01
(1,3614)	1:B:69:VAL:H	1:B:70:GLN:HB3	3	0.01
(1,3614)	1:B:69:VAL:H	1:B:70:GLN:HB2	18	0.01
(1,3614)	1:B:69:VAL:H	1:B:70:GLN:HB3	18	0.01
(1,3614)	1:B:69:VAL:H	1:B:70:GLN:HB2	19	0.01
(1,3614)	1:B:69:VAL:H	1:B:70:GLN:HB3	19	0.01
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB2	6	0.01
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB3	6	0.01
(1,3606)	1:B:69:VAL:HG11	1:B:70:GLN:HB2	1	0.01
(1,3606)	1:B:69:VAL:HG11	1:B:70:GLN:HB3	1	0.01
(1,3606)	1:B:69:VAL:HG12	1:B:70:GLN:HB2	1	0.01
(1,3606)	1:B:69:VAL:HG12	1:B:70:GLN:HB3	1	0.01
(1,3606)	1:B:69:VAL:HG13	1:B:70:GLN:HB2	1	0.01
(1,3606)	1:B:69:VAL:HG13	1:B:70:GLN:HB3	1	0.01
(1,3594)	1:B:66:LEU:HA	1:B:69:VAL:HB	3	0.01
(1,3593)	1:A:66:LEU:HA	1:A:69:VAL:HB	20	0.01



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(1,3592) 1:B:2	20:ASN:HA	1:B:22:ILE:HB	7	
() /		1.D.22.1DD.11D	7	0.01
/	20:ASN:HA	1:B:22:ILE:HB	16	0.01
(1,3592) 1:B:2	20:ASN:HA	1:B:22:ILE:HB	19	0.01
(1,3591) 1:A:2	20:ASN:HA	1:A:22:ILE:HB	7	0.01
(1,3591) 1:A:2	20:ASN:HA	1:A:22:ILE:HB	18	0.01
(1,3562) 1:B:1	5:LYS:HE2	1:B:18:MET:H	16	0.01
(1,3562) 1:B:1	5:LYS:HE3	1:B:18:MET:H	16	0.01
(1,3562) 1:B:1	5:LYS:HE2	1:B:18:MET:H	17	0.01
(1,3562) 1:B:1	5:LYS:HE3	1:B:18:MET:H	17	0.01
(1,3561) 1:A:1	5:LYS:HE2	1:A:18:MET:H	7	0.01
(1,3561) 1:A:1	5:LYS:HE3	1:A:18:MET:H	7	0.01
(1,3558) 1:B:	:15:LYS:H	1:B:15:LYS:HE2	17	0.01
(1,3558) 1:B	:15:LYS:H	1:B:15:LYS:HE3	17	0.01
(1,3531) 1:A:6	68:LYS:HA	1:A:68:LYS:HD3	2	0.01
(1,3530) 1:B:6	68:LYS:HA	1:B:68:LYS:HG3	14	0.01
(1,3530) 1:B:6	68:LYS:HA	1:B:68:LYS:HG3	16	0.01
(1,349) 1:B:18	8:MET:HE1	1:B:21:GLN:HE22	4	0.01
(1,349) 1:B:18	8:MET:HE2	1:B:21:GLN:HE22	4	0.01
(1,349) 1:B:18	8:MET:HE3	1:B:21:GLN:HE22	4	0.01
(1,3484) 1:B:4	1:LYS:HE2	1:B:44:ILE:H	4	0.01
(1,3484) 1:B:4	1:LYS:HE3	1:B:44:ILE:H	4	0.01
(1,3483) 1:A:4	1:LYS:HE2	1:A:44:ILE:H	12	0.01
(1,3483) 1:A:4	1:LYS:HE3	1:A:44:ILE:H	12	0.01
(1,3422) 1:A	:9:ARG:H	1:A:63:MET:HE1	2	0.01
(1,3422) 1:A	:9:ARG:H	1:A:63:MET:HE2	2	0.01
(1,3422) 1:A	:9:ARG:H	1:A:63:MET:HE3	2	0.01
(1,3422) 1:A	:9:ARG:H	1:A:63:MET:HE1	11	0.01
(1,3422) 1:A	:9:ARG:H	1:A:63:MET:HE2	11	0.01
(1,3422) 1:A	:9:ARG:H	1:A:63:MET:HE3	11	0.01
(1,3421) 1:B:63	3:MET:HE1	1:B:77:ARG:H	1	0.01
(1,3421) 1:B:63	3:MET:HE2	1:B:77:ARG:H	1	0.01
(1,3421) 1:B:63	3:MET:HE3	1:B:77:ARG:H	1	0.01
(1,3421) 1:B:63	3:MET:HE1	1:B:77:ARG:H	11	0.01
(1,3421) 1:B:63	3:MET:HE2	1:B:77:ARG:H	11	0.01
(1,3421) 1:B:63	3:MET:HE3	1:B:77:ARG:H	11	0.01
(1,3420) 1:A:63	3:MET:HE1	1:A:77:ARG:H	3	0.01
(1,3420) 1:A:63	3:MET:HE2	1:A:77:ARG:H	3	0.01
(1,3420) 1:A:63	3:MET:HE3	1:A:77:ARG:H	3	0.01
(1,3420) 1:A:63	3:MET:HE1	1:A:77:ARG:H	20	0.01
	3:MET:HE2	1:A:77:ARG:H	20	0.01
(1,3420) 1:A:63	3:MET:HE3	1:A:77:ARG:H	20	0.01
(1,3413) 1:B:63	3:MET:HE1	1:B:76:GLU:HA	7	0.01



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Key	Atom-1	$\mathbf{Atom-2}$	Model	Violation (Å)
(1,3413)	1:B:63:MET:HE2	1:B:76:GLU:HA	7	0.01
(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	7	0.01
(1,3413)	1:B:63:MET:HE1	1:B:76:GLU:HA	17	0.01
(1,3413)	1:B:63:MET:HE2	1:B:76:GLU:HA	17	0.01
(1,3413)	1:B:63:MET:HE3	1:B:76:GLU:HA	17	0.01
(1,3412)	1:A:63:MET:HE1	1:A:76:GLU:HA	11	0.01
(1,3412)	1:A:63:MET:HE2	1:A:76:GLU:HA	11	0.01
(1,3412)	1:A:63:MET:HE3	1:A:76:GLU:HA	11	0.01
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE1	15	0.01
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE2	15	0.01
(1,3394)	1:A:8:ILE:HD11	1:A:63:MET:HE3	15	0.01
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE1	15	0.01
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE2	15	0.01
(1,3394)	1:A:8:ILE:HD12	1:A:63:MET:HE3	15	0.01
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE1	15	0.01
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE2	15	0.01
(1,3394)	1:A:8:ILE:HD13	1:A:63:MET:HE3	15	0.01
(1,3386)	1:A:58:LYS:HZ1	1:A:62:LEU:HD21	18	0.01
(1,3386)	1:A:58:LYS:HZ1	1:A:62:LEU:HD22	18	0.01
(1,3386)	1:A:58:LYS:HZ1	1:A:62:LEU:HD23	18	0.01
(1,3386)	1:A:58:LYS:HZ2	1:A:62:LEU:HD21	18	0.01
(1,3386)	1:A:58:LYS:HZ2	1:A:62:LEU:HD22	18	0.01
(1,3386)	1:A:58:LYS:HZ2	1:A:62:LEU:HD23	18	0.01
(1,3386)	1:A:58:LYS:HZ3	1:A:62:LEU:HD21	18	0.01
(1,3386)	1:A:58:LYS:HZ3	1:A:62:LEU:HD22	18	0.01
(1,3386)	1:A:58:LYS:HZ3	1:A:62:LEU:HD23	18	0.01
(1,3335)	1:B:58:LYS:HE2	1:B:62:LEU:HD11	14	0.01
(1,3335)	1:B:58:LYS:HE2	1:B:62:LEU:HD12	14	0.01
(1,3335)	1:B:58:LYS:HE2	1:B:62:LEU:HD13	14	0.01
(1,3331)	1:B:62:LEU:HD11	1:B:66:LEU:HG	6	0.01
(1,3331)	1:B:62:LEU:HD12	1:B:66:LEU:HG	6	0.01
(1,3331)	1:B:62:LEU:HD13	1:B:66:LEU:HG	6	0.01
(1,3331)	1:B:62:LEU:HD11	1:B:66:LEU:HG	7	0.01
(1,3331)	1:B:62:LEU:HD12	1:B:66:LEU:HG	7	0.01
(1,3331)	1:B:62:LEU:HD13	1:B:66:LEU:HG	7	0.01
(1,3331)	1:B:62:LEU:HD11	1:B:66:LEU:HG	12	0.01
(1,3331)	1:B:62:LEU:HD12	1:B:66:LEU:HG	12	0.01
(1,3331)	1:B:62:LEU:HD13	1:B:66:LEU:HG	12	0.01
(1,3330)	1:A:62:LEU:HD11	1:A:66:LEU:HG	15	0.01
(1,3330)	1:A:62:LEU:HD12	1:A:66:LEU:HG	15	0.01
(1,3330)	1:A:62:LEU:HD13	1:A:66:LEU:HG	15	0.01
(1,3330)	1:A:62:LEU:HD11	1:A:66:LEU:HG	16	0.01



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3330)	1:A:62:LEU:HD12	1:A:66:LEU:HG	16	0.01
(1,3330)	1:A:62:LEU:HD13	1:A:66:LEU:HG	16	0.01
(1,3293)	1:A:58:LYS:HZ1	1:A:61:THR:HG21	18	0.01
(1,3293)	1:A:58:LYS:HZ1	1:A:61:THR:HG22	18	0.01
(1,3293)	1:A:58:LYS:HZ1	1:A:61:THR:HG23	18	0.01
(1,3293)	1:A:58:LYS:HZ2	1:A:61:THR:HG21	18	0.01
(1,3293)	1:A:58:LYS:HZ2	1:A:61:THR:HG22	18	0.01
(1,3293)	1:A:58:LYS:HZ2	1:A:61:THR:HG23	18	0.01
(1,3293)	1:A:58:LYS:HZ3	1:A:61:THR:HG21	18	0.01
(1,3293)	1:A:58:LYS:HZ3	1:A:61:THR:HG22	18	0.01
(1,3293)	1:A:58:LYS:HZ3	1:A:61:THR:HG23	18	0.01
(1,3288)	1:B:61:THR:HG21	1:B:65:LYS:HE2	9	0.01
(1,3288)	1:B:61:THR:HG21	1:B:65:LYS:HE3	9	0.01
(1,3288)	1:B:61:THR:HG22	1:B:65:LYS:HE2	9	0.01
(1,3288)	1:B:61:THR:HG22	1:B:65:LYS:HE3	9	0.01
(1,3288)	1:B:61:THR:HG23	1:B:65:LYS:HE2	9	0.01
(1,3288)	1:B:61:THR:HG23	1:B:65:LYS:HE3	9	0.01
(1,3287)	1:A:61:THR:HG21	1:A:65:LYS:HE2	2	0.01
(1,3287)	1:A:61:THR:HG21	1:A:65:LYS:HE3	2	0.01
(1,3287)	1:A:61:THR:HG22	1:A:65:LYS:HE2	2	0.01
(1,3287)	1:A:61:THR:HG22	1:A:65:LYS:HE3	2	0.01
(1,3287)	1:A:61:THR:HG23	1:A:65:LYS:HE2	2	0.01
(1,3287)	1:A:61:THR:HG23	1:A:65:LYS:HE3	2	0.01
(1,3287)	1:A:61:THR:HG21	1:A:65:LYS:HE2	14	0.01
(1,3287)	1:A:61:THR:HG21	1:A:65:LYS:HE3	14	0.01
(1,3287)	1:A:61:THR:HG22	1:A:65:LYS:HE2	14	0.01
(1,3287)	1:A:61:THR:HG22	1:A:65:LYS:HE3	14	0.01
(1,3287)	1:A:61:THR:HG23	1:A:65:LYS:HE2	14	0.01
(1,3287)	1:A:61:THR:HG23	1:A:65:LYS:HE3	14	0.01
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD21	8	0.01
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD22	8	0.01
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD23	8	0.01
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD21	8	0.01
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD22	8	0.01
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD23	8	0.01
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD21	8	0.01
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD22	8	0.01
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD23	8	0.01
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD21	16	0.01
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD22	16	0.01
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD23	16	0.01
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD21	16	0.01



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Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD22	16	0.01
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD23	16	0.01
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD21	16	0.01
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD22	16	0.01
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD23	16	0.01
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD21	17	0.01
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD22	17	0.01
(1,3223)	1:A:6:ALA:HB1	1:A:59:LEU:HD23	17	0.01
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD21	17	0.01
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD22	17	0.01
(1,3223)	1:A:6:ALA:HB2	1:A:59:LEU:HD23	17	0.01
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD21	17	0.01
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD22	17	0.01
(1,3223)	1:A:6:ALA:HB3	1:A:59:LEU:HD23	17	0.01
(1,3212)	1:B:6:ALA:HB1	1:B:59:LEU:HD11	8	0.01
(1,3212)	1:B:6:ALA:HB1	1:B:59:LEU:HD12	8	0.01
(1,3212)	1:B:6:ALA:HB1	1:B:59:LEU:HD13	8	0.01
(1,3212)	1:B:6:ALA:HB2	1:B:59:LEU:HD11	8	0.01
(1,3212)	1:B:6:ALA:HB2	1:B:59:LEU:HD12	8	0.01
(1,3212)	1:B:6:ALA:HB2	1:B:59:LEU:HD13	8	0.01
(1,3212)	1:B:6:ALA:HB3	1:B:59:LEU:HD11	8	0.01
(1,3212)	1:B:6:ALA:HB3	1:B:59:LEU:HD12	8	0.01
(1,3212)	1:B:6:ALA:HB3	1:B:59:LEU:HD13	8	0.01
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD11	1	0.01
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD12	1	0.01
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD13	1	0.01
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD11	1	0.01
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD12	1	0.01
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD13	1	0.01
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD11	1	0.01
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD12	1	0.01
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD13	1	0.01
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD11	10	0.01
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD12	10	0.01
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD13	10	0.01
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD11	10	0.01
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD12	10	0.01
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD13	10	0.01
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD11	10	0.01
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD12	10	0.01
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD13	10	0.01
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD11	13	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD12	13	0.01
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD13	13	0.01
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD11	13	0.01
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD12	13	0.01
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD13	13	0.01
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD11	13	0.01
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD12	13	0.01
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD13	13	0.01
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD11	17	0.01
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD12	17	0.01
(1,3211)	1:A:6:ALA:HB1	1:A:59:LEU:HD13	17	0.01
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD11	17	0.01
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD12	17	0.01
(1,3211)	1:A:6:ALA:HB2	1:A:59:LEU:HD13	17	0.01
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD11	17	0.01
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD12	17	0.01
(1,3211)	1:A:6:ALA:HB3	1:A:59:LEU:HD13	17	0.01
(1,3130)	1:B:4:PHE:HD1	1:B:56:THR:HG21	1	0.01
(1,3130)	1:B:4:PHE:HD1	1:B:56:THR:HG22	1	0.01
(1,3130)	1:B:4:PHE:HD1	1:B:56:THR:HG23	1	0.01
(1,3130)	1:B:4:PHE:HD2	1:B:56:THR:HG21	1	0.01
(1,3130)	1:B:4:PHE:HD2	1:B:56:THR:HG22	1	0.01
(1,3130)	1:B:4:PHE:HD2	1:B:56:THR:HG23	1	0.01
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG21	5	0.01
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG22	5	0.01
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG23	5	0.01
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG21	5	0.01
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG22	5	0.01
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG23	5	0.01
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD2	7	0.01
(1,3092)	1:B:54:LYS:HA	1:B:54:LYS:HD3	7	0.01
(1,3034)	1:B:53:VAL:HG21	1:B:59:LEU:HA	14	0.01
(1,3034)	1:B:53:VAL:HG22	1:B:59:LEU:HA	14	0.01
(1,3034)	1:B:53:VAL:HG23	1:B:59:LEU:HA	14	0.01
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG11	4	0.01
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG12	4	0.01
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG13	4	0.01
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG11	7	0.01
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG12	7	0.01
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG13	7	0.01
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG11	9	0.01
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG12	9	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,3014)	1:B:4:PHE:H	1:B:53:VAL:HG13	9	0.01
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG11	12	0.01
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG12	12	0.01
(1,3013)	1:A:4:PHE:H	1:A:53:VAL:HG13	12	0.01
(1,3008)	1:B:52:PHE:H	1:B:53:VAL:HG11	9	0.01
(1,3008)	1:B:52:PHE:H	1:B:53:VAL:HG12	9	0.01
(1,3008)	1:B:52:PHE:H	1:B:53:VAL:HG13	9	0.01
(1,3007)	1:A:52:PHE:H	1:A:53:VAL:HG11	7	0.01
(1,3007)	1:A:52:PHE:H	1:A:53:VAL:HG12	7	0.01
(1,3007)	1:A:52:PHE:H	1:A:53:VAL:HG13	7	0.01
(1,3005)	1:A:53:VAL:HG11	1:A:55:ASN:H	1	0.01
(1,3005)	1:A:53:VAL:HG12	1:A:55:ASN:H	1	0.01
(1,3005)	1:A:53:VAL:HG13	1:A:55:ASN:H	1	0.01
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD11	16	0.01
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD12	16	0.01
(1,2950)	1:B:31:THR:H	1:B:51:ILE:HD13	16	0.01
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD11	3	0.01
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD12	3	0.01
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD13	3	0.01
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD11	11	0.01
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD12	11	0.01
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD13	11	0.01
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD11	13	0.01
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD12	13	0.01
(1,2949)	1:A:31:THR:H	1:A:51:ILE:HD13	13	0.01
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	9	0.01
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	9	0.01
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	9	0.01
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	9	0.01
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	9	0.01
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	9	0.01
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	9	0.01
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	9	0.01
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	9	0.01
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD11	14	0.01
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD12	14	0.01
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD13	14	0.01
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD11	14	0.01
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD12	14	0.01
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD13	14	0.01
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD11	15	0.01
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD12	15	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD13	15	0.01
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD11	15	0.01
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD12	15	0.01
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD13	15	0.01
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD11	20	0.01
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD12	20	0.01
(1,2945)	1:A:29:PHE:HD1	1:A:51:ILE:HD13	20	0.01
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD11	20	0.01
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD12	20	0.01
(1,2945)	1:A:29:PHE:HD2	1:A:51:ILE:HD13	20	0.01
(1,2924)	1:B:51:ILE:HD11	1:B:62:LEU:HD21	15	0.01
(1,2924)	1:B:51:ILE:HD11	1:B:62:LEU:HD22	15	0.01
(1,2924)	1:B:51:ILE:HD11	1:B:62:LEU:HD23	15	0.01
(1,2924)	1:B:51:ILE:HD12	1:B:62:LEU:HD21	15	0.01
(1,2924)	1:B:51:ILE:HD12	1:B:62:LEU:HD22	15	0.01
(1,2924)	1:B:51:ILE:HD12	1:B:62:LEU:HD23	15	0.01
(1,2924)	1:B:51:ILE:HD13	1:B:62:LEU:HD21	15	0.01
(1,2924)	1:B:51:ILE:HD13	1:B:62:LEU:HD22	15	0.01
(1,2924)	1:B:51:ILE:HD13	1:B:62:LEU:HD23	15	0.01
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD21	8	0.01
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD22	8	0.01
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD23	8	0.01
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD21	8	0.01
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD22	8	0.01
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD23	8	0.01
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD21	8	0.01
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD22	8	0.01
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD23	8	0.01
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD21	14	0.01
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD22	14	0.01
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD23	14	0.01
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD21	14	0.01
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD22	14	0.01
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD23	14	0.01
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD21	14	0.01
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD22	14	0.01
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD23	14	0.01
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD21	15	0.01
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD22	15	0.01
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD23	15	0.01
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD21	15	0.01
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD22	15	0.01



 $Continued\ from\ previous\ page...$

Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD23	15	0.01
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD21	15	0.01
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD22	15	0.01
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD23	15	0.01
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD21	16	0.01
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD22	16	0.01
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD23	16	0.01
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD21	16	0.01
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD22	16	0.01
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD23	16	0.01
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD21	16	0.01
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD22	16	0.01
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD23	16	0.01
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD21	17	0.01
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD22	17	0.01
(1,2923)	1:A:51:ILE:HD11	1:A:62:LEU:HD23	17	0.01
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD21	17	0.01
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD22	17	0.01
(1,2923)	1:A:51:ILE:HD12	1:A:62:LEU:HD23	17	0.01
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD21	17	0.01
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD22	17	0.01
(1,2923)	1:A:51:ILE:HD13	1:A:62:LEU:HD23	17	0.01
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG21	7	0.01
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG22	7	0.01
(1,2890)	1:B:31:THR:HB	1:B:51:ILE:HG23	7	0.01
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG21	10	0.01
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG22	10	0.01
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG23	10	0.01
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG21	12	0.01
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG22	12	0.01
(1,2889)	1:A:31:THR:HB	1:A:51:ILE:HG23	12	0.01
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG21	6	0.01
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG22	6	0.01
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG23	6	0.01
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG21	9	0.01
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG22	9	0.01
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG23	9	0.01
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG21	17	0.01
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG22	17	0.01
(1,2887)	1:A:33:ILE:HA	1:A:51:ILE:HG23	17	0.01
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD11	2	0.01
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD12	2	0.01



 $Continued\ from\ previous\ page...$

Key	$\frac{1 \text{ from previous page.}}{\text{Atom-1}}$	Atom-2	Model	Violation (Å)
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD13	2	0.01
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD11	2	0.01
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD12	2	0.01
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD13	2	0.01
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD11	2	0.01
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD12	2	0.01
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD13	2	0.01
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD11	9	0.01
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD12	9	0.01
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD13	9	0.01
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD11	9	0.01
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD12	9	0.01
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD13	9	0.01
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD11	9	0.01
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD12	9	0.01
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD13	9	0.01
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD11	15	0.01
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD12	15	0.01
(1,2881)	1:A:8:ILE:HG21	1:A:62:LEU:HD13	15	0.01
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD11	15	0.01
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD12	15	0.01
(1,2881)	1:A:8:ILE:HG22	1:A:62:LEU:HD13	15	0.01
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD11	15	0.01
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD12	15	0.01
(1,2881)	1:A:8:ILE:HG23	1:A:62:LEU:HD13	15	0.01
(1,2829)	1:A:50:MET:HE1	1:A:81:LEU:HA	12	0.01
(1,2829)	1:A:50:MET:HE2	1:A:81:LEU:HA	12	0.01
(1,2829)	1:A:50:MET:HE3	1:A:81:LEU:HA	12	0.01
(1,2816)	1:B:50:MET:HE1	1:B:51:ILE:HG13	13	0.01
(1,2816)	1:B:50:MET:HE2	1:B:51:ILE:HG13	13	0.01
(1,2816)	1:B:50:MET:HE3	1:B:51:ILE:HG13	13	0.01
(1,2816)	1:B:50:MET:HE1	1:B:51:ILE:HG13	16	0.01
(1,2816)	1:B:50:MET:HE2	1:B:51:ILE:HG13	16	0.01
(1,2816)	1:B:50:MET:HE3	1:B:51:ILE:HG13	16	0.01
(1,2815)	1:A:50:MET:HE1	1:A:51:ILE:HG13	13	0.01
(1,2815)	1:A:50:MET:HE2	1:A:51:ILE:HG13	13	0.01
(1,2815)	1:A:50:MET:HE3	1:A:51:ILE:HG13	13	0.01
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	6	0.01
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	3	0.01
(1,2789)	1:A:50:MET:HG3	1:A:51:ILE:H	18	0.01
(1,2773)	1:B:50:MET:HG3	1:B:78:LEU:HD11	15	0.01
(1,2773)	1:B:50:MET:HG3	1:B:78:LEU:HD12	15	0.01



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2773)	1:B:50:MET:HG3	1:B:78:LEU:HD13	15	0.01
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD11	12	0.01
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD12	12	0.01
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD13	12	0.01
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD11	12	0.01
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD12	12	0.01
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD13	12	0.01
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD11	12	0.01
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD12	12	0.01
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD13	12	0.01
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD11	18	0.01
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD12	18	0.01
(1,2714)	1:B:26:ILE:HG21	1:B:49:LEU:HD13	18	0.01
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD11	18	0.01
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD12	18	0.01
(1,2714)	1:B:26:ILE:HG22	1:B:49:LEU:HD13	18	0.01
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD11	18	0.01
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD12	18	0.01
(1,2714)	1:B:26:ILE:HG23	1:B:49:LEU:HD13	18	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD11	1	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD12	1	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD13	1	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD11	1	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD12	1	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD13	1	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD11	1	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD12	1	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD13	1	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD11	2	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD12	2	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD13	2	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD11	2	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD12	2	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD13	2	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD11	2	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD12	2	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD13	2	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD11	9	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD12	9	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD13	9	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD11	9	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD12	9	0.01



 $Continued\ from\ previous\ page...$

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD13	9	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD11	9	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD12	9	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD13	9	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD11	12	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD12	12	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD13	12	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD11	12	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD12	12	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD13	12	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD11	12	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD12	12	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD13	12	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD11	14	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD12	14	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD13	14	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD11	14	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD12	14	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD13	14	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD11	14	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD12	14	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD13	14	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD11	16	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD12	16	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD13	16	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD11	16	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD12	16	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD13	16	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD11	16	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD12	16	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD13	16	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD11	20	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD12	20	0.01
(1,2713)	1:A:26:ILE:HG21	1:A:49:LEU:HD13	20	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD11	20	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD12	20	0.01
(1,2713)	1:A:26:ILE:HG22	1:A:49:LEU:HD13	20	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD11	20	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD12	20	0.01
(1,2713)	1:A:26:ILE:HG23	1:A:49:LEU:HD13	20	0.01
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD21	9	0.01
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD22	9	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2712)	1:B:49:LEU:HD11	1:B:62:LEU:HD23	9	0.01
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD21	9	0.01
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD22	9	0.01
(1,2712)	1:B:49:LEU:HD12	1:B:62:LEU:HD23	9	0.01
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD21	9	0.01
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD22	9	0.01
(1,2712)	1:B:49:LEU:HD13	1:B:62:LEU:HD23	9	0.01
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD21	8	0.01
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD22	8	0.01
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD23	8	0.01
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD21	8	0.01
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD22	8	0.01
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD23	8	0.01
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD21	8	0.01
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD22	8	0.01
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD23	8	0.01
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD21	15	0.01
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD22	15	0.01
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD23	15	0.01
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD21	15	0.01
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD22	15	0.01
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD23	15	0.01
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD21	15	0.01
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD22	15	0.01
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD23	15	0.01
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD21	17	0.01
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD22	17	0.01
(1,2711)	1:A:49:LEU:HD11	1:A:62:LEU:HD23	17	0.01
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD21	17	0.01
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD22	17	0.01
(1,2711)	1:A:49:LEU:HD12	1:A:62:LEU:HD23	17	0.01
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD21	17	0.01
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD22	17	0.01
(1,2711)	1:A:49:LEU:HD13	1:A:62:LEU:HD23	17	0.01
(1,2667)	1:A:23:THR:HG1	1:A:47:CYS:HB3	10	0.01
(1,2640)	1:B:46:THR:HG21	1:B:47:CYS:H	10	0.01
(1,2640)	1:B:46:THR:HG22	1:B:47:CYS:H	10	0.01
(1,2640)	1:B:46:THR:HG23	1:B:47:CYS:H	10	0.01
(1,2640)	1:B:46:THR:HG21	1:B:47:CYS:H	13	0.01
(1,2640)	1:B:46:THR:HG22	1:B:47:CYS:H	13	0.01
(1,2640)	1:B:46:THR:HG23	1:B:47:CYS:H	13	0.01
(1,2639)	1:A:46:THR:HG21	1:A:47:CYS:H	3	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2639)	1:A:46:THR:HG22	1:A:47:CYS:H	3	0.01
(1,2639)	1:A:46:THR:HG23	1:A:47:CYS:H	3	0.01
(1,2639)	1:A:46:THR:HG21	1:A:47:CYS:H	8	0.01
(1,2639)	1:A:46:THR:HG22	1:A:47:CYS:H	8	0.01
(1,2639)	1:A:46:THR:HG23	1:A:47:CYS:H	8	0.01
(1,2639)	1:A:46:THR:HG21	1:A:47:CYS:H	17	0.01
(1,2639)	1:A:46:THR:HG22	1:A:47:CYS:H	17	0.01
(1,2639)	1:A:46:THR:HG23	1:A:47:CYS:H	17	0.01
(1,2639)	1:A:46:THR:HG21	1:A:47:CYS:H	18	0.01
(1,2639)	1:A:46:THR:HG22	1:A:47:CYS:H	18	0.01
(1,2639)	1:A:46:THR:HG23	1:A:47:CYS:H	18	0.01
(1,2618)	1:B:9:ARG:HD2	1:B:46:THR:HG21	13	0.01
(1,2618)	1:B:9:ARG:HD2	1:B:46:THR:HG22	13	0.01
(1,2618)	1:B:9:ARG:HD2	1:B:46:THR:HG23	13	0.01
(1,2618)	1:B:9:ARG:HD3	1:B:46:THR:HG21	13	0.01
(1,2618)	1:B:9:ARG:HD3	1:B:46:THR:HG22	13	0.01
(1,2618)	1:B:9:ARG:HD3	1:B:46:THR:HG23	13	0.01
(1,2617)	1:A:9:ARG:HD2	1:A:46:THR:HG21	19	0.01
(1,2617)	1:A:9:ARG:HD2	1:A:46:THR:HG22	19	0.01
(1,2617)	1:A:9:ARG:HD2	1:A:46:THR:HG23	19	0.01
(1,2617)	1:A:9:ARG:HD3	1:A:46:THR:HG21	19	0.01
(1,2617)	1:A:9:ARG:HD3	1:A:46:THR:HG22	19	0.01
(1,2617)	1:A:9:ARG:HD3	1:A:46:THR:HG23	19	0.01
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG21	4	0.01
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG22	4	0.01
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG23	4	0.01
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG21	18	0.01
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG22	18	0.01
(1,2612)	1:B:44:ILE:HB	1:B:46:THR:HG23	18	0.01
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG21	2	0.01
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG22	2	0.01
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG23	2	0.01
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG21	17	0.01
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG22	17	0.01
(1,2611)	1:A:44:ILE:HB	1:A:46:THR:HG23	17	0.01
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	7	0.01
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	7	0.01
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	7	0.01
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	2	0.01
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	2	0.01
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	2	0.01
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	16	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	16	0.01
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	16	0.01
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD11	3	0.01
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD12	3	0.01
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD13	3	0.01
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD11	17	0.01
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD12	17	0.01
(1,2596)	1:B:44:ILE:H	1:B:44:ILE:HD13	17	0.01
(1,2595)	1:A:44:ILE:H	1:A:44:ILE:HD11	10	0.01
(1,2595)	1:A:44:ILE:H	1:A:44:ILE:HD12	10	0.01
(1,2595)	1:A:44:ILE:H	1:A:44:ILE:HD13	10	0.01
(1,2595)	1:A:44:ILE:H	1:A:44:ILE:HD11	18	0.01
(1,2595)	1:A:44:ILE:H	1:A:44:ILE:HD12	18	0.01
(1,2595)	1:A:44:ILE:H	1:A:44:ILE:HD13	18	0.01
(1,2590)	1:B:44:ILE:HD11	1:B:73:PHE:HD1	12	0.01
(1,2590)	1:B:44:ILE:HD11	1:B:73:PHE:HD2	12	0.01
(1,2590)	1:B:44:ILE:HD12	1:B:73:PHE:HD1	12	0.01
(1,2590)	1:B:44:ILE:HD12	1:B:73:PHE:HD2	12	0.01
(1,2590)	1:B:44:ILE:HD13	1:B:73:PHE:HD1	12	0.01
(1,2590)	1:B:44:ILE:HD13	1:B:73:PHE:HD2	12	0.01
(1,2589)	1:A:44:ILE:HD11	1:A:73:PHE:HD1	2	0.01
(1,2589)	1:A:44:ILE:HD11	1:A:73:PHE:HD2	2	0.01
(1,2589)	1:A:44:ILE:HD12	1:A:73:PHE:HD1	2	0.01
(1,2589)	1:A:44:ILE:HD12	1:A:73:PHE:HD2	2	0.01
(1,2589)	1:A:44:ILE:HD13	1:A:73:PHE:HD1	2	0.01
(1,2589)	1:A:44:ILE:HD13	1:A:73:PHE:HD2	2	0.01
(1,2589)	1:A:44:ILE:HD11	1:A:73:PHE:HD1	14	0.01
(1,2589)	1:A:44:ILE:HD11	1:A:73:PHE:HD2	14	0.01
(1,2589)	1:A:44:ILE:HD12	1:A:73:PHE:HD1	14	0.01
(1,2589)	1:A:44:ILE:HD12	1:A:73:PHE:HD2	14	0.01
(1,2589)	1:A:44:ILE:HD13	1:A:73:PHE:HD1	14	0.01
(1,2589)	1:A:44:ILE:HD13	1:A:73:PHE:HD2	14	0.01
(1,2587)	1:A:44:ILE:HA	1:A:44:ILE:HD11	15	0.01
(1,2587)	1:A:44:ILE:HA	1:A:44:ILE:HD12	15	0.01
(1,2587)	1:A:44:ILE:HA	1:A:44:ILE:HD13	15	0.01
(1,2586)	1:B:13:GLU:HA	1:B:44:ILE:HD11	14	0.01
(1,2586)	1:B:13:GLU:HA	1:B:44:ILE:HD12	14	0.01
(1,2586)	1:B:13:GLU:HA	1:B:44:ILE:HD13	14	0.01
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD11	2	0.01
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD12	2	0.01
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD13	2	0.01
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD11	20	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD12	20	0.01
(1,2585)	1:A:13:GLU:HA	1:A:44:ILE:HD13	20	0.01
(1,2584)	1:B:44:ILE:HD11	1:B:46:THR:HB	18	0.01
(1,2584)	1:B:44:ILE:HD12	1:B:46:THR:HB	18	0.01
(1,2584)	1:B:44:ILE:HD13	1:B:46:THR:HB	18	0.01
(1,2583)	1:A:44:ILE:HD11	1:A:46:THR:HB	4	0.01
(1,2583)	1:A:44:ILE:HD12	1:A:46:THR:HB	4	0.01
(1,2583)	1:A:44:ILE:HD13	1:A:46:THR:HB	4	0.01
(1,2583)	1:A:44:ILE:HD11	1:A:46:THR:HB	12	0.01
(1,2583)	1:A:44:ILE:HD12	1:A:46:THR:HB	12	0.01
(1,2583)	1:A:44:ILE:HD13	1:A:46:THR:HB	12	0.01
(1,2583)	1:A:44:ILE:HD11	1:A:46:THR:HB	13	0.01
(1,2583)	1:A:44:ILE:HD12	1:A:46:THR:HB	13	0.01
(1,2583)	1:A:44:ILE:HD13	1:A:46:THR:HB	13	0.01
(1,2583)	1:A:44:ILE:HD11	1:A:46:THR:HB	17	0.01
(1,2583)	1:A:44:ILE:HD12	1:A:46:THR:HB	17	0.01
(1,2583)	1:A:44:ILE:HD13	1:A:46:THR:HB	17	0.01
(1,2580)	1:B:42:ASP:HB2	1:B:44:ILE:HD11	14	0.01
(1,2580)	1:B:42:ASP:HB2	1:B:44:ILE:HD12	14	0.01
(1,2580)	1:B:42:ASP:HB2	1:B:44:ILE:HD13	14	0.01
(1,2552)	1:B:44:ILE:HG13	1:B:45:PHE:H	9	0.01
(1,2552)	1:B:44:ILE:HG13	1:B:45:PHE:H	10	0.01
(1,2551)	1:A:44:ILE:HG13	1:A:45:PHE:H	3	0.01
(1,2551)	1:A:44:ILE:HG13	1:A:45:PHE:H	8	0.01
(1,2551)	1:A:44:ILE:HG13	1:A:45:PHE:H	18	0.01
(1,2527)	1:A:12:GLY:H	1:A:44:ILE:HB	13	0.01
(1,2526)	1:B:13:GLU:HA	1:B:44:ILE:HB	9	0.01
(1,2526)	1:B:13:GLU:HA	1:B:44:ILE:HB	11	0.01
(1,2525)	1:A:13:GLU:HA	1:A:44:ILE:HB	3	0.01
(1,2524)	1:B:14:ASP:HB3	1:B:43:GLY:HA3	17	0.01
(1,2521)	1:A:14:ASP:HB2	1:A:43:GLY:HA3	4	0.01
(1,2501)	1:A:15:LYS:H	1:A:40:ALA:HB1	15	0.01
(1,2501)	1:A:15:LYS:H	1:A:40:ALA:HB2	15	0.01
(1,2501)	1:A:15:LYS:H	1:A:40:ALA:HB3	15	0.01
(1,2486)	1:B:40:ALA:HA	1:B:45:PHE:HA	9	0.01
(1,2486)	1:B:40:ALA:HA	1:B:45:PHE:HA	16	0.01
(1,2485)	1:A:40:ALA:HA	1:A:45:PHE:HA	6	0.01
(1,2485)	1:A:40:ALA:HA	1:A:45:PHE:HA	8	0.01
(1,2485)	1:A:40:ALA:HA	1:A:45:PHE:HA	11	0.01
(1,2485)	1:A:40:ALA:HA	1:A:45:PHE:HA	18	0.01
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD21	12	0.01
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD22	12	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD23	12	0.01
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD21	20	0.01
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD22	20	0.01
(1,2450)	1:B:37:VAL:HA	1:B:38:LEU:HD23	20	0.01
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD21	6	0.01
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD22	6	0.01
(1,2449)	1:A:37:VAL:HA	1:A:38:LEU:HD23	6	0.01
(1,2448)	1:B:23:THR:HG1	1:B:38:LEU:HD21	10	0.01
(1,2448)	1:B:23:THR:HG1	1:B:38:LEU:HD22	10	0.01
(1,2448)	1:B:23:THR:HG1	1:B:38:LEU:HD23	10	0.01
(1,2432)	1:A:38:LEU:HD21	1:B:35:THR:HG21	2	0.01
(1,2432)	1:A:38:LEU:HD21	1:B:35:THR:HG22	2	0.01
(1,2432)	1:A:38:LEU:HD21	1:B:35:THR:HG23	2	0.01
(1,2432)	1:A:38:LEU:HD22	1:B:35:THR:HG21	2	0.01
(1,2432)	1:A:38:LEU:HD22	1:B:35:THR:HG22	2	0.01
(1,2432)	1:A:38:LEU:HD22	1:B:35:THR:HG23	2	0.01
(1,2432)	1:A:38:LEU:HD23	1:B:35:THR:HG21	2	0.01
(1,2432)	1:A:38:LEU:HD23	1:B:35:THR:HG22	2	0.01
(1,2432)	1:A:38:LEU:HD23	1:B:35:THR:HG23	2	0.01
(1,2432)	1:A:38:LEU:HD21	1:B:35:THR:HG21	16	0.01
(1,2432)	1:A:38:LEU:HD21	1:B:35:THR:HG22	16	0.01
(1,2432)	1:A:38:LEU:HD21	1:B:35:THR:HG23	16	0.01
(1,2432)	1:A:38:LEU:HD22	1:B:35:THR:HG21	16	0.01
(1,2432)	1:A:38:LEU:HD22	1:B:35:THR:HG22	16	0.01
(1,2432)	1:A:38:LEU:HD22	1:B:35:THR:HG23	16	0.01
(1,2432)	1:A:38:LEU:HD23	1:B:35:THR:HG21	16	0.01
(1,2432)	1:A:38:LEU:HD23	1:B:35:THR:HG22	16	0.01
(1,2432)	1:A:38:LEU:HD23	1:B:35:THR:HG23	16	0.01
(1,2424)	1:B:38:LEU:HD11	1:B:39:ASN:H	15	0.01
(1,2424)	1:B:38:LEU:HD12	1:B:39:ASN:H	15	0.01
(1,2424)	1:B:38:LEU:HD13	1:B:39:ASN:H	15	0.01
(1,2424)	1:B:38:LEU:HD11	1:B:39:ASN:H	17	0.01
(1,2424)	1:B:38:LEU:HD12	1:B:39:ASN:H	17	0.01
(1,2424)	1:B:38:LEU:HD13	1:B:39:ASN:H	17	0.01
(1,2424)	1:B:38:LEU:HD11	1:B:39:ASN:H	18	0.01
(1,2424)	1:B:38:LEU:HD12	1:B:39:ASN:H	18	0.01
(1,2424)	1:B:38:LEU:HD13	1:B:39:ASN:H	18	0.01
(1,2417)	1:A:38:LEU:HD11	1:A:45:PHE:HZ	13	0.01
(1,2417)	1:A:38:LEU:HD12	1:A:45:PHE:HZ	13	0.01
(1,2417)	1:A:38:LEU:HD13	1:A:45:PHE:HZ	13	0.01
(1,2417)	1:A:38:LEU:HD11	1:A:45:PHE:HZ	18	0.01
(1,2417)	1:A:38:LEU:HD12	1:A:45:PHE:HZ	18	0.01



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(1,2417) 1:A:38:LEU:HD11 1:A:45:PHE:HZ 18 0.01 (1,2399) 1:A:38:LEU:HD11 1:A:47:CYS:HG 2 0.01 (1,2399) 1:A:38:LEU:HD13 1:A:47:CYS:HG 2 0.01 (1,2399) 1:A:38:LEU:HD13 1:A:47:CYS:HG 2 0.01 (1,2389) 1:B:37:VAL:HG21 1:B:38:LEU:H 3 0.01 (1,2388) 1:B:37:VAL:HG22 1:B:38:LEU:H 3 0.01 (1,2388) 1:B:37:VAL:HG21 1:B:38:LEU:H 6 0.01 (1,2388) 1:B:37:VAL:HG22 1:B:38:LEU:H 6 0.01 (1,2388) 1:B:37:VAL:HG22 1:B:38:LEU:H 6 0.01 (1,2388) 1:B:37:VAL:HG21 1:B:38:LEU:H 8 0.01 (1,2388) 1:B:37:VAL:HG22 1:B:38:LEU:H 8 0.01 (1,2388) 1:B:37:VAL:HG22 1:B:38:LEU:H 8 0.01 (1,2388) 1:B:37:VAL:HG22 1:B:38:LEU:H 8 0.01 (1,2387) 1:A:37:VAL:HG22 1:A:38:LEU:H	Key	Atom-1	Atom-2	Model	Violation (Å)
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		1:A:37:VAL:HG22	1:A:48:ASN:HD22	2	0.01
(1,2379) 1:A:37:VAL:HG21 1:A:48:ASN:HD22 16 0.01	(1,2379)	1:A:37:VAL:HG23	1:A:48:ASN:HD22	2	0.01
	(1,2379)	1:A:37:VAL:HG21	1:A:48:ASN:HD22	16	0.01
(1,2379) 1:A:37:VAL:HG22 1:A:48:ASN:HD22 16 0.01	(1,2379)	1:A:37:VAL:HG22	1:A:48:ASN:HD22	16	0.01
(1,2379) 1:A:37:VAL:HG23 1:A:48:ASN:HD22 16 0.01	(1,2379)	1:A:37:VAL:HG23	1:A:48:ASN:HD22	16	0.01
(1,2379) 1:A:37:VAL:HG21 1:A:48:ASN:HD22 17 0.01	(1,2379)	1:A:37:VAL:HG21	1:A:48:ASN:HD22	17	0.01
(1,2379) 1:A:37:VAL:HG22 1:A:48:ASN:HD22 17 0.01	(1,2379)	1:A:37:VAL:HG22	1:A:48:ASN:HD22	17	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2379)	1:A:37:VAL:HG23	1:A:48:ASN:HD22	17	0.01
(1,2379)	1:A:37:VAL:HG21	1:A:48:ASN:HD22	20	0.01
(1,2379)	1:A:37:VAL:HG22	1:A:48:ASN:HD22	20	0.01
(1,2379)	1:A:37:VAL:HG23	1:A:48:ASN:HD22	20	0.01
(1,2365)	1:A:37:VAL:HG21	1:A:48:ASN:HB3	14	0.01
(1,2365)	1:A:37:VAL:HG22	1:A:48:ASN:HB3	14	0.01
(1,2365)	1:A:37:VAL:HG23	1:A:48:ASN:HB3	14	0.01
(1,235)	1:B:15:LYS:HG2	1:B:19:THR:H	1	0.01
(1,235)	1:B:15:LYS:HG3	1:B:19:THR:H	1	0.01
(1,235)	1:B:15:LYS:HG2	1:B:19:THR:H	12	0.01
(1,235)	1:B:15:LYS:HG3	1:B:19:THR:H	12	0.01
(1,234)	1:A:15:LYS:HG2	1:A:19:THR:H	11	0.01
(1,234)	1:A:15:LYS:HG3	1:A:19:THR:H	11	0.01
(1,2334)	1:B:37:VAL:HB	1:B:48:ASN:HB2	10	0.01
(1,2334)	1:B:37:VAL:HB	1:B:48:ASN:HB2	19	0.01
(1,2326)	1:B:23:THR:H	1:B:36:ILE:HD11	4	0.01
(1,2326)	1:B:23:THR:H	1:B:36:ILE:HD12	4	0.01
(1,2326)	1:B:23:THR:H	1:B:36:ILE:HD13	4	0.01
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD11	6	0.01
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD12	6	0.01
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD13	6	0.01
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD11	8	0.01
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD12	8	0.01
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD13	8	0.01
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD11	13	0.01
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD12	13	0.01
(1,2315)	1:A:23:THR:HG1	1:A:36:ILE:HD13	13	0.01
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	16	0.01
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	16	0.01
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	16	0.01
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	17	0.01
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	17	0.01
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	17	0.01
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	14	0.01
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	14	0.01
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	14	0.01
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	2	0.01
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	2	0.01
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	2	0.01
(1,2287)	1:A:35:THR:HB	1:A:36:ILE:HG21	13	0.01
(1,2287)	1:A:35:THR:HB	1:A:36:ILE:HG22	13	0.01
(1,2287)	1:A:35:THR:HB	1:A:36:ILE:HG23	13	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2282)	1:B:36:ILE:HG21	1:B:37:VAL:HB	1	0.01
(1,2282)	1:B:36:ILE:HG22	1:B:37:VAL:HB	1	0.01
(1,2282)	1:B:36:ILE:HG23	1:B:37:VAL:HB	1	0.01
(1,2282)	1:B:36:ILE:HG21	1:B:37:VAL:HB	4	0.01
(1,2282)	1:B:36:ILE:HG22	1:B:37:VAL:HB	4	0.01
(1,2282)	1:B:36:ILE:HG23	1:B:37:VAL:HB	4	0.01
(1,2281)	1:A:36:ILE:HG21	1:A:37:VAL:HB	8	0.01
(1,2281)	1:A:36:ILE:HG22	1:A:37:VAL:HB	8	0.01
(1,2281)	1:A:36:ILE:HG23	1:A:37:VAL:HB	8	0.01
(1,2258)	1:B:35:THR:HB	1:B:50:MET:HB2	18	0.01
(1,2257)	1:A:35:THR:HB	1:A:50:MET:HB2	4	0.01
(1,2257)	1:A:35:THR:HB	1:A:50:MET:HB2	8	0.01
(1,2257)	1:A:35:THR:HB	1:A:50:MET:HB2	13	0.01
(1,2257)	1:A:35:THR:HB	1:A:50:MET:HB2	15	0.01
(1,2257)	1:A:35:THR:HB	1:A:50:MET:HB2	19	0.01
(1,2257)	1:A:35:THR:HB	1:A:50:MET:HB2	20	0.01
(1,2248)	1:B:33:ILE:HD11	1:B:34:ARG:H	7	0.01
(1,2248)	1:B:33:ILE:HD12	1:B:34:ARG:H	7	0.01
(1,2248)	1:B:33:ILE:HD13	1:B:34:ARG:H	7	0.01
(1,2245)	1:A:33:ILE:H	1:A:33:ILE:HD11	6	0.01
(1,2245)	1:A:33:ILE:H	1:A:33:ILE:HD12	6	0.01
(1,2245)	1:A:33:ILE:H	1:A:33:ILE:HD13	6	0.01
(1,2245)	1:A:33:ILE:H	1:A:33:ILE:HD11	15	0.01
(1,2245)	1:A:33:ILE:H	1:A:33:ILE:HD12	15	0.01
(1,2245)	1:A:33:ILE:H	1:A:33:ILE:HD13	15	0.01
(1,2242)	1:A:33:ILE:HD11	1:B:20:ASN:HD22	14	0.01
(1,2242)	1:A:33:ILE:HD12	1:B:20:ASN:HD22	14	0.01
(1,2242)	1:A:33:ILE:HD13	1:B:20:ASN:HD22	14	0.01
(1,2241)	1:A:20:ASN:HD22	1:B:33:ILE:HD11	2	0.01
(1,2241)	1:A:20:ASN:HD22	1:B:33:ILE:HD12	2	0.01
(1,2241)	1:A:20:ASN:HD22	1:B:33:ILE:HD13	2	0.01
(1,2238)	1:A:33:ILE:HD11	1:B:20:ASN:HA	7	0.01
(1,2238)	1:A:33:ILE:HD12	1:B:20:ASN:HA	7	0.01
(1,2238)	1:A:33:ILE:HD13	1:B:20:ASN:HA	7	0.01
(1,2201)	1:A:31:THR:HG21	1:A:52:PHE:H	15	0.01
(1,2201)	1:A:31:THR:HG22	1:A:52:PHE:H	15	0.01
(1,2201)	1:A:31:THR:HG23	1:A:52:PHE:H	15	0.01
(1,2182)	1:B:29:PHE:HD1	1:B:31:THR:HB	9	0.01
(1,2182)	1:B:29:PHE:HD2	1:B:31:THR:HB	9	0.01
(1,2182)	1:B:29:PHE:HD1	1:B:31:THR:HB	10	0.01
(1,2182)	1:B:29:PHE:HD2	1:B:31:THR:HB	10	0.01
(1,2181)	1:A:29:PHE:HD1	1:A:31:THR:HB	5	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2181)	1:A:29:PHE:HD2	1:A:31:THR:HB	5	0.01
(1,2177)	1:A:28:LYS:HA	1:A:28:LYS:HE2	13	0.01
(1,2177)	1:A:28:LYS:HA	1:A:28:LYS:HE3	13	0.01
(1,2175)	1:A:25:VAL:HA	1:A:28:LYS:HE2	17	0.01
(1,2175)	1:A:25:VAL:HA	1:A:28:LYS:HE3	17	0.01
(1,217)	1:B:18:MET:H	1:B:18:MET:HG3	4	0.01
(1,217)	1:B:18:MET:H	1:B:18:MET:HG3	5	0.01
(1,217)	1:B:18:MET:H	1:B:18:MET:HG3	20	0.01
(1,216)	1:A:18:MET:H	1:A:18:MET:HG3	7	0.01
(1,2151)	1:A:23:THR:HG21	1:A:27:SER:HB3	17	0.01
(1,2151)	1:A:23:THR:HG22	1:A:27:SER:HB3	17	0.01
(1,2151)	1:A:23:THR:HG23	1:A:27:SER:HB3	17	0.01
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	13	0.01
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	13	0.01
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	13	0.01
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG21	1	0.01
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG22	1	0.01
(1,2105)	1:A:21:GLN:HE22	1:A:25:VAL:HG23	1	0.01
(1,2088)	1:B:25:VAL:HG11	1:B:27:SER:H	5	0.01
(1,2088)	1:B:25:VAL:HG12	1:B:27:SER:H	5	0.01
(1,2088)	1:B:25:VAL:HG13	1:B:27:SER:H	5	0.01
(1,2088)	1:B:25:VAL:HG11	1:B:27:SER:H	8	0.01
(1,2088)	1:B:25:VAL:HG12	1:B:27:SER:H	8	0.01
(1,2088)	1:B:25:VAL:HG13	1:B:27:SER:H	8	0.01
(1,2088)	1:B:25:VAL:HG11	1:B:27:SER:H	11	0.01
(1,2088)	1:B:25:VAL:HG12	1:B:27:SER:H	11	0.01
(1,2088)	1:B:25:VAL:HG13	1:B:27:SER:H	11	0.01
(1,2088)	1:B:25:VAL:HG11	1:B:27:SER:H	15	0.01
(1,2088)	1:B:25:VAL:HG12	1:B:27:SER:H	15	0.01
(1,2088)	1:B:25:VAL:HG13	1:B:27:SER:H	15	0.01
(1,2087)	1:A:25:VAL:HG11	1:A:27:SER:H	3	0.01
(1,2087)	1:A:25:VAL:HG12	1:A:27:SER:H	3	0.01
(1,2087)	1:A:25:VAL:HG13	1:A:27:SER:H	3	0.01
(1,2087)	1:A:25:VAL:HG11	1:A:27:SER:H	16	0.01
(1,2087)	1:A:25:VAL:HG12	1:A:27:SER:H	16	0.01
(1,2087)	1:A:25:VAL:HG13	1:A:27:SER:H	16	0.01
(1,2087)	1:A:25:VAL:HG11	1:A:27:SER:H	20	0.01
(1,2087)	1:A:25:VAL:HG12	1:A:27:SER:H	20	0.01
(1,2087)	1:A:25:VAL:HG13	1:A:27:SER:H	20	0.01
(1,2084)	1:B:25:VAL:HG11	1:B:69:VAL:H	18	0.01
(1,2084)	1:B:25:VAL:HG12	1:B:69:VAL:H	18	0.01
(1,2084)	1:B:25:VAL:HG13	1:B:69:VAL:H	18	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2020)	1:B:22:ILE:HA	1:B:22:ILE:HD11	6	0.01
(1,2020)	1:B:22:ILE:HA	1:B:22:ILE:HD12	6	0.01
(1,2020)	1:B:22:ILE:HA	1:B:22:ILE:HD13	6	0.01
(1,2020)	1:B:22:ILE:HA	1:B:22:ILE:HD11	12	0.01
(1,2020)	1:B:22:ILE:HA	1:B:22:ILE:HD12	12	0.01
(1,2020)	1:B:22:ILE:HA	1:B:22:ILE:HD13	12	0.01
(1,2020)	1:B:22:ILE:HA	1:B:22:ILE:HD11	13	0.01
(1,2020)	1:B:22:ILE:HA	1:B:22:ILE:HD12	13	0.01
(1,2020)	1:B:22:ILE:HA	1:B:22:ILE:HD13	13	0.01
(1,2019)	1:A:22:ILE:HA	1:A:22:ILE:HD11	8	0.01
(1,2019)	1:A:22:ILE:HA	1:A:22:ILE:HD12	8	0.01
(1,2019)	1:A:22:ILE:HA	1:A:22:ILE:HD13	8	0.01
(1,1971)	1:B:20:ASN:H	1:B:22:ILE:HG13	3	0.01
(1,1971)	1:B:20:ASN:H	1:B:22:ILE:HG13	9	0.01
(1,1971)	1:B:20:ASN:H	1:B:22:ILE:HG13	15	0.01
(1,1970)	1:A:20:ASN:H	1:A:22:ILE:HG13	14	0.01
(1,1970)	1:A:20:ASN:H	1:A:22:ILE:HG13	18	0.01
(1,1941)	1:B:22:ILE:HB	1:B:47:CYS:HG	4	0.01
(1,1941)	1:B:22:ILE:HB	1:B:47:CYS:HG	10	0.01
(1,1940)	1:A:22:ILE:HB	1:A:47:CYS:HG	2	0.01
(1,1940)	1:A:22:ILE:HB	1:A:47:CYS:HG	8	0.01
(1,1933)	1:B:21:GLN:HE21	1:B:22:ILE:HA	1	0.01
(1,1933)	1:B:21:GLN:HE21	1:B:22:ILE:HA	4	0.01
(1,1933)	1:B:21:GLN:HE21	1:B:22:ILE:HA	5	0.01
(1,1933)	1:B:21:GLN:HE21	1:B:22:ILE:HA	6	0.01
(1,1933)	1:B:21:GLN:HE21	1:B:22:ILE:HA	7	0.01
(1,1933)	1:B:21:GLN:HE21	1:B:22:ILE:HA	16	0.01
(1,1932)	1:A:21:GLN:HE21	1:A:22:ILE:HA	1	0.01
(1,1932)	1:A:21:GLN:HE21	1:A:22:ILE:HA	5	0.01
(1,1932)	1:A:21:GLN:HE21	1:A:22:ILE:HA	8	0.01
(1,1932)	1:A:21:GLN:HE21	1:A:22:ILE:HA	16	0.01
(1,1864)	1:A:18:MET:HE1	1:A:45:PHE:HE1	20	0.01
(1,1864)	1:A:18:MET:HE1	1:A:45:PHE:HE2	20	0.01
(1,1864)	1:A:18:MET:HE2	1:A:45:PHE:HE1	20	0.01
(1,1864)	1:A:18:MET:HE2	1:A:45:PHE:HE2	20	0.01
(1,1864)	1:A:18:MET:HE3	1:A:45:PHE:HE1	20	0.01
(1,1864)	1:A:18:MET:HE3	1:A:45:PHE:HE2	20	0.01
(1,1861)	1:B:18:MET:HE1	1:B:71:GLY:HA2	11	0.01
(1,1861)	1:B:18:MET:HE2	1:B:71:GLY:HA2	11	0.01
(1,1861)	1:B:18:MET:HE3	1:B:71:GLY:HA2	11	0.01
(1,1861)	1:B:18:MET:HE1	1:B:71:GLY:HA2	15	0.01
(1,1861)	1:B:18:MET:HE2	1:B:71:GLY:HA2	15	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1861)	1:B:18:MET:HE3	1:B:71:GLY:HA2	15	0.01
(1,1861)		1:B:71:GLY:HA2	17	0.01
(1,1861)	1:B:18:MET:HE2	1:B:71:GLY:HA2	17	0.01
(1,1861)	1:B:18:MET:HE3	1:B:71:GLY:HA2	17	0.01
(1,1861)	1:B:18:MET:HE1	1:B:71:GLY:HA2	19	0.01
(1,1861)	1:B:18:MET:HE2	1:B:71:GLY:HA2	19	0.01
(1,1861)	1:B:18:MET:HE3	1:B:71:GLY:HA2	19	0.01
(1,1860)	1:A:18:MET:HE1	1:A:71:GLY:HA2	4	0.01
(1,1860)	1:A:18:MET:HE2	1:A:71:GLY:HA2	4	0.01
(1,1860)	1:A:18:MET:HE3	1:A:71:GLY:HA2	4	0.01
(1,1860)	1:A:18:MET:HE1	1:A:71:GLY:HA2	12	0.01
(1,1860)	1:A:18:MET:HE2	1:A:71:GLY:HA2	12	0.01
(1,1860)	1:A:18:MET:HE3	1:A:71:GLY:HA2	12	0.01
(1,1860)	1:A:18:MET:HE1	1:A:71:GLY:HA2	13	0.01
(1,1860)	1:A:18:MET:HE2	1:A:71:GLY:HA2	13	0.01
(1,1860)	1:A:18:MET:HE3	1:A:71:GLY:HA2	13	0.01
(1,1860)	1:A:18:MET:HE1	1:A:71:GLY:HA2	15	0.01
(1,1860)	1:A:18:MET:HE2	1:A:71:GLY:HA2	15	0.01
(1,1860)	1:A:18:MET:HE3	1:A:71:GLY:HA2	15	0.01
(1,1860)	1:A:18:MET:HE1	1:A:71:GLY:HA2	19	0.01
(1,1860)	1:A:18:MET:HE2	1:A:71:GLY:HA2	19	0.01
(1,1860)	1:A:18:MET:HE3	1:A:71:GLY:HA2	19	0.01
(1,1844)	1:B:17:GLY:H	1:B:18:MET:HG3	13	0.01
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	4	0.01
(1,1838)	1:B:18:MET:HA	1:B:21:GLN:HG2	7	0.01
(1,1838)	1:B:18:MET:HA	1:B:21:GLN:HG3	7	0.01
(1,1838)	1:B:18:MET:HA	1:B:21:GLN:HG2	14	0.01
(1,1838)	1:B:18:MET:HA	1:B:21:GLN:HG3	14	0.01
(1,1837)	1:A:18:MET:HA	1:A:21:GLN:HG2	3	0.01
(1,1837)	1:A:18:MET:HA	1:A:21:GLN:HG3	3	0.01
(1,1825)	1:B:15:LYS:HA	1:B:15:LYS:HE2	7	0.01
(1,1825)	1:B:15:LYS:HA	1:B:15:LYS:HE3	7	0.01
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG21	10	0.01
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG22	10	0.01
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG23	10	0.01
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG21	10	0.01
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG22	10	0.01
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG23	10	0.01
(1,1814)	1:A:68:LYS:HE2	1:A:69:VAL:HG21	5	0.01
(1,1814)	1:A:68:LYS:HE2	1:A:69:VAL:HG22	5	0.01
(1,1814)	1:A:68:LYS:HE2	1:A:69:VAL:HG23	5	0.01
(1,1814)	1:A:68:LYS:HE3	1:A:69:VAL:HG21	5	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1814)	1:A:68:LYS:HE3	1:A:69:VAL:HG22	5	0.01
(1,1814)	1:A:68:LYS:HE3	1:A:69:VAL:HG23	5	0.01
(1,1814)	1:A:68:LYS:HE2	1:A:69:VAL:HG21	20	0.01
(1,1814)	1:A:68:LYS:HE2	1:A:69:VAL:HG22	20	0.01
(1,1814)	1:A:68:LYS:HE2	1:A:69:VAL:HG23	20	0.01
(1,1814)	1:A:68:LYS:HE3	1:A:69:VAL:HG21	20	0.01
(1,1814)	1:A:68:LYS:HE3	1:A:69:VAL:HG22	20	0.01
(1,1814)	1:A:68:LYS:HE3	1:A:69:VAL:HG23	20	0.01
(1,181)	1:A:15:LYS:H	1:A:44:ILE:HA	18	0.01
(1,1774)	1:A:13:GLU:HG2	1:A:44:ILE:HA	19	0.01
(1,1774)	1:A:13:GLU:HG3	1:A:44:ILE:HA	19	0.01
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG11	12	0.01
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG12	12	0.01
(1,1761)	1:B:13:GLU:HG2	1:B:69:VAL:HG13	12	0.01
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG11	12	0.01
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG12	12	0.01
(1,1761)	1:B:13:GLU:HG3	1:B:69:VAL:HG13	12	0.01
(1,176)	1:B:15:LYS:H	1:B:18:MET:HG2	9	0.01
(1,172)	1:B:13:GLU:HG2	1:B:15:LYS:H	3	0.01
(1,172)	1:B:13:GLU:HG3	1:B:15:LYS:H	3	0.01
(1,1699)	1:B:11:VAL:HG21	1:B:45:PHE:HE1	6	0.01
(1,1699)	1:B:11:VAL:HG21	1:B:45:PHE:HE2	6	0.01
(1,1699)	1:B:11:VAL:HG22	1:B:45:PHE:HE1	6	0.01
(1,1699)	1:B:11:VAL:HG22	1:B:45:PHE:HE2	6	0.01
(1,1699)	1:B:11:VAL:HG23	1:B:45:PHE:HE1	6	0.01
(1,1699)	1:B:11:VAL:HG23	1:B:45:PHE:HE2	6	0.01
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	11	0.01
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	11	0.01
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	11	0.01
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	2	0.01
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	2	0.01
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	2	0.01
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	2	0.01
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	2	0.01
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG23	2	0.01
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	2	0.01
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	2	0.01
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	2	0.01
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	11	0.01
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	11	0.01
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	11	0.01
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	11	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	11	0.01
-		1:B:46:THR:HG23	11	0.01
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	11	0.01
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	11	0.01
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	11	0.01
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG21	20	0.01
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG22	20	0.01
(1,1687)	1:B:11:VAL:HG21	1:B:46:THR:HG23	20	0.01
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG21	20	0.01
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG22	20	0.01
(1,1687)	1:B:11:VAL:HG22	1:B:46:THR:HG23	20	0.01
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG21	20	0.01
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG22	20	0.01
(1,1687)	1:B:11:VAL:HG23	1:B:46:THR:HG23	20	0.01
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG21	3	0.01
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG22	3	0.01
(1,1686)	1:A:11:VAL:HG21	1:A:46:THR:HG23	3	0.01
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG21	3	0.01
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG22	3	0.01
(1,1686)	1:A:11:VAL:HG22	1:A:46:THR:HG23	3	0.01
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG21	3	0.01
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG22	3	0.01
(1,1686)	1:A:11:VAL:HG23	1:A:46:THR:HG23	3	0.01
(1,168)	1:B:15:LYS:H	1:B:18:MET:HE1	9	0.01
(1,168)	1:B:15:LYS:H	1:B:18:MET:HE2	9	0.01
(1,168)	1:B:15:LYS:H	1:B:18:MET:HE3	9	0.01
(1,1677)	1:B:10:ILE:HD11	1:B:49:LEU:H	5	0.01
(1,1677)	1:B:10:ILE:HD12	1:B:49:LEU:H	5	0.01
(1,1677)	1:B:10:ILE:HD13	1:B:49:LEU:H	5	0.01
(1,1676)	1:A:10:ILE:HD11	1:A:49:LEU:H	8	0.01
(1,1676)	1:A:10:ILE:HD12	1:A:49:LEU:H	8	0.01
(1,1676)	1:A:10:ILE:HD13	1:A:49:LEU:H	8	0.01
(1,167)	1:A:15:LYS:H	1:A:18:MET:HE1	6	0.01
(1,167)	1:A:15:LYS:H	1:A:18:MET:HE2	6	0.01
(1,167)	1:A:15:LYS:H	1:A:18:MET:HE3	6	0.01
(1,1667)	1:B:10:ILE:HD11	1:B:11:VAL:H	14	0.01
(1,1667)	1:B:10:ILE:HD12	1:B:11:VAL:H	14	0.01
(1,1667)	1:B:10:ILE:HD13	1:B:11:VAL:H	14	0.01
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD11	1	0.01
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD12	1	0.01
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD13	1	0.01
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD11	9	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD12	9	0.01
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD13	9	0.01
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD11	17	0.01
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD12	17	0.01
(1,1641)	1:B:8:ILE:HB	1:B:10:ILE:HD13	17	0.01
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD11	8	0.01
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD12	8	0.01
(1,1640)	1:A:8:ILE:HB	1:A:10:ILE:HD13	8	0.01
(1,160)	1:A:13:GLU:H	1:A:73:PHE:H	8	0.01
(1,1577)	1:B:9:ARG:HD2	1:B:11:VAL:HB	3	0.01
(1,1577)	1:B:9:ARG:HD3	1:B:11:VAL:HB	3	0.01
(1,1576)	1:A:9:ARG:HD2	1:A:11:VAL:HB	5	0.01
(1,1576)	1:A:9:ARG:HD3	1:A:11:VAL:HB	5	0.01
(1,1576)	1:A:9:ARG:HD2	1:A:11:VAL:HB	6	0.01
(1,1576)	1:A:9:ARG:HD3	1:A:11:VAL:HB	6	0.01
(1,1576)	1:A:9:ARG:HD2	1:A:11:VAL:HB	9	0.01
(1,1576)	1:A:9:ARG:HD3	1:A:11:VAL:HB	9	0.01
(1,1558)	1:B:24:GLY:H	1:B:26:ILE:HD11	5	0.01
(1,1558)	1:B:24:GLY:H	1:B:26:ILE:HD12	5	0.01
(1,1558)	1:B:24:GLY:H	1:B:26:ILE:HD13	5	0.01
(1,1557)	1:A:24:GLY:H	1:A:26:ILE:HD11	4	0.01
(1,1557)	1:A:24:GLY:H	1:A:26:ILE:HD12	4	0.01
(1,1557)	1:A:24:GLY:H	1:A:26:ILE:HD13	4	0.01
(1,1550)	1:B:23:THR:HA	1:B:26:ILE:HD11	4	0.01
(1,1550)	1:B:23:THR:HA	1:B:26:ILE:HD12	4	0.01
(1,1550)	1:B:23:THR:HA	1:B:26:ILE:HD13	4	0.01
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	9	0.01
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	9	0.01
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	9	0.01
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	9	0.01
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	9	0.01
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	9	0.01
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	9	0.01
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	9	0.01
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	9	0.01
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	1	0.01
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	1	0.01
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	1	0.01
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	1	0.01
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	1	0.01
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	1	0.01
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	10	0.01



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Key			Model	Violation (Å)
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	10	0.01
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	10	0.01
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	10	0.01
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	10	0.01
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	10	0.01
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	12	0.01
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	12	0.01
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	12	0.01
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	12	0.01
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	12	0.01
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	12	0.01
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD2	19	0.01
(1,1520)	1:B:8:ILE:HG21	1:B:77:ARG:HD3	19	0.01
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD2	19	0.01
(1,1520)	1:B:8:ILE:HG22	1:B:77:ARG:HD3	19	0.01
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD2	19	0.01
(1,1520)	1:B:8:ILE:HG23	1:B:77:ARG:HD3	19	0.01
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	7	0.01
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	7	0.01
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	7	0.01
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	7	0.01
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	7	0.01
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	7	0.01
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	18	0.01
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	18	0.01
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	18	0.01
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	18	0.01
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	18	0.01
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	18	0.01
(1,1517)	1:A:8:ILE:HG21	1:A:63:MET:HG2	13	0.01
(1,1517)	1:A:8:ILE:HG21	1:A:63:MET:HG3	13	0.01
(1,1517)	1:A:8:ILE:HG22	1:A:63:MET:HG2	13	0.01
(1,1517)	1:A:8:ILE:HG22	1:A:63:MET:HG3	13	0.01
(1,1517)	1:A:8:ILE:HG23	1:A:63:MET:HG2	13	0.01
(1,1517)	1:A:8:ILE:HG23	1:A:63:MET:HG3	13	0.01
(1,151)	1:B:13:GLU:H	1:B:44:ILE:HA	11	0.01
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	7	0.01
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	7	0.01
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	7	0.01
(1,1480)	1:B:5:LEU:HD21	1:B:52:PHE:HA	9	0.01
(1,1480)	1:B:5:LEU:HD22	1:B:52:PHE:HA	9	0.01
(1,1480)	1:B:5:LEU:HD23	1:B:52:PHE:HA	9	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1477)	1477) 1:A:5:LEU:HD21 1:A:5		4	0.01
(1,1477) 1:A:5:LEU:HD22		1:A:51:ILE:HA	4	0.01
(1,1477)	1:A:5:LEU:HD23	1:A:51:ILE:HA	4	0.01
(1,144)	1:A:13:GLU:H	1:A:13:GLU:HG2	7	0.01
(1,144)	1:A:13:GLU:H	1:A:13:GLU:HG3	7	0.01
(1,1429)	1:A:5:LEU:HG	1:A:52:PHE:HE1	8	0.01
(1,1429)	1:A:5:LEU:HG	1:A:52:PHE:HE2	8	0.01
(1,1413)	1:A:3:ASP:HB2	1:A:53:VAL:H	19	0.01
(1,1378)	1:B:40:ALA:H	1:B:41:LYS:HD2	2	0.01
(1,1378)	1:B:40:ALA:H	1:B:41:LYS:HD3	2	0.01
(1,1378)	1:B:40:ALA:H	1:B:41:LYS:HD2	12	0.01
(1,1378)	1:B:40:ALA:H	1:B:41:LYS:HD3	12	0.01
(1,1310)	1:B:77:ARG:H	1:B:77:ARG:HD2	14	0.01
(1,1310)	1:B:77:ARG:H	1:B:77:ARG:HD3	14	0.01
(1,1266)	1:B:74:THR:HG21	1:B:75:VAL:H	17	0.01
(1,1266)	1:B:74:THR:HG22	1:B:75:VAL:H	17	0.01
(1,1266)	1:B:74:THR:HG23	1:B:75:VAL:H	17	0.01
(1,1265)	1:A:74:THR:HG21	1:A:75:VAL:H	7	0.01
(1,1265)	1:A:74:THR:HG22	1:A:75:VAL:H	7	0.01
(1,1265)	1:A:74:THR:HG23	1:A:75:VAL:H	7	0.01
(1,1212)	1:B:69:VAL:HG11	1:B:71:GLY:H	12	0.01
(1,1212)	1:B:69:VAL:HG12	1:B:71:GLY:H	12	0.01
(1,1212)	1:B:69:VAL:HG13	1:B:71:GLY:H	12	0.01
(1,1212)	1:B:69:VAL:HG11	1:B:71:GLY:H	20	0.01
(1,1212)	1:B:69:VAL:HG12	1:B:71:GLY:H	20	0.01
(1,1212)	1:B:69:VAL:HG13	1:B:71:GLY:H	20	0.01
(1,1211)	1:A:69:VAL:HG11	1:A:71:GLY:H	20	0.01
(1,1211)	1:A:69:VAL:HG12	1:A:71:GLY:H	20	0.01
(1,1211)	1:A:69:VAL:HG13	1:A:71:GLY:H	20	0.01
(1,1196)	1:B:69:VAL:H	1:B:70:GLN:H	8	0.01
(1,1196)	1:B:69:VAL:H	1:B:70:GLN:H	16	0.01
(1,1196)	1:B:69:VAL:H	1:B:70:GLN:H	17	0.01
(1,1195)	1:A:69:VAL:H	1:A:70:GLN:H	10	0.01
(1,1192)	1:B:69:VAL:H	1:B:72:VAL:H	2	0.01
(1,1191)	1:A:69:VAL:H	1:A:72:VAL:H	16	0.01
(1,1158)	1:B:68:LYS:H	1:B:75:VAL:HG21	11	0.01
(1,1158)	1:B:68:LYS:H	1:B:75:VAL:HG22	11	0.01
(1,1158)	1:B:68:LYS:H	1:B:75:VAL:HG23	11	0.01
(1,1150)	1:B:67:ARG:HE	1:B:75:VAL:HB	15	0.01
(1,1150)	1:B:67:ARG:HE	1:B:75:VAL:HB	16	0.01
(1,1149)	1:A:67:ARG:HE	1:A:75:VAL:HB	15	0.01
(1,1139)	1:A:67:ARG:H	1:A:67:ARG:HE	8	0.01



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Key Atom-1		Atom-2	Model	Violation (Å)
(1,1124)	1:B:67:ARG:H	1:B:69:VAL:HG21	7	0.01
(1,1124)	1:B:67:ARG:H	1:B:69:VAL:HG22	7	0.01
(1,1124)	1:B:67:ARG:H	1:B:69:VAL:HG23	7	0.01
(1,1106)	1:B:62:LEU:HD11	1:B:66:LEU:H	1	0.01
(1,1106)	1:B:62:LEU:HD12	1:B:66:LEU:H	1	0.01
(1,1106)	1:B:62:LEU:HD13	1:B:66:LEU:H	1	0.01
(1,1106)	1:B:62:LEU:HD11	1:B:66:LEU:H	7	0.01
(1,1106)	1:B:62:LEU:HD12	1:B:66:LEU:H	7	0.01
(1,1106)	1:B:62:LEU:HD13	1:B:66:LEU:H	7	0.01
(1,1106)	1:B:62:LEU:HD11	1:B:66:LEU:H	9	0.01
(1,1106)	1:B:62:LEU:HD12	1:B:66:LEU:H	9	0.01
(1,1106)	1:B:62:LEU:HD13	1:B:66:LEU:H	9	0.01
(1,1106)	1:B:62:LEU:HD11	1:B:66:LEU:H	13	0.01
(1,1106)	1:B:62:LEU:HD12	1:B:66:LEU:H	13	0.01
(1,1106)	1:B:62:LEU:HD13	1:B:66:LEU:H	13	0.01
(1,1106)	1:B:62:LEU:HD11	1:B:66:LEU:H	17	0.01
(1,1106)	1:B:62:LEU:HD12	1:B:66:LEU:H	17	0.01
(1,1106)	1:B:62:LEU:HD13	1:B:66:LEU:H	17	0.01
(1,1106)	1:B:62:LEU:HD11	1:B:66:LEU:H	19	0.01
(1,1106)	1:B:62:LEU:HD12	1:B:66:LEU:H	19	0.01
(1,1106)	1:B:62:LEU:HD13	1:B:66:LEU:H	19	0.01
(1,1105)	1:A:62:LEU:HD11	1:A:66:LEU:H	20	0.01
(1,1105)	1:A:62:LEU:HD12	1:A:66:LEU:H	20	0.01
(1,1105)	1:A:62:LEU:HD13	1:A:66:LEU:H	20	0.01
(1,1104)	1:B:62:LEU:HD11	1:B:65:LYS:H	5	0.01
(1,1104)	1:B:62:LEU:HD12	1:B:65:LYS:H	5	0.01
(1,1104)	1:B:62:LEU:HD13	1:B:65:LYS:H	5	0.01
(1,1104)	1:B:62:LEU:HD11	1:B:65:LYS:H	18	0.01
(1,1104)	1:B:62:LEU:HD12	1:B:65:LYS:H	18	0.01
(1,1104)	1:B:62:LEU:HD13	1:B:65:LYS:H	18	0.01
(1,1103)	1:A:62:LEU:HD11	1:A:65:LYS:H	9	0.01
(1,1103)	1:A:62:LEU:HD12	1:A:65:LYS:H	9	0.01
(1,1103)	1:A:62:LEU:HD13	1:A:65:LYS:H	9	0.01
(1,1103)	1:A:62:LEU:HD11	1:A:65:LYS:H	13	0.01
(1,1103)	1:A:62:LEU:HD12	1:A:65:LYS:H	13	0.01
(1,1103)	1:A:62:LEU:HD13	1:A:65:LYS:H	13	0.01
(1,1103)	1:A:62:LEU:HD11	1:A:65:LYS:H	16	0.01
(1,1103)	1:A:62:LEU:HD12	1:A:65:LYS:H	16	0.01
(1,1103)	1:A:62:LEU:HD13	1:A:65:LYS:H	16	0.01
(1,1103)	1:A:62:LEU:HD11	1:A:65:LYS:H	18	0.01
(1,1103)	1:A:62:LEU:HD12	1:A:65:LYS:H	18	0.01
(1,1103)	1:A:62:LEU:HD13	1:A:65:LYS:H	18	0.01



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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1103)	1:A:62:LEU:HD11	1:A:65:LYS:H	20	0.01
(1,1103)	1:A:62:LEU:HD12	1:A:65:LYS:H	20	0.01
(1,1103)	1:A:62:LEU:HD13	1:A:65:LYS:H	20	0.01
(1,1067)	1:B:64:ASP:H	1:B:75:VAL:HG11	7	0.01
(1,1067)	1:B:64:ASP:H	1:B:75:VAL:HG12	7	0.01
(1,1067)	1:B:64:ASP:H	1:B:75:VAL:HG13	7	0.01
(1,1066)	1:A:64:ASP:H	1:A:75:VAL:HG11	4	0.01
(1,1066)	1:A:64:ASP:H	1:A:75:VAL:HG12	4	0.01
(1,1066)	1:A:64:ASP:H	1:A:75:VAL:HG13	4	0.01
(1,1066)	1:A:64:ASP:H	1:A:75:VAL:HG11	18	0.01
(1,1066)	1:A:64:ASP:H	1:A:75:VAL:HG12	18	0.01
(1,1066)	1:A:64:ASP:H	1:A:75:VAL:HG13	18	0.01
(1,1047)	1:B:58:LYS:HZ1	1:B:62:LEU:H	4	0.01
(1,1047)	1:B:58:LYS:HZ2	1:B:62:LEU:H	4	0.01
(1,1047)	1:B:58:LYS:HZ3	1:B:62:LEU:H	4	0.01
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	5	0.01
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	5	0.01
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	5	0.01
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	8	0.01
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	8	0.01
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	8	0.01



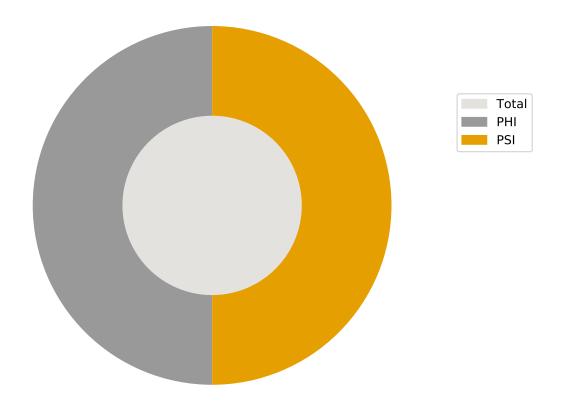
9 Dihedral angle restraints analysis

9.1 Dihedral angle restraints summary

Angle name	Count	%
PHI	116	50.0
PSI	116	50.0
Total	232	100.0

9.1.1 Pie chart : Dihedral angle restraints

There are 0 unmapped restraints



9.2 Dihedral angle violations

The following table provides the summary of violated restraints. Restraints that are violated at least in one model are counted as violated.

Angle name	Count	$\%^1$	$\%^2$
PHI	30	25.9	30.6
PSI	68	58.6	69.4

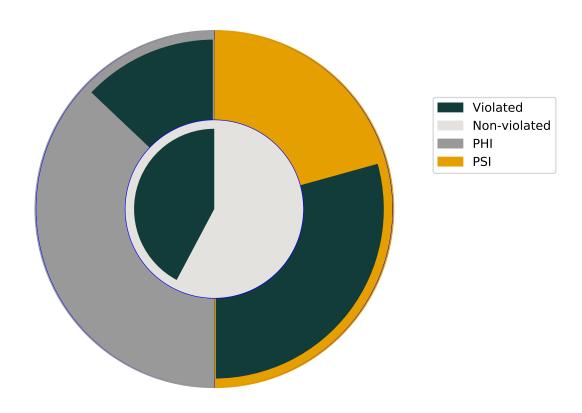


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Angle name	Count	$\frac{1}{\%^{1}}$	$\%^{2}$
Total	98	42.2	100.0

¹percentage of violated restraints in that particular angle type, ²percentage of violation in total violations.

9.2.1 Pie chart: Dihedral angle violations



9.3 Consistent dihedral angle violations

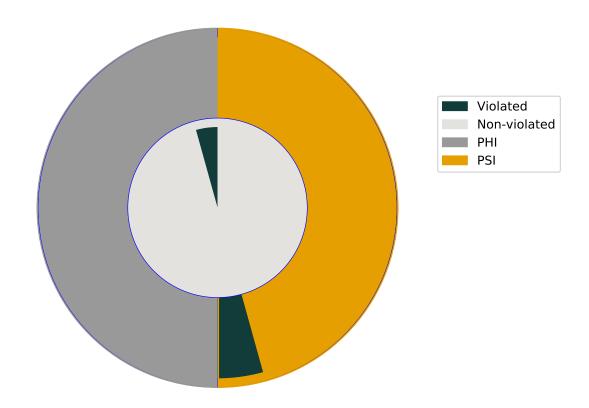
The following table provides the summary of consistently violated restraints. Restraints that are violated in all models are counted as consistently violated.

Angle name	Count	$\%^1$	$\%^2$
PHI	0	0.0	0.0
PSI	10	8.6	100.0
Total	10	4.3	100.0

 1 percentage of violated restraints in that particular angle type, 2 percentage of violation in total violations.



9.3.1 Pie chart: Consistent dihedral angle violations



9.4 Residual dihedral angle violations

Violation are counted in different bin sizes and listed below

Range (\circ)	Avg. No. of violated restraints per model	$ \text{Max violation } (\circ) $
0.0-5.0	30.4	3.59
5.0-10.0	0.4	9.93
10.0-20.0	2.4	18.2
20.0-40.0	3.3	39.94
40.0-80.0	3.0	69.43
80.0<	None	None

9.5 Dihedral angle violations in the ensemble

The restraints are grouped based on the number of violated models and listed here.

No.	of vio	lated restraints	No. of violated models		
PHI	PSI	Total	No. of violated models		
9	11	20	1		

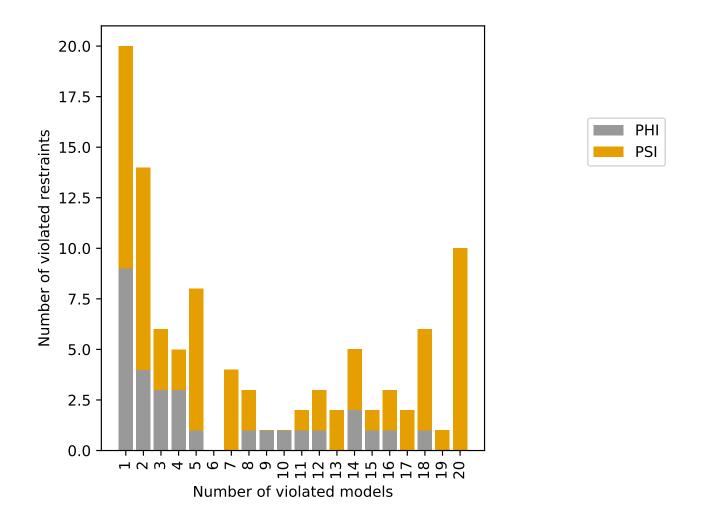


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		$\overline{ m plated\ restraints}$			
PHI	PSI	Total	No. of violated models		
4	10	14	2		
3	3	6	3		
3	2	5	4		
1	7	8	5		
0	0	0	6		
0	4	4	7		
1	2	3	8		
1	0	1	9		
1	0	1	10		
1	1	2	11		
1	2	3	12		
0	2	2	13		
2	3	5	14		
1	1	2	15		
1	2	3	16		
0	2	2	17		
1	5	6	18		
0	1	1	19		
0	10	10	20		



9.5.1 Bar graph: No. of models vs No. of violations



9.6 Violations in each model

The following table lists the violation count in each model in the ensemble

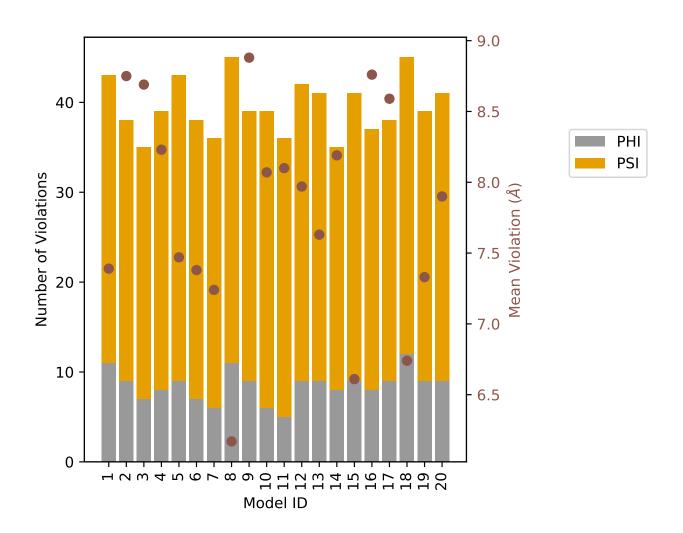
Model ID	No. of violations		Moon (a)	Mov (a)	
Model 1D	PHI	PSI	Total	$\mathbf{Mean} \; (\; \circ \;)$	$\mathbf{Max} (\circ)$
1	11	32	43	7.39	46.36
2	9	29	38	8.75	54.01
3	7	28	35	8.69	66.02
4	8	31	39	8.23	58.06
5	9	34	43	7.47	56.54
6	7	31	38	7.38	68.8
7	6	30	36	7.24	55.69
8	11	34	45	6.17	46.53
9	9	30	39	8.88	59.13



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Model ID	No. of violations			Moon (a)	Mary (a)
Model 1D	PHI	PSI	Total	$ \mathbf{Mean} (\circ) $	$\mathbf{Max} (\circ)$
10	6	33	39	8.07	47.84
11	5	31	36	8.1	48.02
12	9	33	42	7.97	63.57
13	9	32	41	7.63	57.23
14	8	27	35	8.19	54.95
15	9	32	41	6.61	46.56
16	8	29	37	8.76	55.54
17	9	29	38	8.59	61.48
18	12	33	45	6.74	60.03
19	9	30	39	7.33	62.38
20	9	32	41	7.9	69.43

9.6.1 Bar graph: Violations in each model

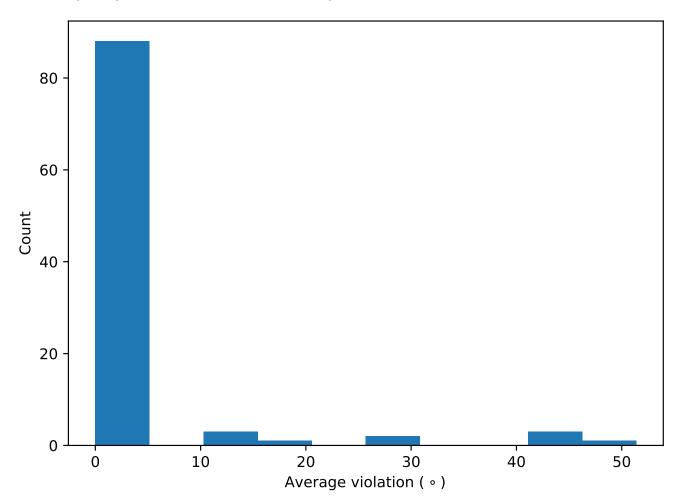




9.7 Most violated dihedral angle restraints

9.7.1 Histogram: Distribution of mean dihedral angle violations

The following histogram shows the distribution of average violation of each restraint



9.7.2 Table: Most violated dihedral angle restraints

The following tale lists the average violation of each restraint sorted by number of violated models

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models	Mean (o)	Max (°)
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	18	46.16	69.43
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	19	51.38	68.8
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	20	45.51	48.14
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	20	42.79	48.02
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	20	27.54	35.74
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	20	28.07	33.55
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	14	16.22	25.52
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	16	12.85	25.09
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	20	11.43	15.68
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	20	11.82	14.38



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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models	Mean (°)	Max (∘)
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	18	1.59	3.59
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	18	1.77	3.0
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	20	2.06	2.99
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	20	2.15	2.94
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	16	1.37	2.71
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	12	1.73	2.59
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	20	1.35	2.58
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	17	1.35	2.36
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	18	1.23	2.25
(1,170)	1:B:37:VAL:N	1:B:37:VAL:CA	1:B:37:VAL:C	1:B:38:LEU:N	7	0.96	2.21
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	14	1.1	2.17
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	15	1.05	2.14
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	13	0.96	2.1
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	20	0.77	1.93
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	13	1.05	1.85
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	18	0.74	1.66
(1,28)	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	1:A:21:GLN:N	12	0.73	1.54
(1,60)	1:A:40:ALA:N	1:A:40:ALA:CA	1:A:40:ALA:C	1:A:41:LYS:N	1	1.5	1.5
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	17	0.8	1.48
(1,96)	1:A:63:MET:N	1:A:63:MET:CA	1:A:63:MET:C	1:A:64:ASP:N	3	0.52	1.48
(1,128)	1:B:9:ARG:N	1:B:9:ARG:CA	1:B:9:ARG:C	1:B:10:ILE:N	7	0.79	1.4
(1,182)	1:B:46:THR:N	1:B:46:THR:CA	1:B:46:THR:C	1:B:47:CYS:N	4	0.77	1.34
(1,212)	1:B:63:MET:N	1:B:63:MET:CA	1:B:63:MET:C	1:B:64:ASP:N	5	0.51	1.26
(1,204)	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	1:B:60:THR:N	14	0.47	1.25
(1,12)	1:A:9:ARG:N	1:A:9:ARG:CA	1:A:9:ARG:C	1:A:10:ILE:N	2	1.02	1.22
(1,196)	1:B:53:VAL:N	1:B:53:VAL:CA	1:B:53:VAL:C	1:B:54:LYS:N	5	0.66	1.21
(1,90)	1:A:60:THR:N	1:A:60:THR:CA	1:A:60:THR:C	1:A:61:THR:N	5	0.42	1.17
(1,110)	1:A:74:THR:N	1:A:74:THR:CA	1:A:74:THR:C	1:A:75:VAL:N	2	0.76	1.16
(1,120)	1:B:5:LEU:N	1:B:5:LEU:CA	1:B:5:LEU:C	1:B:6:ALA:N	5	0.43	1.06
(1,166)	1:B:35:THR:N	1:B:35:THR:CA	1:B:35:THR:C	1:B:36:ILE:N	8	0.52	1.06
(1,206)	1:B:60:THR:N	1:B:60:THR:CA	1:B:60:THR:C	1:B:61:THR:N	8	0.64	1.04
(1,98)	1:A:64:ASP:N	1:A:64:ASP:CA	1:A:64:ASP:C	1:A:65:LYS:N	1	1.03	1.03
(1,66)	1:A:46:THR:N	1:A:46:THR:CA	1:A:46:THR:C	1:A:47:CYS:N	5	0.46	0.98
(1,144)	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	1:B:21:GLN:N	11	0.46	0.89
(1,80)	1:A:53:VAL:N	1:A:53:VAL:CA	1:A:53:VAL:C	1:A:54:LYS:N	5	0.37	0.8
(1,50)	1:A:35:THR:N	1:A:35:THR:CA	1:A:35:THR:C	1:A:36:ILE:N	7	0.31	0.79
(1,218)	1:B:66:LEU:N	1:B:66:LEU:CA	1:B:66:LEU:C	1:B:67:ARG:N	3	0.37	0.79
(1,172)	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	1:B:39:ASN:N	2	0.63	0.79
(1,4)	1:A:5:LEU:N	1:A:5:LEU:CA	1:A:5:LEU:C	1:A:6:ALA:N	7	0.42	0.77
(1,226)	1:B:74:THR:N	1:B:74:THR:CA	1:B:74:THR:C	1:B:75:VAL:N	5	0.49	0.72
(1,174)	1:B:39:ASN:N	1:B:39:ASN:CA	1:B:39:ASN:C	1:B:40:ALA:N	2	0.39	0.68
(1,224)	1:B:69:VAL:N	1:B:69:VAL:CA	1:B:69:VAL:C	1:B:70:GLN:N	2	0.46	0.63
(1,152)	1:B:24:GLY:N	1:B:24:GLY:CA	1:B:24:GLY:C	1:B:25:VAL:N	4	0.4	0.56
(1,178)	1:B:44:ILE:N	1:B:44:ILE:CA	1:B:44:ILE:C	1:B:45:PHE:N	1	0.53	0.53
(1,116)	1:A:77:ARG:N	1:A:77:ARG:CA	1:A:77:ARG:C	1:A:78:LEU:N	1	0.47	0.47
(1,110) $(1,48)$	1:A:33:ILE:N	1:A:33:ILE:CA	1:A:33:ILE:C	1:A:34:ARG:N	2	0.28	0.41
(1,36)	1:A:24:GLY:N	1:A:24:GLY:CA	1:A:24:GLY:C	1:A:25:VAL:N	2	0.32	0.41
(1,114)	1:A:76:GLU:N	1:A:76:GLU:CA	1:A:76:GLU:C	1:A:77:ARG:N	2	0.3	0.4
(1,714) $(1,70)$	1:A:48:ASN:N	1:A:48:ASN:CA	1:A:48:ASN:C	1:A:49:LEU:N	3	0.23	0.37
(1,62)	1:A:44:ILE:N	1:A:44:ILE:CA	1:A:44:ILE:C	1:A:45:PHE:N	1	0.36	0.36
(1,02) $(1,214)$	1:B:64:ASP:N	1:B:64:ASP:CA	1:B:64:ASP:C	1:B:65:LYS:N	1	0.36	0.36
(1,414)	T.D.04.1701 .11	1.D.04.1101 .OA	1.101.F0.G1.	1.0.00.110.11	1	Continued on	



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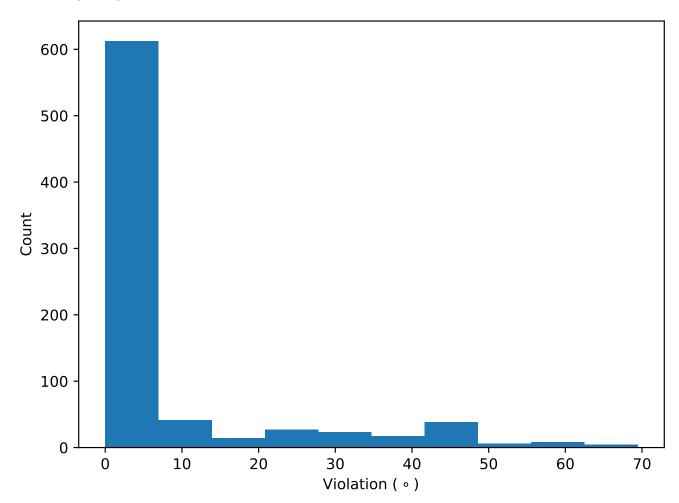
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models	Mean (o)	Max (°)
(1,102)	1:A:66:LEU:N	1:A:66:LEU:CA	1:A:66:LEU:C	1:A:67:ARG:N	2	0.15	0.24
(1,142)	1:B:19:THR:N	1:B:19:THR:CA	1:B:19:THR:C	1:B:20:ASN:N	1	0.23	0.23
(1,230)	1:B:76:GLU:N	1:B:76:GLU:CA	1:B:76:GLU:C	1:B:77:ARG:N	1	0.22	0.22
(1,186)	1:B:48:ASN:N	1:B:48:ASN:CA	1:B:48:ASN:C	1:B:49:LEU:N	2	0.15	0.16
(1,184)	1:B:47:CYS:N	1:B:47:CYS:CA	1:B:47:CYS:C	1:B:48:ASN:N	1	0.12	0.12
(1,210)	1:B:62:LEU:N	1:B:62:LEU:CA	1:B:62:LEU:C	1:B:63:MET:N	1	0.1	0.1
(1,232)	1:B:77:ARG:N	1:B:77:ARG:CA	1:B:77:ARG:C	1:B:78:LEU:N	1	0.02	0.02
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	14	0.94	2.47
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	16	0.96	2.14
(1,55)	1:A:37:VAL:C	1:A:38:LEU:N	1:A:38:LEU:CA	1:A:38:LEU:C	4	1.3	2.06
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	14	0.69	1.99
(1,171)	1:B:37:VAL:C	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	9	1.13	1.9
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	18	0.62	1.76
(1,139)	1:B:17:GLY:C	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	5	0.8	1.62
(1,23)	1:A:17:GLY:C	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	3	0.7	1.21
(1,85)	1:A:57:ASP:C	1:A:58:LYS:N	1:A:58:LYS:CA	1:A:58:LYS:C	10	0.68	1.14
(1,27)	1:A:19:THR:C	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	11	0.41	1.08
(1,5)	1:A:5:LEU:C	1:A:6:ALA:N	1:A:6:ALA:CA	1:A:6:ALA:C	8	0.45	1.01
(1,187)	1:B:48:ASN:C	1:B:49:LEU:N	1:B:49:LEU:CA	1:B:49:LEU:C	15	0.59	1.0
(1,33)	1:A:22:ILE:C	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	4	0.49	0.94
(1,121)	1:B:5:LEU:C	1:B:6:ALA:N	1:B:6:ALA:CA	1:B:6:ALA:C	3	0.66	0.92
(1,149)	1:B:22:ILE:C	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	4	0.39	0.87
(1,143)	1:B:19:THR:C	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	12	0.34	0.82
(1,31)	1:A:21:GLN:C	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	2	0.42	0.66
(1,87)	1:A:58:LYS:C	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1	0.62	0.62
(1,69)	1:A:47:CYS:C	1:A:48:ASN:N	1:A:48:ASN:CA	1:A:48:ASN:C	1	0.51	0.51
(1,57)	1:A:38:LEU:C	1:A:39:ASN:N	1:A:39:ASN:CA	1:A:39:ASN:C	2	0.29	0.5
(1,211)	1:B:62:LEU:C	1:B:63:MET:N	1:B:63:MET:CA	1:B:63:MET:C	3	0.24	0.46
(1,203)	1:B:58:LYS:C	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	1	0.33	0.33
(1,59)	1:A:39:ASN:C	1:A:40:ALA:N	1:A:40:ALA:CA	1:A:40:ALA:C	1	0.26	0.26
(1,197)	1:B:53:VAL:C	1:B:54:LYS:N	1:B:54:LYS:CA	1:B:54:LYS:C	1	0.24	0.24
(1,145)	1:B:20:ASN:C	1:B:21:GLN:N	1:B:21:GLN:CA	1:B:21:GLN:C	2	0.14	0.22
(1,185)	1:B:47:CYS:C	1:B:48:ASN:N	1:B:48:ASN:CA	1:B:48:ASN:C	2	0.14	0.18
(1,153)	1:B:24:GLY:C	1:B:25:VAL:N	1:B:25:VAL:CA	1:B:25:VAL:C	1	0.17	0.17
(1,147)	1:B:21:GLN:C	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1	0.14	0.14
(1,39)	1:A:25:VAL:C	1:A:26:ILE:N	1:A:26:ILE:CA	1:A:26:ILE:C	1	0.08	0.08
(1,97)	1:A:63:MET:C	1:A:64:ASP:N	1:A:64:ASP:CA	1:A:64:ASP:C	1	0.01	0.01



9.8 All violated dihedral angleeee restraints

9.8.1 Histogram : Distribution of violations

The following histogram shows the distribution of violations in the ensemble.



9.8.2 Table: All violated dihedral angle restraints

The following table lists the violations in the ensemble sorted by violation value

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	$\textbf{Violation} \ (\ \circ\)$
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	20	69.43
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	6	68.8
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	3	66.02
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	12	63.57
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	19	62.38
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	17	61.48
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	18	60.03
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	9	59.13
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	4	58.06
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	13	57.23



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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (o)
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	5	56.54
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	7	55.69
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	16	55.54
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	14	54.95
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	2	54.01
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	9	53.6
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	18	52.47
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	4	49.61
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	16	48.14
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	11	48.02
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	6	47.88
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	10	47.84
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	9	47.83
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	13	47.78
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	12	47.1
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	9	47.05
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	11	46.77
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	20	46.69
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	15	46.56
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	2	46.54
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	8	46.53
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	4	46.47
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	8	46.42
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	1	46.36
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	5	46.33
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	13	46.19
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	14	46.13
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	17	45.91
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	17	45.91
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	19	45.84
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	12	45.4
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	17	45.38
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	14	45.24
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	14	45.2
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	4	45.16
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	5	44.95
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	15	44.9
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	2	44.53
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	16	44.13
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	13	43.72
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	1	43.68
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	10	43.65
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	3	43.2
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	15	42.82
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	20	42.7
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	15	42.06
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	11	41.51
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	12	41.47
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	18	40.73
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	16	40.68
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	6	40.04



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Key	$rac{\textbf{Atom-1}}{\mathbf{Atom-1}}$	Atom-2	Atom-3	Atom-4	Model	Violation (o)
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ILE:N	7	39.94
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	11	39.74
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	20	39.1
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	1	38.96
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	10	38.25
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	18	37.75
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	1	37.39
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	7	36.98
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	5	36.82
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	17	35.74
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	8	35.58
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	19	35.31
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	2	33.85
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	10	33.62
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	2	33.55
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	19	31.88
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	5	31.51
(1,124)	1:B:7:GLY:N	1:B:7:GLY:CA	1:B:7:GLY:C	1:B:8:ILE:N	3	30.86
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	3	30.82
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	10	30.71
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	3	30.66
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	9	30.5
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	10	30.5
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	20	30.24
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	19	30.11
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	17	30.09
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	13	30.05
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	16	29.86
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	20	29.84
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	18	29.44
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	15	29.31
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	12	29.23
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	8	28.96
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	4	28.72
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	4	28.45
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	18	27.63
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	7	27.52
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	9	27.45
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	16	27.33
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	7	27.32
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	11	27.19
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	3	26.96
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	11	26.92
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	1	26.71
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	1	26.66
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	6	26.13
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	15	25.97
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	5	25.83
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	8	25.78
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	8	25.52
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	3	25.12



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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (o)
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	1	25.09
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	2	24.56
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	2	23.58
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	12	23.57
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	6	22.96
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	10	22.66
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	13	22.65
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	14	22.39
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	1	22.06
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	6	21.82
(1,118)	1:B:4:PHE:N	1:B:4:PHE:CA	1:B:4:PHE:C	1:B:5:LEU:N	14	20.92
(1,2)	1:A:4:PHE:N	1:A:4:PHE:CA	1:A:4:PHE:C	1:A:5:LEU:N	19	20.66
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	2	20.49
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	7	20.2
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	5	20.04
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	16	18.2
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	19	17.94
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	12	17.17
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	17	16.57
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	9	16.28
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	20	15.68
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	11	14.69
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	10	14.49
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	11	14.38
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	5	14.1
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	14	13.69
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	3	13.66
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	6	13.65
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	8	13.62
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	9	13.6
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	7	13.57
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	12	13.41
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	15	13.22
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	10	12.9
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	16	12.71
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	2	12.62
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	12	12.59
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	9	12.55
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	8	12.51
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	2	12.47
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	4	12.43
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	13	12.27
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	3	12.25
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	20	12.16
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	4	12.1
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	1	11.82
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	7	11.65
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	5	11.36
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	17	11.21
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	17	11.19
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	8 Continu	11.11



 $Continued\ from\ previous\ page...$

Key	ea from previous p Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (o)
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	9	11.04
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	18	11.02
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	16	10.98
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	4	10.86
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	19	10.79
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	14	10.59
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	10	10.57
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	13	10.41
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	16	10.32
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	18	10.29
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	12	10.24
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	6	9.93
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	13	8.21
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	11	7.7
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	19	7.56
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	20	6.3
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	6	6.25
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	13	6.06
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	5	5.35
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	18	3.59
(1,76)	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	1:A:52:PHE:N	1	3.53
(1,192)	1:B:51:ILE:N	1:B:51:ILE:CA	1:B:51:ILE:C	1:B:52:PHE:N	15	3.07
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	5	3.0
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	10	2.99
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	17	2.98
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	18	2.94
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	11	2.76
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	4	2.72
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	8	2.71
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	9	2.69
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	2	2.67
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	2	2.65
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	9	2.59
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	16	2.58
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	9	2.57
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	12	2.56
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	10	2.55
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	20	2.49
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	9	2.47
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	4	2.45
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	12	2.43
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	19	2.43
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	17	2.43
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	8	2.42
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	3	2.41
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	5	2.4
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	12	2.4
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	20	2.4
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	13	2.39
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	14	2.37
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	Continu	2.37



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Key	ed from previous p Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (o)
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	13	2.36
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	1	2.34
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	7	2.33
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	14	2.32
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	7	2.32
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	5	2.3
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	3	2.3
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	12	2.28
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	5	2.27
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	6	2.25
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	20	2.23
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	20	2.22
(1,170)	1:B:37:VAL:N	1:B:37:VAL:CA	1:B:37:VAL:C	1:B:38:LEU:N	14	2.21
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	16	2.18
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	1	2.18
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	9	2.17
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	10	2.17
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	7	2.16
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	15	2.15
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	15	2.14
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	5	2.14
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	3	2.13
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	5	2.11
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	1	2.1
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	13	2.1
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	10	2.1
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	11	2.1
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	9	2.1
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	7	2.08
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	9	2.08
(1,55)	1:A:37:VAL:C	1:A:38:LEU:N	1:A:38:LEU:CA	1:A:38:LEU:C	8	2.06
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	10	2.06
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	8	2.06
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	18	2.06
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	1	2.05
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	3	2.05
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	19	2.05
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	13	2.03
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	20	2.0
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	14	1.99
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	13	1.98
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	4	1.97
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	1	1.97
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	13	1.97
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	20	1.97
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	4	1.93
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	12	1.92
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	2	1.92
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	16	1.91
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	1	1.91
(1,171)	1:B:37:VAL:C	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	13	d on next page



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Key	$\frac{ed\ from\ previous\ p}{\mathbf{Atom-1}}$	Atom-2	Atom-3	Atom-4	Model	Violation (o)
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	1	1.9
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	6	1.88
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	4	1.87
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	17	1.86
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	18	1.85
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	2	1.84
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	11	1.84
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	16	1.84
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	18	1.83
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	1	1.82
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	11	1.82
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	7	1.79
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	8	1.77
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	6	1.76
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	17	1.75
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	1	1.74
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	14	1.74
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	11	1.72
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	6	1.71
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	12	1.71
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	8	1.69
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	19	1.69
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	10	1.69
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	3	1.69
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	2	1.68
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	16	1.68
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	18	1.67
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	12	1.67
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	2	1.66
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	14	1.66
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	15	1.66
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	14	1.64
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	1	1.64
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	17	1.64
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	18	1.64
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	10	1.63
(1,139)	1:B:17:GLY:C	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	6	1.62
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	14	1.61
(1,171)	1:B:37:VAL:C	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	16	1.59
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	14	1.59
(1,55)	1:A:37:VAL:C	1:A:38:LEU:N	1:A:38:LEU:CA	1:A:38:LEU:C	11	1.58
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	18	1.57
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	4	1.57
(1,28)	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	1:A:21:GLN:N	20	1.54
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	16	1.54
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	15	1.52
(1,60)	1:A:40:ALA:N	1:A:40:ALA:CA	1:A:40:ALA:C	1:A:41:LYS:N	7	1.5
(1,170)	1:B:37:VAL:N	1:B:37:VAL:CA	1:B:37:VAL:C	1:B:38:LEU:N	1	1.5
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	3	1.49
(1,96)	1:A:63:MET:N	1:A:63:MET:CA	1:A:63:MET:C	1:A:64:ASP:N	1	1.48
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	4	d on next nage



 $Continued\ from\ previous\ page...$

	Key	ea from previous p Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (o)
(1,42) 1:A-27:SER:N 1:A-27:SER:CA 1:A-22:LE:CC 1:A-28:LIN:N 8 1.42 (1,32) 1:A-22:LE:N 1:A-22:LE:CA 1:A-22:LE:CC 1:A-23:THR:N 7 1.42 (1,34) 1:A-23:THR:N 1:A-23:THR:CA 1:B-18:MET:C 1:B-19:THR:N 1 1.42 (1,34) 1:A-23:THR:N 1:A-23:THR:CA 1:B-18:MET:C 1:B-19:THR:N 1 1.42 (1,34) 1:A-23:THR:N 1:A-23:THR:CA 1:B-18:NALC 1:B-19:THR:N 1 1.42 (1,14) 1:A-10:LE:N 1:A-10:LE:CA 1:A-18:TA-CA 1:B-18:TA-CA 1:B-19:TARCN 1:A-24:TA-CA 1:B-19:TARCN 1:A-24:TA-CA		1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	12	1.48
(1,34) 1:A-22:LEEN	(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	14	1.42
(1,120	(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	8	1.42
(1,243) 1:A-23:THR.N 1:A-23:THR.CA 1:A-23:THR.C 1:A-24:GLY.N 10 1.41 (1,228) 1:B-75:VAL.N 1:B:75:VAL.CA 1:B:75:VAL.C 1:B:76:GLU.N 9 1.4 (1,128) 1:B-10:ELEN 1:A-10:ELECA 1:A-10:ELECA 1:A-10:ELEN 20 1.4 (1,128) 1:B-9:ARG.N 1:B-9:ARG.CA 1:B-9:ARG.C 1:B-10:ELEN 20 1.4 (1,105) 1:A-67:ARG.C 1:A-68:LYS.N 1:A-68:LYS.CA 1:B-10:ELEN 20 1.4 (1,104) 1:A-67:ARG.N 1:A-67:ARG.CA 1:A-68:LYS.CA 1:A-68:LYS.CA 1:A-68:LYS.CA 1.4 (1,104) 1:A-67:ARG.N 1:A-67:ARG.CA 1:A-67:ARG.C 1:A-68:LYS.N 8 1.4 (1,130) 1:B-10:ELEN 1:B-10:ELE.CA 1:B-10:ELE.C 1:B-11:VAL.N 15 1.39 (1,130) 1:B-10:ELEN 1:B-10:ELE.CA 1:B-10:ELE.C 1:B-11:VAL.N 15 1.38 (1,28) 1:A-67:ARG.N 1:A-67-ARG.CA 1:A-67-ARG.C 1:A-68:LYS.N 16 1.38 (1,28) 1:A-67-ARG.N 1:A-67-ARG.CA 1:A-67-ARG.C 1:A-68:LYS.N 4 1.35 (1,104) 1:A-67-ARG.N 1:A-67-ARG.CA 1:A-67-ARG.C 1:A-68:LYS.N 4 1.35 (1,104) 1:B-16-HLEN 1:B-1	(' /	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	7	1.42
(1,23) 1:A-23:THR:N 1:A-23:THR:CA 1:A-23:THR:C 1:A-24:GIY:N 10 1.41 (1,228) 1:B:75:VAL:N 1:B:75:VAL:CA 1:B:75:VAL:C 1:B:76:GLU:N 9 1.4 (1,128) 1:B:95:RG:N 1:B:94RG:CA 1:B:94RG:C 1:A:10:VAL:N 8 1.4 (1,128) 1:B:94RG:N 1:B:94RG:CA 1:B:94RG:C 1:B:10:ILE:N 20 1.4 (1,105) 1:A:67:ARG:C 1:A:68:LYS:N 1:A:68:LYS:CA 1:A:68:LYS:C 2 1.4 (1,104) 1:A:67:ARG:N 1:A:67:ARG:CA 1:A:68:LYS:CA 1:A:68:LYS:C 2 1.4 (1,104) 1:A:67:ARG:N 1:A:67:ARG:CA 1:A:67:ARG:C 1:A:68:LYS:N 8 1.4 (1,130) 1:B:10:ILE:N 1:B:10:ILE:CA 1:B:10:ILE:C 1:B:11:VAL:N 1:5 1.39 (1,130) 1:B:10:ILE:N 1:B:10:ILE:CA 1:B:10:ILE:C 1:B:11:VAL:N 1:D:10:ILE:N 1:D:10:ILE	_ ` '	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	1	1.42
(1,128) 18-75-VAL-N 18-75-VAL-CA 18-75-VAL-C 18-76-GIU-N 9 1.4 (1,14) 1-A:10:ILE-N 1-A:10:ILE-CA 1-A:10:ILE-C 1-A:11:VAL-N 8 1.4 (1,128) 18-9:ARG-N 18-9:ARG-CA 1-A:10:ILE-C 1-A:11:VAL-N 8 1.4 (1,128) 18-9:ARG-N 18-9:ARG-CA 1-A:68:IVS-CA 1-A:68:IVS-C 2 1.4 (1,104) 1-A:67-ARG-C 1-A:68:IVS-N 1-A:68:IVS-N 2 1.4 (1,104) 1-A:67-ARG-N 1-A:67-ARG-CA 1-A:68:IVS-N 8 1.4 (1,130) 18-10:ILE-N 1-B:10:ILE-CA 1-B:10:ILE-C 1-B:11:VAL-N 15 1.39 (1,130) 1-B:10:ILE-N 1-B:10:ILE-CA 1-B:10:ILE-C 1-B:11:VAL-N 2 1.38 (1,130) 1-B:10:ILE-N 1-B:10:ILE-CA 1-B:10:ILE-C 1-B:11:VAL-N 2 1.38 (1,28) 1-A:26-ASN-N 1-A:26-ASN-CA 1-A:20-ASN-C 1-A:21:GLN-N 4 1.37 (1,171) 1-B:37-VAL-C 1-B:38:ILE-N 1-B:38:ILE-C 1-B:38:ILE-N 1-A:65-ARG-N 1-A:67-ARG-N 1-A:68-IVS-N 1-A:68-IVS-N 1-A:67-ARG-N 1-A:67-ARG-N 1-A:67-ARG-N 1-A:67-ARG-N 1-A:67-ARG-N 1-A:68-IVS-N 1-A:	_ ` '	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	10	1.41
(1,128) 1.B.9.4.R.G.N 1.B.9.4.R.G.C 1.B.9.4.R.G.C 1.B.10.1.L.E.N 2.0 1.4 (1,105) 12.4.67.4.R.G.C 1.4.68.1.Y.S.N 1.4.68.1.Y.S.N 1.4.68.1.Y.S.N 2. 1.4 (1,104) 12.4.67.4.R.G.C 1.4.68.1.Y.S.N 3. 1.4 (1,130) 1.B.10.1.L.E.N 1.B.10.1.L.E.C 1.B.10.1.L.E.C 1.B.11.Y.A.L.N 1.5 1.39 (1,130) 1.B.10.1.L.E.N 1.B.10.1.L.E.C 1.B.10.1.L.E.C 1.B.11.Y.A.L.N 1.5 1.39 (1,130) 1.B.10.1.L.E.N 1.B.10.1.L.E.C 1.B.10.1.L.E.C 1.B.11.Y.A.L.N 2. 1.38 (1,104) 1.4.67.4.R.G.N 1.4.67.4.R.G.C 1.4.67.4.R.G.C 1.4.68.1.Y.S.N 1.6. 1.38 (1,28) 1.4.20.4.S.N.N 1.4.20.4.S.N.C 1.4.20.4.S.N.C 1.4.21.G.L.N.N 4. 1.37 (1,171) 1.B.37.Y.A.L.C 1.B.38.L.L.U.N 1.B.38.L.L.U.C 1.B.38.L.L.U.C 1.2 1.35 (1,104) 1.2.67.4.R.G.N 1.4.67.4.R.G.C 1.4.67.4.R.G.C 1.4.68.1.Y.S.N 4. 1.35 (1,104) 1.4.67.4.R.G.N 1.4.67.4.R.G.C 1.B.36.T.H.R.C 1.B.36.T.H.	(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	9	1.4
(1,105)	(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	8	1.4
(1,104)	(1,128)	1:B:9:ARG:N	1:B:9:ARG:CA	1:B:9:ARG:C	1:B:10:ILE:N	20	1.4
(1,130) 1.B.10:1LEN 1.B.10:1LE:CA 1.B.10:1LE:C 1.B.11:VAL:N 15 1.39 (1,130) 1.B.10:1LE:N 1.B.10:1LE:CA 1.B.10:1LE:C 1.B.11:VAL:N 2 1.38 (1,130) 1.B.10:1LE:N 1.B.10:1LE:CA 1.B.10:1LE:C 1.B.11:VAL:N 2 1.38 (1,28) 1.A.667.ARG:N 1.A.667.ARG:CA 1.A.677.ARG:C 1.A.667.ARG:N 1.A.667.ARG:CA 1.A.20:ASN:C 1.A.21:GIN:N 4 1.37 (1,171) 1.B.37:VAL:C 1.B.38.LEU:N 1.B.38.LEU:CA 1.B.38.LEU:C 1.2 1.35 (1,104) 1.A.667.ARG:N 1.A.667.ARG:CA 1.A.667.ARG:CA 1.A.667.ARG:N 1.A.667.ARG:N 1.A.667.ARG:CA 1.A.667.ARG:CA 1.A.667.ARG:N 1.A.667.ARG:N 1.A.667.ARG:CA 1.A.667.ARG:C 1.A.668.LYS:N 4 1.35 (1,182) 1.B.467.THR:N 1.B.36.THR:CA 1.B.46.THR:C 1.B.47.CYS:N 8 1.34 (1,104) 1.A.67.ARG:N 1.A.20.ASN:CA 1.A.20.ASN:CA 1.A.20.ASN:CA 1.A.20.ASN:CA 1.A.20.ASN:CA 1.A.20.ASN:CA 1.A.20.ASN:N 1.A.20.ASN:CA 1.A.20.AS	(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	2	1.4
(1,130) 1:B:10:ILE:N 1:B:10:ILE:CA 1:B:10:ILE:C 1:B:11:VAL:N 2 1.38 (1,104) 1:A:67:ARG:N 1:A:67:ARG:CA 1:A:67:ARG:C 1:A:68:LYS:N 16 1.38 (1,28) 1:A:20:ASN:N 1:A:20:ASN:C 1:A:20:ASN	(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	8	1.4
(1,104) 1:A:67:ARG:N 1:A:67:ARG:CA 1:A:67:ARG:C 1:A:26:ARG:C 1:A:21:GLN:N 4 1.37 (1,171) 1:B:37:VAL:C 1:B:38:LEU:N 1:B:38:LEU:CA 1:CA 1:CA 1:CA 1:CA 1:CA 1:CA 1:CA 1	(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	15	1.39
(1,28)	(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	2	1.38
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(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	4	1.15
(1,171)	1:B:37:VAL:C	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	5	1.15
(1,85)	1:A:57:ASP:C	1:A:58:LYS:N	1:A:58:LYS:CA	1:A:58:LYS:C	8	1.14
(1,85)	1:A:57:ASP:C	1:A:58:LYS:N	1:A:58:LYS:CA	1:A:58:LYS:C	11	1.14
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	19	1.14
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	1	1.12
(1,55)	1:A:37:VAL:C	1:A:38:LEU:N	1:A:38:LEU:CA	1:A:38:LEU:C	9	1.12
(1,170)	1:B:37:VAL:N	1:B:37:VAL:CA	1:B:37:VAL:C	1:B:38:LEU:N	20	1.12
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	10	1.12
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	12	1.11
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	13	1.11
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	2	1.11
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	5	1.09
(1,27)	1:A:19:THR:C	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	20	1.08
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	7	1.08
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	18	1.07
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	15	1.06
(1,166)	1:B:35:THR:N	1:B:35:THR:CA	1:B:35:THR:C	1:B:36:ILE:N	4	1.06
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	5	1.06
(1,120)	1:B:5:LEU:N	1:B:5:LEU:CA	1:B:5:LEU:C	1:B:6:ALA:N	17	1.06
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	9	1.05
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	18	1.05
(1,206)	1:B:60:THR:N	1:B:60:THR:CA	1:B:60:THR:C	1:B:61:THR:N	15	1.04
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	18	1.04
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	13	1.04
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	17	1.04
(1,98)	1:A:64:ASP:N	1:A:64:ASP:CA	1:A:64:ASP:C	1:A:65:LYS:N	18	1.03
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	12	1.03
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	3	1.03
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	8	1.02
(1,128)	1:B:9:ARG:N	1:B:9:ARG:CA	1:B:9:ARG:C	1:B:10:ILE:N	19	1.02
(1,5)	1:A:5:LEU:C	1:A:6:ALA:N	1:A:6:ALA:CA	1:A:6:ALA:C	18	1.01
(1,5)	1:A:5:LEU:C	1:A:6:ALA:N	1:A:6:ALA:CA	1:A:6:ALA:C	20	1.01
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	13	1.01
(1,139)	1:B:17:GLY:C	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	2	1.01
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	18	1.0
(1,187)	1:B:48:ASN:C	1:B:49:LEU:N	1:B:49:LEU:CA	1:B:49:LEU:C	18	1.0
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	18	1.0
(1,139)	1:B:17:GLY:C	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	18	0.99
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	10	0.98
(1,66)	1:A:46:THR:N	1:A:46:THR:CA	1:A:46:THR:C	1:A:47:CYS:N	13	0.98
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	16	0.98
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	19	0.98
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	8	0.98
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	15	0.97
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	18	0.97
(1,204)	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	1:B:60:THR:N	11	0.97
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	13	0.97
(1,85)	1:A:57:ASP:C	1:A:58:LYS:N	1:A:58:LYS:CA	1:A:58:LYS:C	15	0.96
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	4	0.96
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	18	0.96



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Key	ed from previous p Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (o)
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	17	0.96
(1,128)	1:B:9:ARG:N	1:B:9:ARG:CA	1:B:9:ARG:C	1:B:10:ILE:N	15	0.96
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	3	0.95
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	7	0.94
(1,33)	1:A:22:ILE:C	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	20	0.94
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	15	0.94
(1,204)	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	1:B:60:THR:N	12	0.93
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	20	0.92
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	15	0.92
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	11	0.92
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	8	0.92
(1,121)	1:B:5:LEU:C	1:B:6:ALA:N	1:B:6:ALA:CA	1:B:6:ALA:C	4	0.92
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	10	0.91
(1,170)	1:B:37:VAL:N	1:B:37:VAL:CA	1:B:37:VAL:C	1:B:38:LEU:N	11	0.91
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	6	0.91
(1,85)	1:A:57:ASP:C	1:A:58:LYS:N	1:A:58:LYS:CA	1:A:58:LYS:C	7	0.9
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	5	0.9
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	7	0.89
(1,187)	1:B:48:ASN:C	1:B:49:LEU:N	1:B:49:LEU:CA	1:B:49:LEU:C	1	0.89
(1,144)	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	1:B:21:GLN:N	3	0.89
(1,187)	1:B:48:ASN:C	1:B:49:LEU:N	1:B:49:LEU:CA	1:B:49:LEU:C	17	0.88
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	1	0.88
(1,85)	1:A:57:ASP:C	1:A:58:LYS:N	1:A:58:LYS:CA	1:A:58:LYS:C	10	0.87
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	12	0.87
(1,206)	1:B:60:THR:N	1:B:60:THR:CA	1:B:60:THR:C	1:B:61:THR:N	14	0.87
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	6	0.87
(1,149)	1:B:22:ILE:C	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	17	0.87
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	16	0.86
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	13	0.86
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	7	0.86
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	7	0.86
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	11	0.85
(1,204)	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	1:B:60:THR:N	6	0.85
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	19	0.85
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	17	0.84
(1,12)	1:A:9:ARG:N	1:A:9:ARG:CA	1:A:9:ARG:C	1:A:10:ILE:N	12	0.83
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	12	0.83
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	8	0.82
(1,171)	1:B:37:VAL:C	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	9	0.82
(1,143)	1:B:19:THR:C	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	6	0.82
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	19	0.81
(1,187)	1:B:48:ASN:C	1:B:49:LEU:N	1:B:49:LEU:CA	1:B:49:LEU:C	10	0.81
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	4	0.8
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	12	0.8
(1,80)	1:A:53:VAL:N	1:A:53:VAL:CA	1:A:53:VAL:C	1:A:54:LYS:N	18	0.8
(1,187)	1:B:48:ASN:C	1:B:49:LEU:N	1:B:49:LEU:CA	1:B:49:LEU:C	16	0.8
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	16	0.79
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	7	0.79
(1,50)	1:A:35:THR:N	1:A:35:THR:CA	1:A:35:THR:C	1:A:36:ILE:N	13	0.79
(1,218)	1:B:66:LEU:N	1:B:66:LEU:CA	1:B:66:LEU:C	1:B:67:ARG:N	3	0.79
(1,212)	1:B:63:MET:N	1:B:63:MET:CA	1:B:63:MET:C	1:B:64:ASP:N	8	ed on next nage



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Key	ea from previous p Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (o)
(1,206)	1:B:60:THR:N	1:B:60:THR:CA	1:B:60:THR:C	1:B:61:THR:N	2	0.79
(1,172)	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	1:B:39:ASN:N	19	0.79
(1,171)	1:B:37:VAL:C	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	2	0.79
(1,171)	1:B:37:VAL:C	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	19	0.79
(1,206)	1:B:60:THR:N	1:B:60:THR:CA	1:B:60:THR:C	1:B:61:THR:N	11	0.78
(1,144)	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	1:B:21:GLN:N	1	0.78
(1,4)	1:A:5:LEU:N	1:A:5:LEU:CA	1:A:5:LEU:C	1:A:6:ALA:N	12	0.77
(1,206)	1:B:60:THR:N	1:B:60:THR:CA	1:B:60:THR:C	1:B:61:THR:N	18	0.77
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	4	0.77
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	19	0.76
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	5	0.76
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	10	0.76
(1,66)	1:A:46:THR:N	1:A:46:THR:CA	1:A:46:THR:C	1:A:47:CYS:N	6	0.75
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	16	0.75
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	10	0.75
(1,196)	1:B:53:VAL:N	1:B:53:VAL:CA	1:B:53:VAL:C	1:B:54:LYS:N	11	0.75
(1,196)	1:B:53:VAL:N	1:B:53:VAL:CA	1:B:53:VAL:C	1:B:54:LYS:N	19	0.75
(1,28)	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	1:A:21:GLN:N	19	0.74
(1,128)	1:B:9:ARG:N	1:B:9:ARG:CA	1:B:9:ARG:C	1:B:10:ILE:N	6	0.74
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	13	0.73
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	5	0.73
(1,28)	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	1:A:21:GLN:N	15	0.73
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	20	0.73
(1,27)	1:A:19:THR:C	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	6	0.72
(1,226)	1:B:74:THR:N	1:B:74:THR:CA	1:B:74:THR:C	1:B:75:VAL:N	17	0.72
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	19	0.71
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	4	0.71
(1,182)	1:B:46:THR:N	1:B:46:THR:CA	1:B:46:THR:C	1:B:47:CYS:N	10	0.71
(1,28)	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	1:A:21:GLN:N	2	0.7
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	8	0.7
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	15	0.7
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	19	0.69
(1,226)	1:B:74:THR:N	1:B:74:THR:CA	1:B:74:THR:C	1:B:75:VAL:N	12	0.69
(1,187)	1:B:48:ASN:C	1:B:49:LEU:N	1:B:49:LEU:CA	1:B:49:LEU:C	4	0.69
(1,187)	1:B:48:ASN:C	1:B:49:LEU:N	1:B:49:LEU:CA	1:B:49:LEU:C	9	0.69
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	12	0.69
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	3	0.68
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	10	0.68
(1,28)	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	1:A:21:GLN:N	5	0.68
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	15	0.68
(1,174)	1:B:39:ASN:N	1:B:39:ASN:CA	1:B:39:ASN:C	1:B:40:ALA:N	4	0.68
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	3	0.68
(1,226)	1:B:74:THR:N	1:B:74:THR:CA	1:B:74:THR:C	1:B:75:VAL:N	4	0.67
(1,187)	1:B:48:ASN:C	1:B:49:LEU:N	1:B:49:LEU:CA	1:B:49:LEU:C	5	0.67
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	13	0.67
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	17	0.66
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	9	0.66
(1,31)	1:A:21:GLN:C	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	20	0.66
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	5	0.66
(1,182)	1:B:46:THR:N	1:B:46:THR:CA	1:B:46:THR:C	1:B:47:CYS:N	15	0.66
(1,166)	1:B:35:THR:N	1:B:35:THR:CA	1:B:35:THR:C	1:B:36:ILE:N	2	0.66



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Key	ea from previous p Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (o)
(1,128)	1:B:9:ARG:N	1:B:9:ARG:CA	1:B:9:ARG:C	1:B:10:ILE:N	18	0.66
(1,33)	1:A:22:ILE:C	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	19	0.64
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	12	0.64
(1,166)	1:B:35:THR:N	1:B:35:THR:CA	1:B:35:THR:C	1:B:36:ILE:N	9	0.64
(1,28)	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	1:A:21:GLN:N	3	0.63
(1,224)	1:B:69:VAL:N	1:B:69:VAL:CA	1:B:69:VAL:C	1:B:70:GLN:N	14	0.63
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	20	0.63
(1,144)	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	1:B:21:GLN:N	7	0.63
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	14	0.63
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	15	0.62
(1,87)	1:A:58:LYS:C	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	16	0.62
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	2	0.62
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	5	0.62
(1,166)	1:B:35:THR:N	1:B:35:THR:CA	1:B:35:THR:C	1:B:36:ILE:N	11	0.61
(1,120)	1:B:5:LEU:N	1:B:5:LEU:CA	1:B:5:LEU:C	1:B:6:ALA:N	16	0.61
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	4	0.6
(1,187)	1:B:48:ASN:C	1:B:49:LEU:N	1:B:49:LEU:CA	1:B:49:LEU:C	8	0.6
(1,171)	1:B:37:VAL:C	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	17	0.6
(1,85)	1:A:57:ASP:C	1:A:58:LYS:N	1:A:58:LYS:CA	1:A:58:LYS:C	18	0.59
(1,4)	1:A:5:LEU:N	1:A:5:LEU:CA	1:A:5:LEU:C	1:A:6:ALA:N	13	0.59
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	16	0.59
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	15	0.59
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	1	0.58
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	6	0.58
(1,121)	1:B:5:LEU:C	1:B:6:ALA:N	1:B:6:ALA:CA	1:B:6:ALA:C	8	0.58
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	6	0.56
(1,27)	1:A:19:THR:C	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	13	0.56
(1,152)	1:B:24:GLY:N	1:B:24:GLY:CA	1:B:24:GLY:C	1:B:25:VAL:N	15	0.56
(1,144)	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	1:B:21:GLN:N	11	0.56
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	3	0.55
(1,28)	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	1:A:21:GLN:N	1	0.54
(1,166)	1:B:35:THR:N	1:B:35:THR:CA	1:B:35:THR:C	1:B:36:ILE:N	14	0.54
(1,178)	1:B:44:ILE:N	1:B:44:ILE:CA	1:B:44:ILE:C	1:B:45:PHE:N	12	0.53
(1,143)	1:B:19:THR:C	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	1	0.53
(1,90)	1:A:60:THR:N	1:A:60:THR:CA	1:A:60:THR:C	1:A:61:THR:N	4	0.52
(1,187)	1:B:48:ASN:C	1:B:49:LEU:N	1:B:49:LEU:CA	1:B:49:LEU:C	7	0.52
(1,144)	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	1:B:21:GLN:N	20	0.52
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	14	0.52
(1,69)	1:A:47:CYS:C	1:A:48:ASN:N	1:A:48:ASN:CA	1:A:48:ASN:C	2	0.51
(1,4)	1:A:5:LEU:N	1:A:5:LEU:CA	1:A:5:LEU:C	1:A:6:ALA:N	1	0.51
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	2	0.51
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	20	0.51
(1,143)	1:B:19:THR:C	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	9	0.51
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	19	0.51
(1,57)	1:A:38:LEU:C	1:A:39:ASN:N	1:A:39:ASN:CA	1:A:39:ASN:C	18	0.5
(1,23)	1:A:17:GLY:C	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	6	0.5
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	9	0.5
(1,80)	1:A:53:VAL:N	1:A:53:VAL:CA	1:A:53:VAL:C	1:A:54:LYS:N	1	0.49
(1,143)	1:B:19:THR:C	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	12	0.49
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	15	0.49
(1,121)	1:B:5:LEU:C	1:B:6:ALA:N	1:B:6:ALA:CA	1:B:6:ALA:C	1	0.49
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Key	ea from previous p Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (o)
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	8	0.48
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	19	0.48
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	2	0.47
(1,4)	1:A:5:LEU:N	1:A:5:LEU:CA	1:A:5:LEU:C	1:A:6:ALA:N	17	0.47
(1,170)	1:B:37:VAL:N	1:B:37:VAL:CA	1:B:37:VAL:C	1:B:38:LEU:N	18	0.47
(1,116)	1:A:77:ARG:N	1:A:77:ARG:CA	1:A:77:ARG:C	1:A:78:LEU:N	8	0.47
(1,211)	1:B:62:LEU:C	1:B:63:MET:N	1:B:63:MET:CA	1:B:63:MET:C	19	0.46
(1,204)	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	1:B:60:THR:N	2	0.46
(1,172)	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	1:B:39:ASN:N	10	0.46
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	11	0.46
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	3	0.45
(1,5)	1:A:5:LEU:C	1:A:6:ALA:N	1:A:6:ALA:CA	1:A:6:ALA:C	17	0.45
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	10	0.45
(1,206)	1:B:60:THR:N	1:B:60:THR:CA	1:B:60:THR:C	1:B:61:THR:N	4	0.45
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	2	0.45
(1,143)	1:B:19:THR:C	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	3	0.45
(1,55)	1:A:37:VAL:C	1:A:38:LEU:N	1:A:38:LEU:CA	1:A:38:LEU:C	13	0.44
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	11	0.44
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	13	0.44
(1,27)	1:A:19:THR:C	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	19	0.44
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	15	0.44
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	16	0.43
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	15	0.43
(1,187)	1:B:48:ASN:C	1:B:49:LEU:N	1:B:49:LEU:CA	1:B:49:LEU:C	14	0.43
(1,143)	1:B:19:THR:C	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	2	0.43
(1,143)	1:B:19:THR:C	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	7	0.43
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	5	0.42
(1,50)	1:A:35:THR:N	1:A:35:THR:CA	1:A:35:THR:C	1:A:36:ILE:N	1	0.42
(1,204)	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	1:B:60:THR:N	10	0.42
(1,187)	1:B:48:ASN:C	1:B:49:LEU:N	1:B:49:LEU:CA	1:B:49:LEU:C	20	0.42
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	9	0.42
(1,48)	1:A:33:ILE:N	1:A:33:ILE:CA	1:A:33:ILE:C	1:A:34:ARG:N	7	0.41
(1,144)	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	1:B:21:GLN:N	17	0.41
(1,128)	1:B:9:ARG:N	1:B:9:ARG:CA	1:B:9:ARG:C	1:B:10:ILE:N	8	0.41
(1,50)	1:A:35:THR:N	1:A:35:THR:CA	1:A:35:THR:C	1:A:36:ILE:N	8	0.4
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	7	0.4
(1,36)	1:A:24:GLY:N	1:A:24:GLY:CA	1:A:24:GLY:C	1:A:25:VAL:N	11	0.4
(1,23)	1:A:17:GLY:C	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	13	0.4
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	3	0.4
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	11	0.4
(1,114)	1:A:76:GLU:N	1:A:76:GLU:CA	1:A:76:GLU:C	1:A:77:ARG:N	8	0.4
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	6	0.4
(1,85)	1:A:57:ASP:C	1:A:58:LYS:N	1:A:58:LYS:CA	1:A:58:LYS:C	2	0.39
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	12	0.39
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	20	0.39
(1,5)	1:A:5:LEU:C	1:A:6:ALA:N	1:A:6:ALA:CA	1:A:6:ALA:C	1	0.39
(1,27)	1:A:19:THR:C	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	3	0.39
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	7	0.39
(1,27)	1:A:19:THR:C	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	14	0.38
(1,152)	1:B:24:GLY:N	1:B:24:GLY:CA	1:B:24:GLY:C	1:B:25:VAL:N	5	0.38
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	6 Continu	0.38



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Key	ed from previous p Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (o)
(1,85)	1:A:57:ASP:C	1:A:58:LYS:N	1:A:58:LYS:CA	1:A:58:LYS:C	16	0.37
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	14	0.37
(1,70)	1:A:48:ASN:N	1:A:48:ASN:CA	1:A:48:ASN:C	1:A:49:LEU:N	12	0.37
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	6	0.37
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	1	0.37
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	17	0.36
(1,62)	1:A:44:ILE:N	1:A:44:ILE:CA	1:A:44:ILE:C	1:A:45:PHE:N	20	0.36
(1,214)	1:B:64:ASP:N	1:B:64:ASP:CA	1:B:64:ASP:C	1:B:65:LYS:N	3	0.36
(1,204)	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	1:B:60:THR:N	19	0.36
(1,182)	1:B:46:THR:N	1:B:46:THR:CA	1:B:46:THR:C	1:B:47:CYS:N	13	0.36
(1,139)	1:B:17:GLY:C	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	13	0.36
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	8	0.36
(1,110)	1:A:74:THR:N	1:A:74:THR:CA	1:A:74:THR:C	1:A:75:VAL:N	17	0.36
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	6	0.35
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	7	0.35
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	9	0.35
(1,204)	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	1:B:60:THR:N	7	0.35
(1,166)	1:B:35:THR:N	1:B:35:THR:CA	1:B:35:THR:C	1:B:36:ILE:N	19	0.35
(1,149)	1:B:22:ILE:C	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	9	0.35
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	18	0.34
(1,152)	1:B:24:GLY:N	1:B:24:GLY:CA	1:B:24:GLY:C	1:B:25:VAL:N	3	0.34
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	11	0.34
(1,27)	1:A:19:THR:C	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	1	0.33
(1,212)	1:B:63:MET:N	1:B:63:MET:CA	1:B:63:MET:C	1:B:64:ASP:N	9	0.33
(1,203)	1:B:58:LYS:C	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	6	0.33
(1,144)	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	1:B:21:GLN:N	5	0.33
(1,85)	1:A:57:ASP:C	1:A:58:LYS:N	1:A:58:LYS:CA	1:A:58:LYS:C	12	0.32
(1,27)	1:A:19:THR:C	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	5	0.32
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	8	0.32
(1,149)	1:B:22:ILE:C	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	8	0.32
(1,128)	1:B:9:ARG:N	1:B:9:ARG:CA	1:B:9:ARG:C	1:B:10:ILE:N	2	0.32
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	4	0.31
(1,204)	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	1:B:60:THR:N	5	0.31
(1,170)	1:B:37:VAL:N	1:B:37:VAL:CA	1:B:37:VAL:C	1:B:38:LEU:N	7	0.31
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	11	0.31
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	9	0.3
(1,80)	1:A:53:VAL:N	1:A:53:VAL:CA	1:A:53:VAL:C	1:A:54:LYS:N	10	0.3
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	1	0.3
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	14	0.3
(1,33)	1:A:22:ILE:C	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	9	0.3
(1,28)	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	1:A:21:GLN:N	10	0.3
(1,196)	1:B:53:VAL:N	1:B:53:VAL:CA	1:B:53:VAL:C	1:B:54:LYS:N	2	0.3
(1,152)	1:B:24:GLY:N	1:B:24:GLY:CA	1:B:24:GLY:C	1:B:25:VAL:N	18	0.3
(1,144)	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	1:B:21:GLN:N	6	0.3
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	19	0.29
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	14	0.28
(1,224)	1:B:69:VAL:N	1:B:69:VAL:CA	1:B:69:VAL:C	1:B:70:GLN:N	7	0.28
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	10	0.28
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	19	0.28
(1,66)	1:A:46:THR:N	1:A:46:THR:CA	1:A:46:THR:C	1:A:47:CYS:N	17	0.27
(1,4)	1:A:5:LEU:N	1:A:5:LEU:CA	1:A:5:LEU:C	1:A:6:ALA:N	8	0.27



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Key	ed from previous p Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (o)
(1,196)	1:B:53:VAL:N	1:B:53:VAL:CA	1:B:53:VAL:C	1:B:54:LYS:N	5	0.27
(1,187)	1:B:48:ASN:C	1:B:49:LEU:N	1:B:49:LEU:CA	1:B:49:LEU:C	15	0.27
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	8	0.27
(1,59)	1:A:39:ASN:C	1:A:40:ALA:N	1:A:40:ALA:CA	1:A:40:ALA:C	10	0.26
(1,50)	1:A:35:THR:N	1:A:35:THR:CA	1:A:35:THR:C	1:A:36:ILE:N	9	0.26
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	12	0.26
(1,144)	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	1:B:21:GLN:N	4	0.26
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	20	0.25
(1,211)	1:B:62:LEU:C	1:B:63:MET:N	1:B:63:MET:CA	1:B:63:MET:C	16	0.25
(1,206)	1:B:60:THR:N	1:B:60:THR:CA	1:B:60:THR:C	1:B:61:THR:N	7	0.25
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	9	0.25
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	5	0.24
(1,50)	1:A:35:THR:N	1:A:35:THR:CA	1:A:35:THR:C	1:A:36:ILE:N	18	0.24
(1,204)	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	1:B:60:THR:N	13	0.24
(1,197)	1:B:53:VAL:C	1:B:54:LYS:N	1:B:54:LYS:CA	1:B:54:LYS:C	4	0.24
(1,143)	1:B:19:THR:C	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	17	0.24
(1,102)	1:A:66:LEU:N	1:A:66:LEU:CA	1:A:66:LEU:C	1:A:67:ARG:N	5	0.24
(1,70)	1:A:48:ASN:N	1:A:48:ASN:CA	1:A:48:ASN:C	1:A:49:LEU:N	15	0.23
(1,66)	1:A:46:THR:N	1:A:46:THR:CA	1:A:46:THR:C	1:A:47:CYS:N	4	0.23
(1,36)	1:A:24:GLY:N	1:A:24:GLY:CA	1:A:24:GLY:C	1:A:25:VAL:N	9	0.23
(1,226)	1:B:74:THR:N	1:B:74:THR:CA	1:B:74:THR:C	1:B:75:VAL:N	6	0.23
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	5	0.23
(1,142)	1:B:19:THR:N	1:B:19:THR:CA	1:B:19:THR:C	1:B:20:ASN:N	20	0.23
(1,5)	1:A:5:LEU:C	1:A:6:ALA:N	1:A:6:ALA:CA	1:A:6:ALA:C	15	0.22
(1,230)	1:B:76:GLU:N	1:B:76:GLU:CA	1:B:76:GLU:C	1:B:77:ARG:N	6	0.22
(1,170)	1:B:37:VAL:N	1:B:37:VAL:CA	1:B:37:VAL:C	1:B:38:LEU:N	8	0.22
(1,166)	1:B:35:THR:N	1:B:35:THR:CA	1:B:35:THR:C	1:B:36:ILE:N	13	0.22
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	18	0.22
(1,145)	1:B:20:ASN:C	1:B:21:GLN:N	1:B:21:GLN:CA	1:B:21:GLN:C	13	0.22
(1,120)	1:B:5:LEU:N	1:B:5:LEU:CA	1:B:5:LEU:C	1:B:6:ALA:N	20	0.22
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	9	0.22
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	11	0.21
(1,5)	1:A:5:LEU:C	1:A:6:ALA:N	1:A:6:ALA:CA	1:A:6:ALA:C	8	0.21
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	15	0.21
(1,218)	1:B:66:LEU:N	1:B:66:LEU:CA	1:B:66:LEU:C	1:B:67:ARG:N	5	0.21
(1,120)	1:B:5:LEU:N	1:B:5:LEU:CA	1:B:5:LEU:C	1:B:6:ALA:N	1	0.21
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	19	0.2
(1,144)	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	1:B:21:GLN:N	16	0.2
(1,80)	1:A:53:VAL:N	1:A:53:VAL:CA	1:A:53:VAL:C	1:A:54:LYS:N	2	0.19
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	13	0.19
(1,4)	1:A:5:LEU:N	1:A:5:LEU:CA	1:A:5:LEU:C	1:A:6:ALA:N	16	0.19
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	13	0.19
(1,114)	1:A:76:GLU:N	1:A:76:GLU:CA	1:A:76:GLU:C	1:A:77:ARG:N	18	0.19
(1,31)	1:A:21:GLN:C	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	19	0.18
(1,206)	1:B:60:THR:N	1:B:60:THR:CA	1:B:60:THR:C	1:B:61:THR:N	19	0.18
(1,185)	1:B:47:CYS:C	1:B:48:ASN:N	1:B:48:ASN:CA	1:B:48:ASN:C	20	0.18
(1,5)	1:A:5:LEU:C	1:A:6:ALA:N	1:A:6:ALA:CA	1:A:6:ALA:C	9	0.17
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	2	0.17
(1,153)	1:B:24:GLY:C	1:B:25:VAL:N	1:B:25:VAL:CA	1:B:25:VAL:C	14	0.17
(1,144)	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	1:B:21:GLN:N	9	0.17
(1,90)	1:A:60:THR:N	1:A:60:THR:CA	1:A:60:THR:C	1:A:61:THR:N	20	0.16



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Key	$rac{\textbf{Atom-1}}{\mathbf{Atom-1}}$	Atom-2	Atom-3	Atom-4	Model	Violation (o)
(1,226)	1:B:74:THR:N	1:B:74:THR:CA	1:B:74:THR:C	1:B:75:VAL:N	18	0.16
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	11	0.16
(1,186)	1:B:48:ASN:N	1:B:48:ASN:CA	1:B:48:ASN:C	1:B:49:LEU:N	10	0.16
(1,90)	1:A:60:THR:N	1:A:60:THR:CA	1:A:60:THR:C	1:A:61:THR:N	17	0.15
(1,48)	1:A:33:ILE:N	1:A:33:ILE:CA	1:A:33:ILE:C	1:A:34:ARG:N	11	0.15
(1,4)	1:A:5:LEU:N	1:A:5:LEU:CA	1:A:5:LEU:C	1:A:6:ALA:N	20	0.15
(1,28)	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	1:A:21:GLN:N	17	0.15
(1,204)	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	1:B:60:THR:N	3	0.15
(1,204)	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	1:B:60:THR:N	15	0.15
(1,186)	1:B:48:ASN:N	1:B:48:ASN:CA	1:B:48:ASN:C	1:B:49:LEU:N	18	0.15
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	3	0.14
(1,27)	1:A:19:THR:C	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	8	0.14
(1,187)	1:B:48:ASN:C	1:B:49:LEU:N	1:B:49:LEU:CA	1:B:49:LEU:C	3	0.14
(1,147)	1:B:21:GLN:C	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	17	0.14
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	15	0.14
(1,85)	1:A:57:ASP:C	1:A:58:LYS:N	1:A:58:LYS:CA	1:A:58:LYS:C	4	0.13
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	12	0.13
(1,204)	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	1:B:60:THR:N	17	0.13
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	2	0.12
(1,184)	1:B:47:CYS:N	1:B:47:CYS:CA	1:B:47:CYS:C	1:B:48:ASN:N	5	0.12
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	17	0.12
(1,90)	1:A:60:THR:N	1:A:60:THR:CA	1:A:60:THR:C	1:A:61:THR:N	16	0.11
(1,218)	1:B:66:LEU:N	1:B:66:LEU:CA	1:B:66:LEU:C	1:B:67:ARG:N	15	0.11
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	15	0.11
(1,5)	1:A:5:LEU:C	1:A:6:ALA:N	1:A:6:ALA:CA	1:A:6:ALA:C	16	0.1
(1,33)	1:A:22:ILE:C	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1	0.1
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	5	0.1
(1,210)	1:B:62:LEU:N	1:B:62:LEU:CA	1:B:62:LEU:C	1:B:63:MET:N	6	0.1
(1,143)	1:B:19:THR:C	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	5	0.1
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	14	0.1
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	4	0.1
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	18	0.09
(1,57)	1:A:38:LEU:C	1:A:39:ASN:N	1:A:39:ASN:CA	1:A:39:ASN:C	1	0.09
(1,185)	1:B:47:CYS:C	1:B:48:ASN:N	1:B:48:ASN:CA	1:B:48:ASN:C	18	0.09
(1,174)	1:B:39:ASN:N	1:B:39:ASN:CA	1:B:39:ASN:C	1:B:40:ALA:N	10	0.09
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	19	0.09
(1,70)	1:A:48:ASN:N	1:A:48:ASN:CA	1:A:48:ASN:C	1:A:49:LEU:N	16	0.08
(1,50)	1:A:35:THR:N	1:A:35:THR:CA	1:A:35:THR:C	1:A:36:ILE:N	17	0.08
(1,39)	1:A:25:VAL:C	1:A:26:ILE:N	1:A:26:ILE:CA	1:A:26:ILE:C	17	0.08
(1,212)	1:B:63:MET:N	1:B:63:MET:CA	1:B:63:MET:C	1:B:64:ASP:N	10	0.08
(1,28)	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	1:A:21:GLN:N	8	0.07
(1,212)	1:B:63:MET:N	1:B:63:MET:CA	1:B:63:MET:C	1:B:64:ASP:N	14	0.07
(1,96)	1:A:63:MET:N	1:A:63:MET:CA	1:A:63:MET:C	1:A:64:ASP:N	13	0.06
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	15	0.06
(1,66)	1:A:46:THR:N	1:A:46:THR:CA	1:A:46:THR:C	1:A:47:CYS:N	7	0.06
(1,27)	1:A:19:THR:C	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	4	0.06
(1,27)	1:A:19:THR:C	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	12	0.06
(1,145)	1:B:20:ASN:C	1:B:21:GLN:N	1:B:21:GLN:CA	1:B:21:GLN:C	8	0.06
(1,120)	1:B:5:LEU:N	1:B:5:LEU:CA	1:B:5:LEU:C	1:B:6:ALA:N	13	0.06
(1,102)	1:A:66:LEU:N	1:A:66:LEU:CA	1:A:66:LEU:C	1:A:67:ARG:N	9	0.06
(1,80)	1:A:53:VAL:N	1:A:53:VAL:CA	1:A:53:VAL:C	1:A:54:LYS:N	5	0.05



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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (\circ)
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	5	0.05
(1,187)	1:B:48:ASN:C	1:B:49:LEU:N	1:B:49:LEU:CA	1:B:49:LEU:C	12	0.04
(1,166)	1:B:35:THR:N	1:B:35:THR:CA	1:B:35:THR:C	1:B:36:ILE:N	12	0.04
(1,143)	1:B:19:THR:C	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	15	0.04
(1,143)	1:B:19:THR:C	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	20	0.04
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	6	0.04
(1,204)	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	1:B:60:THR:N	18	0.03
(1,139)	1:B:17:GLY:C	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	15	0.03
(1,96)	1:A:63:MET:N	1:A:63:MET:CA	1:A:63:MET:C	1:A:64:ASP:N	12	0.02
(1,232)	1:B:77:ARG:N	1:B:77:ARG:CA	1:B:77:ARG:C	1:B:78:LEU:N	8	0.02
(1,211)	1:B:62:LEU:C	1:B:63:MET:N	1:B:63:MET:CA	1:B:63:MET:C	18	0.02
(1,149)	1:B:22:ILE:C	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	18	0.02
(1,143)	1:B:19:THR:C	1:B:20:ASN:N	1:B:20:ASN:CA	1:B:20:ASN:C	11	0.02
(1,97)	1:A:63:MET:C	1:A:64:ASP:N	1:A:64:ASP:CA	1:A:64:ASP:C	14	0.01
(1,50)	1:A:35:THR:N	1:A:35:THR:CA	1:A:35:THR:C	1:A:36:ILE:N	6	0.01

