



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 3, 2023 – 09:48 PM EDT

PDB ID : 7LOI  
BMRB ID : 30856  
Title : Model of the HIV-1 gp41 membrane-proximal external region, transmembrane domain and cytoplasmic tail  
Authors : Piai, A.; Fu, Q.; Sharp, A.K.; Bigli, B.; Brown, A.M.; Chou, J.J.  
Deposited on : 2021-02-10

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.33

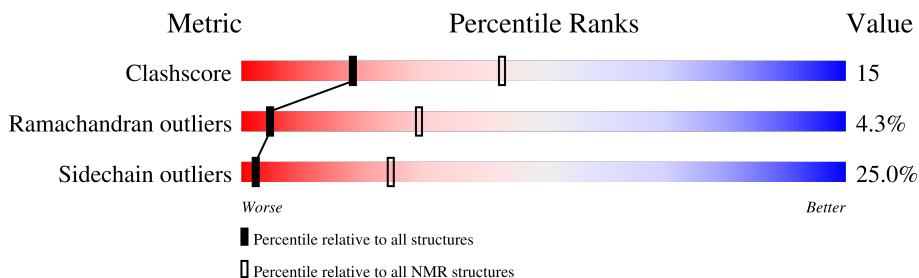
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 8%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	197	
1	B	197	
1	C	197	

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:660-A:716, A:739-A:856, B:660-B:716, B:739-B:856, C:660-C:716, C:739-C:856 (525)	1.58	4

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

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

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

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8940 atoms, of which 4563 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	175	2980	949	1521	267	243	0
1	B	175	2980	949	1521	267	243	0
1	C	175	2980	949	1521	267	243	0

There are 27 discrepancies between the modelled and reference sequences:

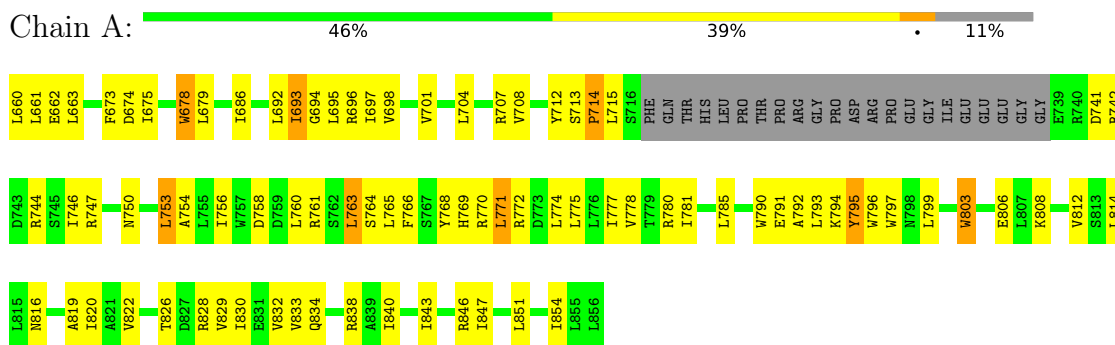
Chain	Residue	Modelled	Actual	Comment	Reference
A	674	ASP	ASN	conflict	UNP A0A386YSI0
A	683	ARG	LYS	conflict	UNP A0A386YSI0
A	687	ILE	MET	conflict	UNP A0A386YSI0
A	691	SER	GLY	conflict	UNP A0A386YSI0
A	693	ILE	VAL	conflict	UNP A0A386YSI0
A	704	LEU	ILE	conflict	UNP A0A386YSI0
A	764	SER	CYS	engineered mutation	UNP A0A386YSI0
A	823	GLY	ALA	engineered mutation	UNP A0A386YSI0
A	837	SER	CYS	engineered mutation	UNP A0A386YSI0
B	674	ASP	ASN	conflict	UNP A0A386YSI0
B	683	ARG	LYS	conflict	UNP A0A386YSI0
B	687	ILE	MET	conflict	UNP A0A386YSI0
B	691	SER	GLY	conflict	UNP A0A386YSI0
B	693	ILE	VAL	conflict	UNP A0A386YSI0
B	704	LEU	ILE	conflict	UNP A0A386YSI0
B	764	SER	CYS	engineered mutation	UNP A0A386YSI0
B	823	GLY	ALA	engineered mutation	UNP A0A386YSI0
B	837	SER	CYS	engineered mutation	UNP A0A386YSI0
C	674	ASP	ASN	conflict	UNP A0A386YSI0
C	683	ARG	LYS	conflict	UNP A0A386YSI0
C	687	ILE	MET	conflict	UNP A0A386YSI0
C	691	SER	GLY	conflict	UNP A0A386YSI0
C	693	ILE	VAL	conflict	UNP A0A386YSI0
C	704	LEU	ILE	conflict	UNP A0A386YSI0
C	764	SER	CYS	engineered mutation	UNP A0A386YSI0
C	823	GLY	ALA	engineered mutation	UNP A0A386YSI0
C	837	SER	CYS	engineered mutation	UNP A0A386YSI0

## 4 Residue-property plots [i](#)

### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Transmembrane protein gp41

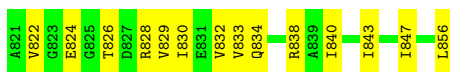


- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41





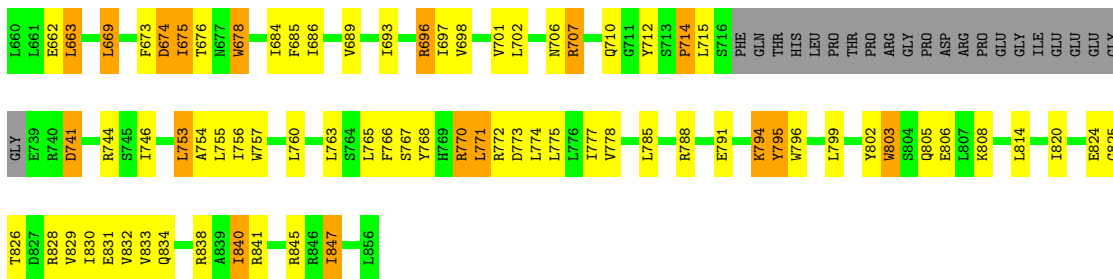
## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

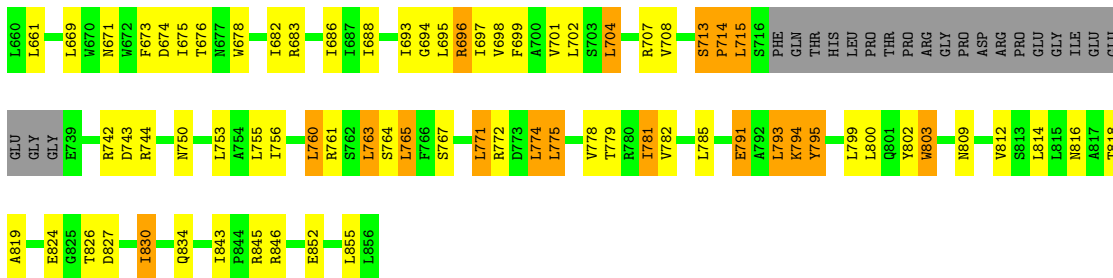
- Molecule 1: Transmembrane protein gp41

Chain A: 51% 29% 9% 11%



- Molecule 1: Transmembrane protein gp41

Chain B: 52% 28% 9% 11%



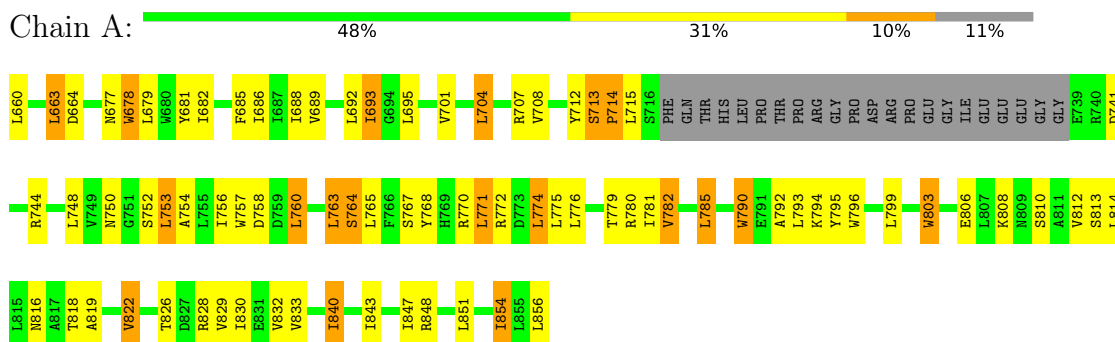
- Molecule 1: Transmembrane protein gp41

Chain C: 45% 34% 10% 11%

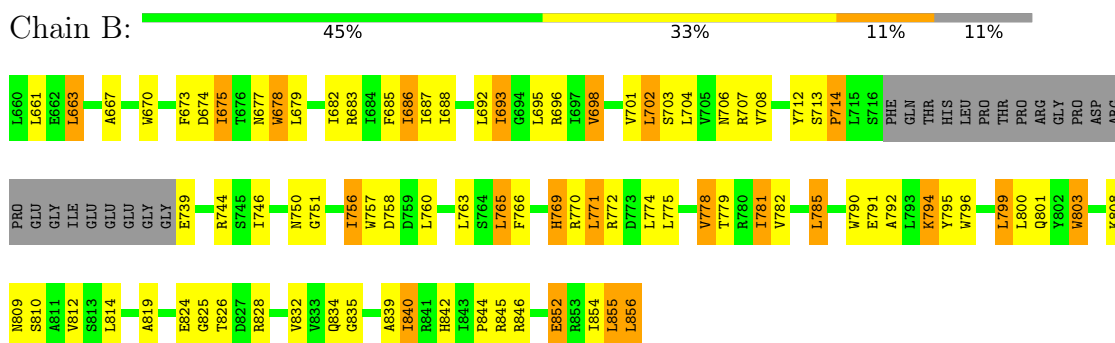


### 4.2.2 Score per residue for model 2

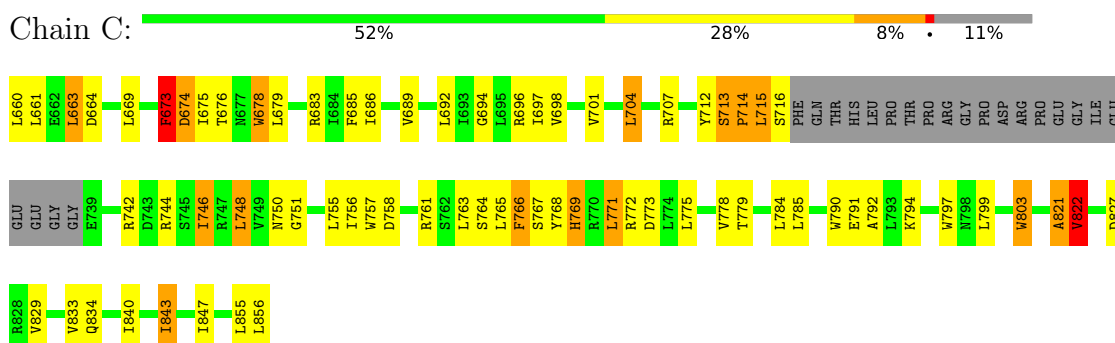
- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41

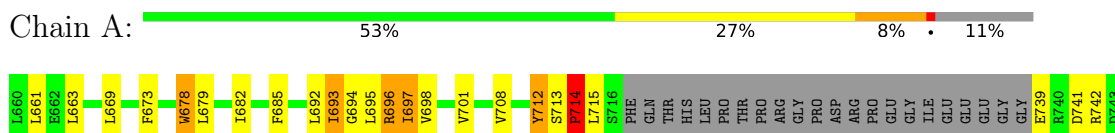


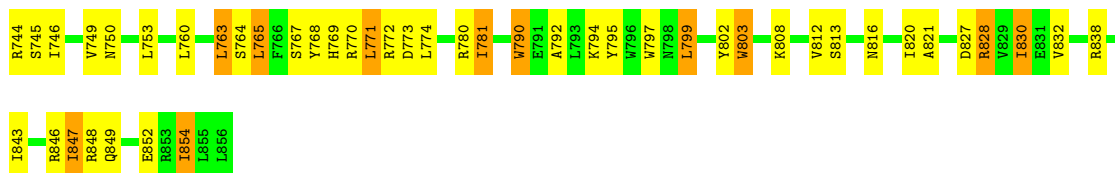
- Molecule 1: Transmembrane protein gp41



### 4.2.3 Score per residue for model 3

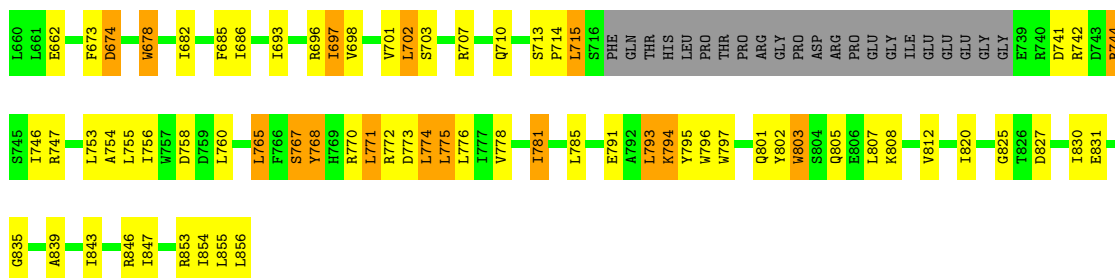
- Molecule 1: Transmembrane protein gp41





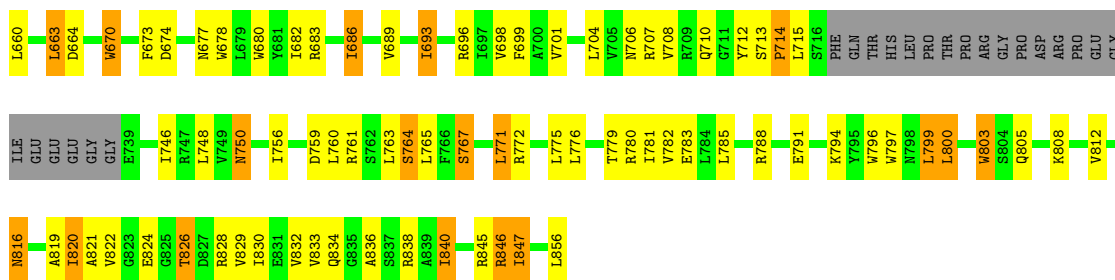
- Molecule 1: Transmembrane protein gp41

Chain B: 53% 27% 8% 11%



- Molecule 1: Transmembrane protein gp41

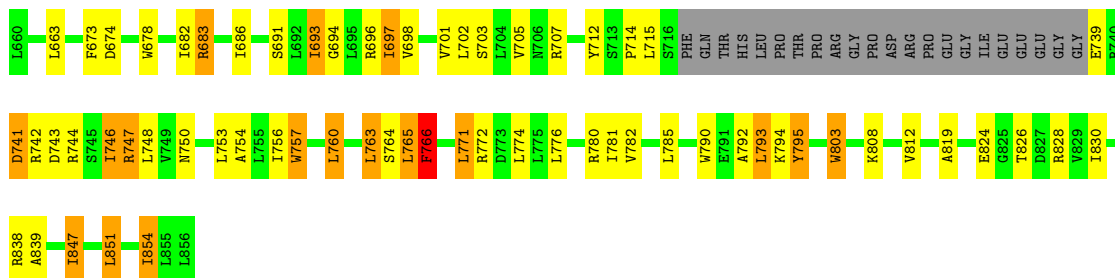
Chain C: 49% 31% 9% 11%



#### 4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Transmembrane protein gp41

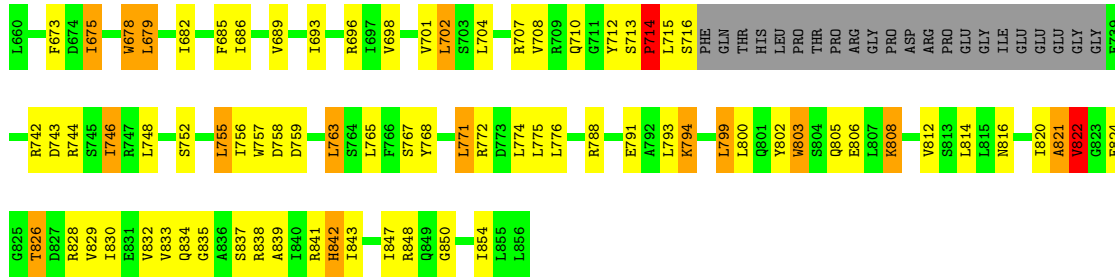
Chain A: 56% 24% 9% 11%



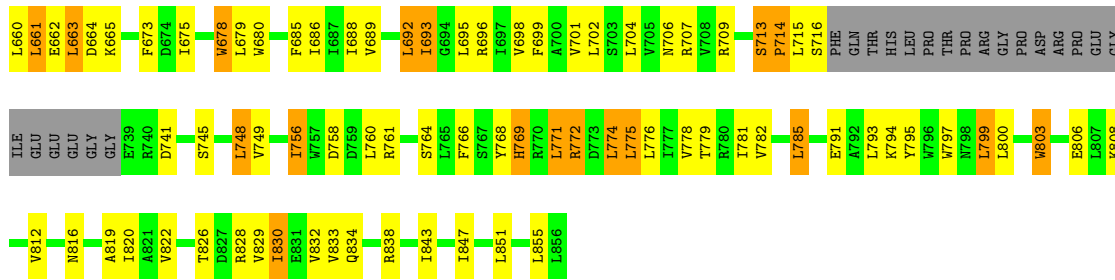
- Molecule 1: Transmembrane protein gp41

Chain B: 49% 31% 8% 11%



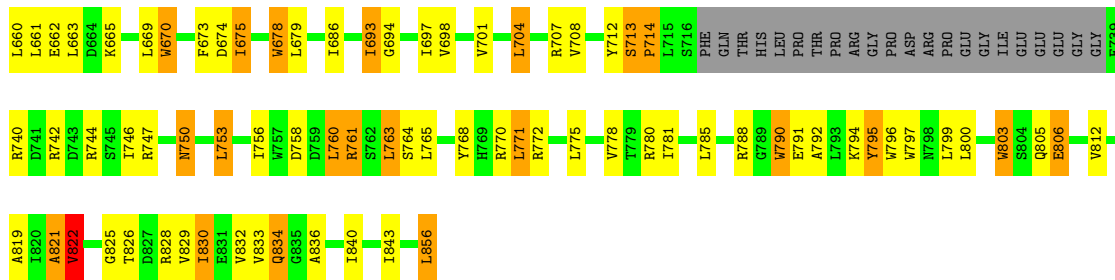


• Molecule 1: Transmembrane protein gp41

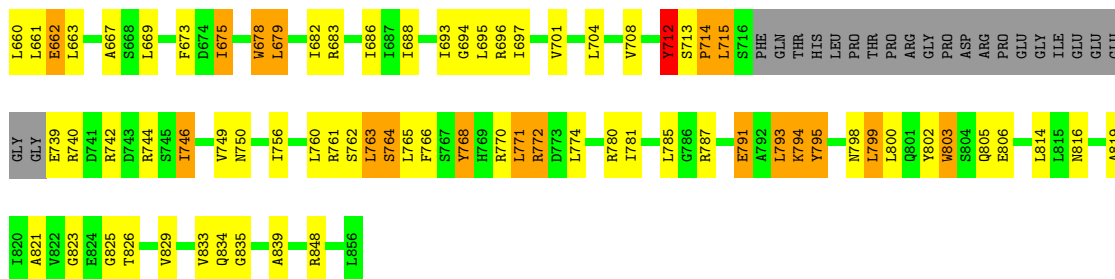


4.2.5 Score per residue for model 5

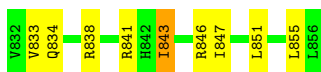
• Molecule 1: Transmembrane protein gp41



• Molecule 1: Transmembrane protein gp41



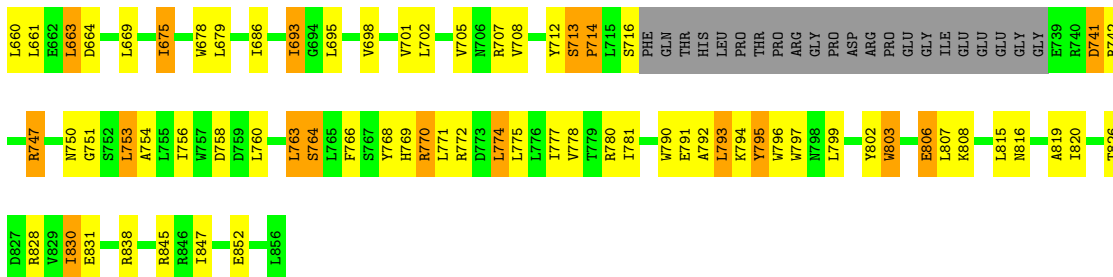




#### 4.2.7 Score per residue for model 7

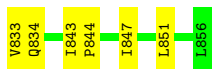
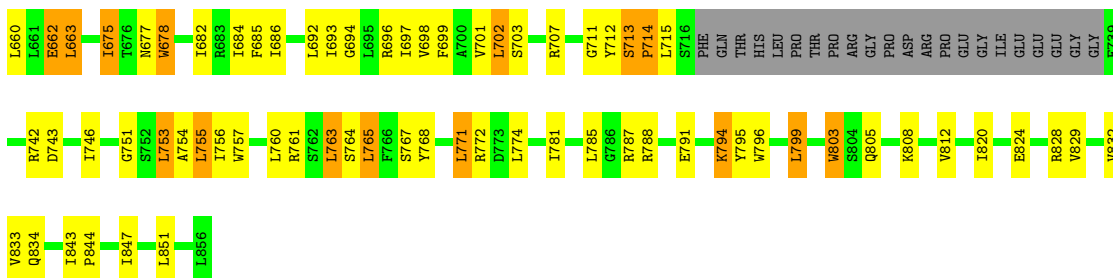
- Molecule 1: Transmembrane protein gp41

Chain A: 53% 27% 9% 11%



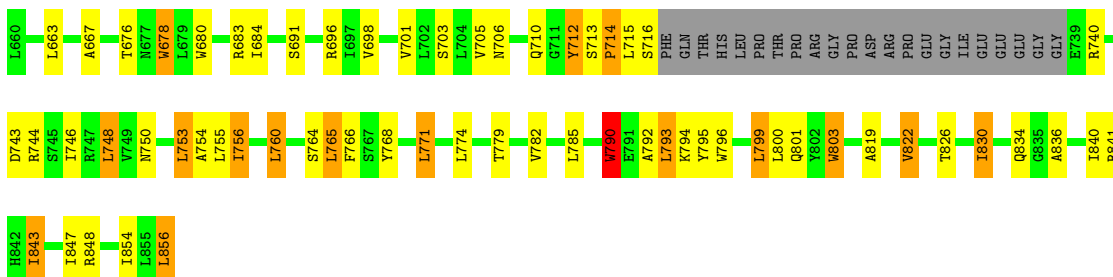
- Molecule 1: Transmembrane protein gp41

Chain B: 54% 27% 8% 11%



- Molecule 1: Transmembrane protein gp41

Chain C: 57% 23% 8% 11%



#### 4.2.8 Score per residue for model 8

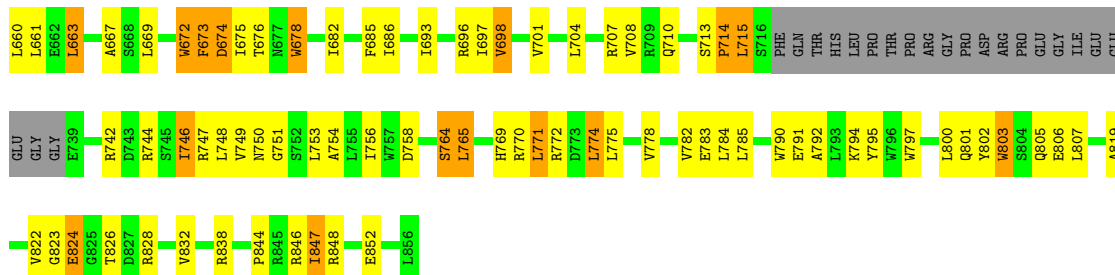
- Molecule 1: Transmembrane protein gp41





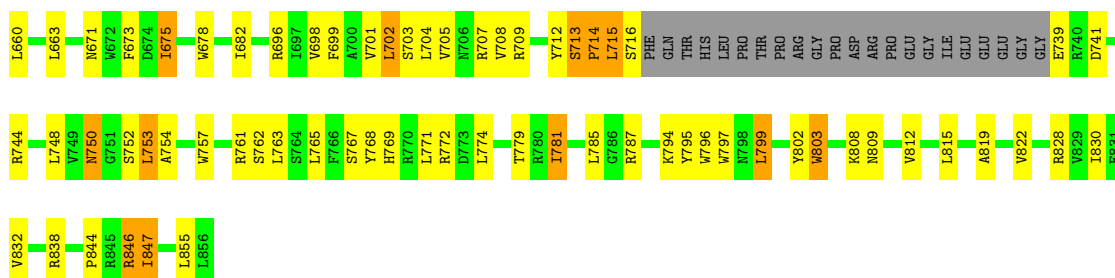
- Molecule 1: Transmembrane protein gp41

Chain B: 50% 31% 8% 11%



- Molecule 1: Transmembrane protein gp41

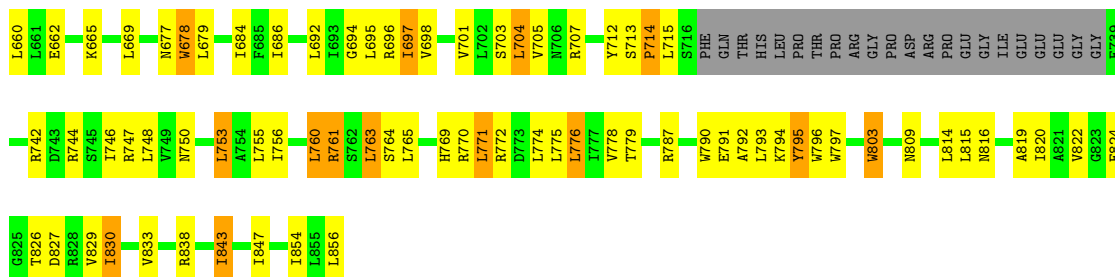
Chain C: 55% 28% 6% 11%



#### 4.2.10 Score per residue for model 10

- Molecule 1: Transmembrane protein gp41

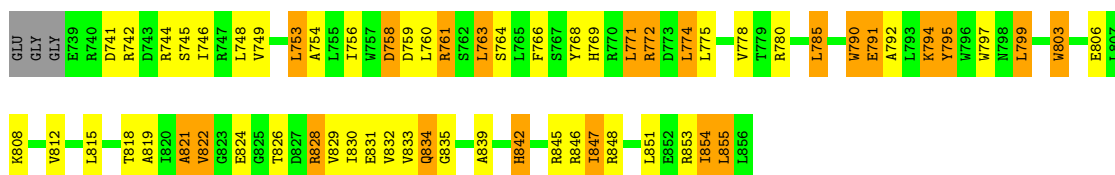
Chain A: 51% 31% 7% 11%



- Molecule 1: Transmembrane protein gp41

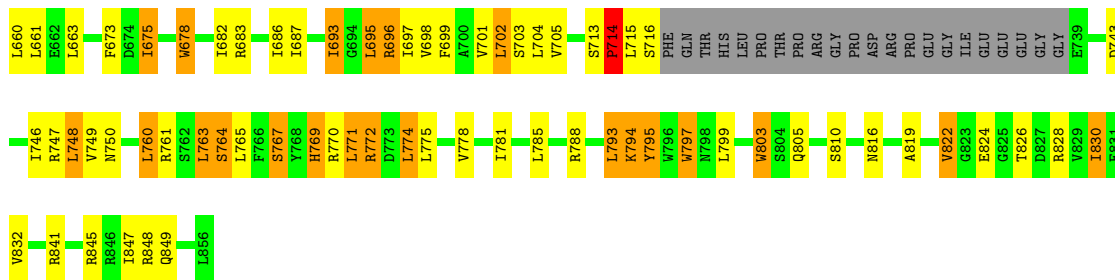
Chain B: 43% 32% 14% 11%





- Molecule 1: Transmembrane protein gp41

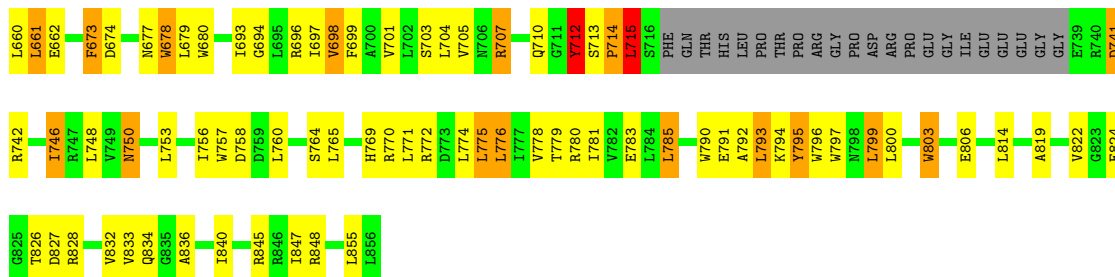
Chain C: 54% 23% 11% 11%



#### 4.2.11 Score per residue for model 11

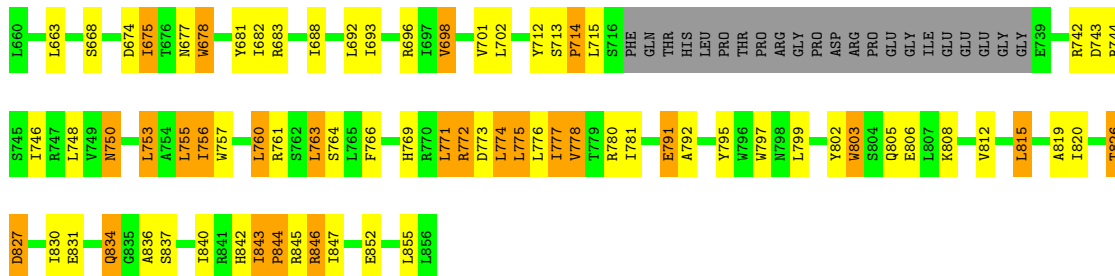
- Molecule 1: Transmembrane protein gp41

Chain A: 49% 30% 8% 11%



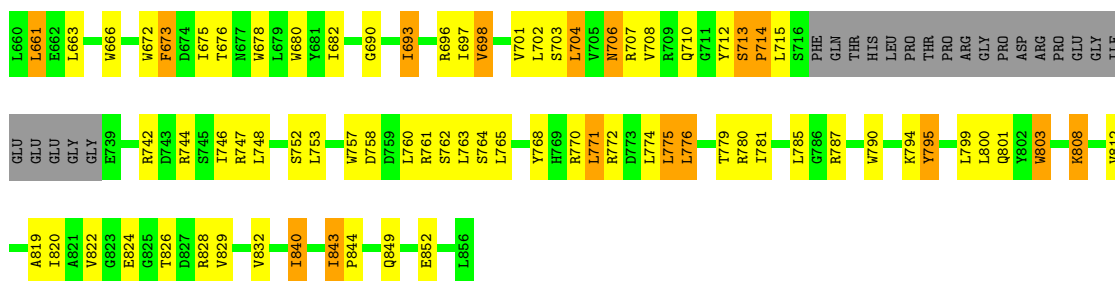
- Molecule 1: Transmembrane protein gp41

Chain B: 50% 26% 13% 11%



- Molecule 1: Transmembrane protein gp41

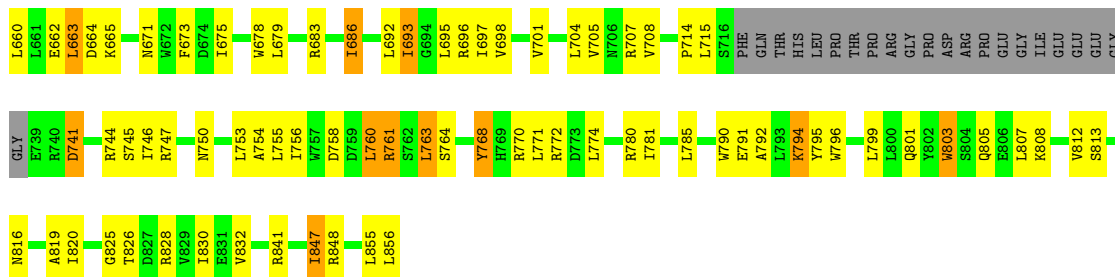
Chain C: 50% 30% 8% 11%



#### 4.2.12 Score per residue for model 12

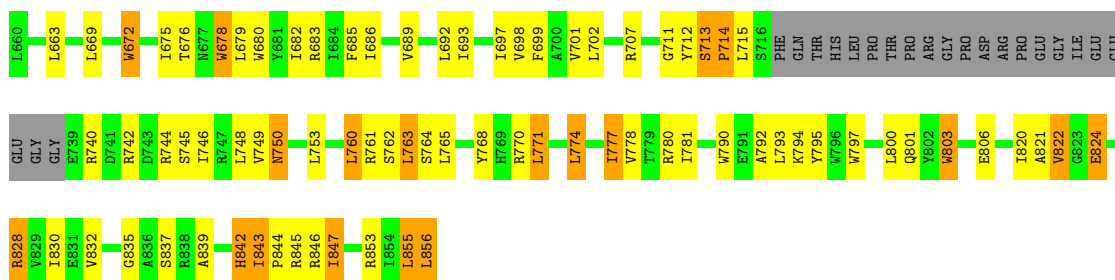
- Molecule 1: Transmembrane protein gp41

Chain A: 51% 32% 6% 11%



- Molecule 1: Transmembrane protein gp41

Chain B: 49% 30% 10% 11%



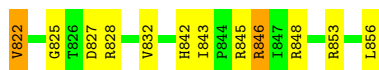
- Molecule 1: Transmembrane protein gp41

Chain C: 50% 28% 11% 11%





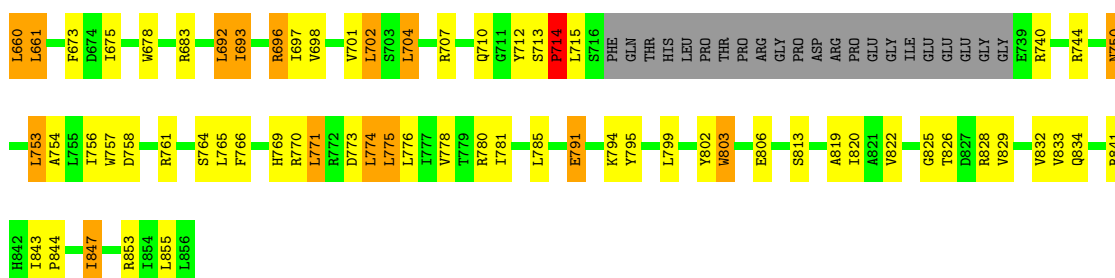




• Molecule 1: Transmembrane protein gp41

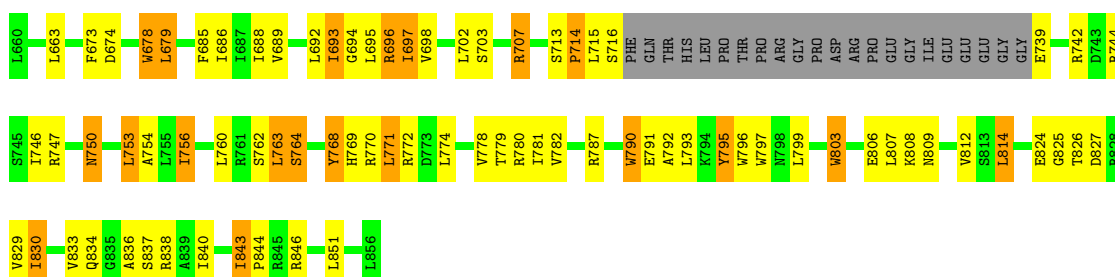


• Molecule 1: Transmembrane protein gp41



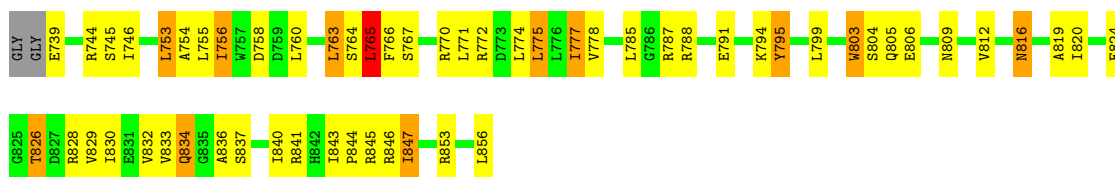
4.2.15 Score per residue for model 15

• Molecule 1: Transmembrane protein gp41



• Molecule 1: Transmembrane protein gp41





- Molecule 1: Transmembrane protein gp41

Chain C: 54% 27% 6% • 11%



## 5 Refinement protocol and experimental data overview

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

Of the 150 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	
X-PLOR NIH	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	657
Number of shifts mapped to atoms	622
Number of unparsed shifts	0
Number of shifts with mapping errors	35
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	8%

## 6 Model quality i

### 6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.79±0.01	0±0/1490 ( 0.0± 0.0%)	0.97±0.01	0±1/2021 ( 0.0± 0.0%)
1	B	0.79±0.01	0±0/1490 ( 0.0± 0.0%)	0.96±0.01	0±1/2021 ( 0.0± 0.0%)
1	C	0.79±0.01	0±0/1490 ( 0.0± 0.0%)	0.96±0.01	0±0/2021 ( 0.0± 0.0%)
All	All	0.79	0/67050 ( 0.0%)	0.97	12/90945 ( 0.0%)

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

Mol	Chain	Chirality	Planarity
1	B	0.0±0.0	0.1±0.2
All	All	0	1

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	795	TYR	CB-CG-CD1	-7.20	116.68	121.00	4	1
1	B	795	TYR	CB-CG-CD1	-6.27	117.24	121.00	6	1
1	A	707	ARG	NE-CZ-NH2	5.66	123.13	120.30	1	2
1	A	685	PHE	CB-CG-CD2	-5.65	116.85	120.80	15	1
1	C	790	TRP	CD1-NE1-CE2	5.44	113.89	109.00	7	1
1	B	712	TYR	CB-CG-CD2	-5.33	117.80	121.00	5	1
1	B	795	TYR	CB-CG-CD2	-5.29	117.83	121.00	8	2
1	C	761	ARG	NE-CZ-NH2	5.11	122.85	120.30	5	1
1	A	795	TYR	CB-CG-CD2	5.09	124.05	121.00	4	1
1	C	696	ARG	NE-CZ-NH2	5.01	122.80	120.30	14	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	B	770	ARG	Sidechain	1

## 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	1459	1521	1515	55±5
1	B	1459	1521	1515	52±8
1	C	1459	1521	1515	48±6
All	All	65655	68445	68175	1955

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:746:ILE:HG23	1:C:781:ILE:HD12	1.00	1.27	11	1
1:C:819:ALA:HB3	1:C:826:THR:HG21	0.97	1.35	14	1
1:B:819:ALA:HB1	1:B:826:THR:HG23	0.90	1.41	1	1
1:A:686:ILE:HD11	1:C:686:ILE:HG21	0.90	1.43	4	4
1:B:669:LEU:HD13	1:B:676:THR:HG21	0.89	1.43	8	1
1:A:781:ILE:HG21	1:B:746:ILE:HG23	0.84	1.46	9	2
1:A:663:LEU:HD21	1:B:660:LEU:HD23	0.83	1.49	13	1
1:A:686:ILE:HG21	1:B:686:ILE:HD12	0.82	1.50	9	1
1:A:753:LEU:HD13	1:A:754:ALA:N	0.82	1.89	14	5
1:C:695:LEU:O	1:C:698:VAL:HG22	0.79	1.78	12	1
1:B:774:LEU:HD13	1:B:777:ILE:HD12	0.79	1.52	6	2
1:A:799:LEU:HD13	1:B:756:ILE:HD11	0.78	1.54	14	2
1:A:763:LEU:HD23	1:A:764:SER:N	0.78	1.93	5	4
1:C:753:LEU:HD13	1:C:754:ALA:N	0.76	1.93	7	4
1:A:760:LEU:HD13	1:A:761:ARG:N	0.76	1.96	12	4
1:C:713:SER:O	1:C:714:PRO:O	0.75	2.04	11	10
1:C:775:LEU:HD13	1:C:776:LEU:N	0.75	1.96	11	2
1:B:698:VAL:O	1:B:701:VAL:HG22	0.74	1.82	15	13
1:C:715:LEU:HD13	1:C:716:SER:N	0.74	1.97	2	1

*Continued on next page...*

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:763:LEU:HD22	1:A:764:SER:N	0.74	1.97	12	8
1:B:771:LEU:HD23	1:B:772:ARG:N	0.74	1.98	14	2
1:C:678:TRP:O	1:C:682:ILE:HD12	0.73	1.83	8	1
1:A:819:ALA:O	1:A:822:VAL:HG12	0.73	1.83	10	1
1:A:698:VAL:O	1:A:701:VAL:HG22	0.73	1.84	12	11
1:C:698:VAL:O	1:C:701:VAL:HG22	0.73	1.84	2	13
1:A:713:SER:O	1:A:714:PRO:O	0.73	2.06	7	8
1:C:715:LEU:HD13	1:C:715:LEU:O	0.73	1.83	7	2
1:A:819:ALA:HB3	1:A:827:ASP:OD2	0.72	1.84	10	1
1:C:819:ALA:O	1:C:822:VAL:HG22	0.72	1.84	9	7
1:C:771:LEU:HD22	1:C:772:ARG:N	0.72	1.99	10	1
1:B:771:LEU:HD22	1:B:772:ARG:N	0.72	1.98	5	1
1:A:705:VAL:HG11	1:A:748:LEU:HD12	0.72	1.60	11	1
1:C:774:LEU:HD13	1:C:775:LEU:N	0.72	1.99	12	1
1:C:753:LEU:HD13	1:C:754:ALA:H	0.72	1.45	7	3
1:B:777:ILE:HD12	1:B:778:VAL:N	0.72	2.00	14	1
1:B:763:LEU:O	1:B:774:LEU:HD13	0.71	1.84	1	1
1:B:822:VAL:HG12	1:B:826:THR:HG22	0.71	1.60	8	1
1:C:704:LEU:O	1:C:708:VAL:HG23	0.71	1.85	13	4
1:B:795:TYR:CG	1:C:756:ILE:HG21	0.71	2.21	15	2
1:A:750:ASN:ND2	1:C:785:LEU:HD22	0.71	2.01	3	3
1:B:763:LEU:HD22	1:B:764:SER:N	0.71	2.01	12	6
1:B:795:TYR:CD2	1:C:756:ILE:HG21	0.71	2.21	15	1
1:A:746:ILE:HG21	1:C:781:ILE:CG2	0.71	2.15	1	4
1:B:764:SER:CB	1:B:771:LEU:HD12	0.71	2.16	10	3
1:B:781:ILE:CG2	1:C:746:ILE:HG21	0.71	2.16	12	2
1:C:748:LEU:HD13	1:C:749:VAL:N	0.70	2.01	4	2
1:A:693:ILE:HD13	1:A:694:GLY:N	0.70	2.01	3	1
1:B:777:ILE:HD13	1:B:778:VAL:N	0.70	2.01	12	3
1:B:763:LEU:O	1:B:774:LEU:HD21	0.70	1.87	2	1
1:A:707:ARG:CB	1:C:704:LEU:HD11	0.70	2.16	4	1
1:C:663:LEU:HD13	1:C:664:ASP:N	0.70	2.02	4	3
1:A:764:SER:CB	1:A:771:LEU:HD22	0.70	2.16	13	1
1:A:746:ILE:HG21	1:C:781:ILE:HG23	0.69	1.64	15	3
1:B:760:LEU:O	1:B:760:LEU:HD22	0.69	1.87	11	7
1:A:771:LEU:HD22	1:A:772:ARG:N	0.69	2.02	15	1
1:A:819:ALA:HB1	1:A:826:THR:CG2	0.69	2.17	9	1
1:B:667:ALA:HB2	1:C:660:LEU:HD11	0.69	1.63	2	1
1:B:715:LEU:HD12	1:B:716:SER:N	0.69	2.02	4	1
1:B:715:LEU:HD22	1:B:715:LEU:O	0.69	1.87	9	2
1:B:797:TRP:CG	1:B:847:ILE:HD11	0.69	2.23	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:777:ILE:HD13	1:A:778:VAL:N	0.69	2.03	14	1
1:A:756:ILE:HD11	1:C:796:TRP:CD1	0.69	2.22	7	1
1:B:751:GLY:O	1:C:715:LEU:HD12	0.69	1.87	7	1
1:B:795:TYR:CB	1:C:756:ILE:HG21	0.69	2.18	14	2
1:A:685:PHE:O	1:A:689:VAL:HG22	0.69	1.88	8	1
1:A:799:LEU:CD1	1:B:756:ILE:HD11	0.69	2.18	14	1
1:C:771:LEU:HD13	1:C:772:ARG:H	0.69	1.47	4	1
1:B:713:SER:O	1:B:714:PRO:O	0.68	2.11	10	11
1:B:760:LEU:HD13	1:B:761:ARG:N	0.68	2.04	14	5
1:C:771:LEU:H	1:C:771:LEU:HD23	0.68	1.47	15	2
1:A:715:LEU:O	1:A:715:LEU:HD13	0.68	1.89	15	3
1:C:819:ALA:O	1:C:822:VAL:HG12	0.68	1.89	11	3
1:A:781:ILE:HD13	1:B:746:ILE:CG1	0.68	2.17	3	1
1:A:781:ILE:HG21	1:B:746:ILE:CG2	0.68	2.17	9	3
1:A:660:LEU:O	1:C:663:LEU:HD22	0.68	1.87	5	1
1:A:771:LEU:H	1:A:771:LEU:HD13	0.68	1.48	15	8
1:B:753:LEU:HD13	1:B:754:ALA:N	0.68	2.04	7	2
1:C:763:LEU:HD22	1:C:764:SER:N	0.68	2.04	10	1
1:A:756:ILE:O	1:A:760:LEU:HD12	0.68	1.88	12	3
1:A:685:PHE:O	1:A:689:VAL:HG23	0.68	1.88	1	3
1:B:751:GLY:CA	1:C:715:LEU:HD11	0.68	2.19	2	1
1:B:669:LEU:HD13	1:B:669:LEU:O	0.67	1.89	1	2
1:B:686:ILE:HG21	1:C:686:ILE:HD11	0.67	1.67	2	2
1:A:757:TRP:CZ3	1:B:715:LEU:HD13	0.67	2.24	4	1
1:B:775:LEU:O	1:B:775:LEU:HD22	0.67	1.89	11	2
1:B:803:TRP:CH2	1:C:760:LEU:HD22	0.67	2.23	4	1
1:B:852:GLU:O	1:B:855:LEU:HD12	0.67	1.90	2	1
1:A:693:ILE:HD11	1:B:696:ARG:NE	0.67	2.05	7	5
1:A:746:ILE:HG23	1:C:781:ILE:CD1	0.67	2.12	11	1
1:A:694:GLY:O	1:A:697:ILE:HD12	0.67	1.89	3	3
1:C:748:LEU:HD22	1:C:748:LEU:O	0.67	1.90	8	2
1:B:669:LEU:CD1	1:B:676:THR:HG21	0.67	2.20	8	1
1:B:704:LEU:HD11	1:C:707:ARG:CB	0.67	2.20	2	1
1:B:682:ILE:HD12	1:B:683:ARG:N	0.67	2.04	1	6
1:B:775:LEU:O	1:B:778:VAL:HG22	0.67	1.90	6	5
1:B:781:ILE:HG23	1:C:746:ILE:HG21	0.67	1.67	12	1
1:A:753:LEU:HD22	1:A:753:LEU:C	0.66	2.11	6	4
1:C:702:LEU:HD22	1:C:702:LEU:O	0.66	1.90	12	3
1:C:830:ILE:H	1:C:830:ILE:HD13	0.66	1.49	6	1
1:A:756:ILE:HD13	1:C:796:TRP:NE1	0.66	2.05	9	1
1:B:750:ASN:O	1:B:753:LEU:HD12	0.66	1.90	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:678:TRP:O	1:B:682:ILE:HG23	0.66	1.90	1	8
1:B:704:LEU:O	1:B:708:VAL:HG23	0.66	1.90	15	3
1:A:705:VAL:HG21	1:A:748:LEU:HD12	0.66	1.68	10	2
1:A:675:ILE:HD13	1:A:675:ILE:O	0.66	1.90	7	4
1:C:797:TRP:CD1	1:C:847:ILE:HD11	0.66	2.25	12	2
1:C:774:LEU:O	1:C:774:LEU:HD22	0.66	1.91	12	1
1:A:682:ILE:HD12	1:A:683:ARG:N	0.66	2.06	4	1
1:B:793:LEU:HD13	1:B:793:LEU:O	0.66	1.91	13	4
1:B:785:LEU:HD23	1:C:750:ASN:OD1	0.66	1.89	5	1
1:B:779:THR:O	1:B:782:VAL:HG22	0.65	1.91	14	2
1:B:795:TYR:HB3	1:C:756:ILE:HG21	0.65	1.67	14	2
1:A:791:GLU:O	1:A:794:LYS:HG3	0.65	1.91	12	1
1:C:760:LEU:HD22	1:C:760:LEU:O	0.65	1.91	1	1
1:A:785:LEU:HD13	1:A:785:LEU:O	0.65	1.90	14	3
1:A:803:TRP:CH2	1:B:760:LEU:HD23	0.65	2.26	13	1
1:B:781:ILE:HD12	1:B:782:VAL:N	0.65	2.07	6	1
1:A:663:LEU:HD22	1:A:663:LEU:O	0.65	1.90	14	1
1:A:819:ALA:O	1:A:826:THR:HG21	0.65	1.91	2	2
1:B:753:LEU:HD22	1:B:754:ALA:N	0.65	2.07	6	1
1:A:802:TYR:CD1	1:B:760:LEU:HD21	0.65	2.26	7	1
1:A:829:VAL:O	1:A:833:VAL:HG22	0.65	1.91	1	6
1:A:754:ALA:CB	1:B:715:LEU:HD11	0.65	2.21	4	1
1:B:675:ILE:HD13	1:B:675:ILE:O	0.65	1.92	8	2
1:A:776:LEU:HD13	1:A:776:LEU:H	0.65	1.51	10	1
1:C:695:LEU:HD22	1:C:695:LEU:C	0.65	2.12	10	1
1:C:746:ILE:O	1:C:749:VAL:HG22	0.64	1.92	8	2
1:B:755:LEU:HD13	1:B:755:LEU:O	0.64	1.93	7	2
1:A:663:LEU:HD12	1:A:664:ASP:N	0.64	2.07	12	1
1:A:763:LEU:HD23	1:A:764:SER:H	0.64	1.52	8	1
1:B:702:LEU:O	1:B:702:LEU:HD22	0.64	1.92	14	3
1:A:755:LEU:HD13	1:A:756:ILE:N	0.64	2.06	8	1
1:A:750:ASN:OD1	1:C:785:LEU:HD23	0.64	1.91	10	1
1:A:715:LEU:HD12	1:C:754:ALA:O	0.64	1.92	15	1
1:A:753:LEU:HD23	1:C:791:GLU:HB3	0.64	1.67	6	3
1:B:702:LEU:C	1:B:702:LEU:HD13	0.64	2.13	2	5
1:A:763:LEU:H	1:A:763:LEU:HD13	0.64	1.50	4	8
1:A:775:LEU:O	1:A:778:VAL:HG12	0.64	1.91	5	7
1:A:854:ILE:O	1:A:854:ILE:HD13	0.64	1.92	4	2
1:A:816:ASN:N	1:A:830:ILE:HD11	0.64	2.06	13	2
1:B:669:LEU:HD11	1:B:675:ILE:HG23	0.64	1.69	9	1
1:C:764:SER:OG	1:C:771:LEU:HD12	0.64	1.92	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:822:VAL:HG21	1:C:826:THR:HG21	0.64	1.69	8	1
1:C:775:LEU:O	1:C:778:VAL:HG22	0.64	1.93	4	4
1:B:855:LEU:HD22	1:B:855:LEU:O	0.63	1.93	2	2
1:A:799:LEU:O	1:A:803:TRP:CE3	0.63	2.51	3	4
1:C:799:LEU:HD23	1:C:800:LEU:N	0.63	2.08	3	1
1:C:771:LEU:H	1:C:771:LEU:HD13	0.63	1.52	10	7
1:A:774:LEU:O	1:A:777:ILE:HG22	0.63	1.92	6	1
1:C:797:TRP:NE1	1:C:847:ILE:HD11	0.63	2.08	9	1
1:C:692:LEU:HD23	1:C:693:ILE:N	0.63	2.07	14	1
1:A:715:LEU:HD12	1:C:751:GLY:CA	0.63	2.23	2	1
1:A:750:ASN:ND2	1:C:785:LEU:HD23	0.63	2.09	2	6
1:A:756:ILE:CG2	1:A:760:LEU:HD12	0.63	2.22	6	1
1:B:764:SER:HB3	1:B:771:LEU:HD12	0.63	1.70	7	4
1:A:755:LEU:HD22	1:A:755:LEU:O	0.63	1.93	8	1
1:B:799:LEU:HD23	1:B:800:LEU:N	0.63	2.08	2	1
1:A:756:ILE:HD13	1:C:795:TYR:HB3	0.63	1.68	10	2
1:C:768:TYR:CD2	1:C:771:LEU:HD11	0.63	2.28	13	1
1:C:675:ILE:O	1:C:675:ILE:HD13	0.63	1.94	10	3
1:B:785:LEU:HD23	1:C:750:ASN:ND2	0.63	2.09	15	2
1:C:678:TRP:O	1:C:682:ILE:HG23	0.63	1.94	15	2
1:C:819:ALA:HB1	1:C:826:THR:CG2	0.63	2.23	11	1
1:B:756:ILE:HD13	1:B:756:ILE:O	0.63	1.93	2	2
1:C:828:ARG:O	1:C:832:VAL:HG23	0.63	1.94	13	4
1:C:776:LEU:O	1:C:779:THR:HG22	0.63	1.94	4	2
1:B:686:ILE:HG21	1:C:686:ILE:CD1	0.63	2.24	5	1
1:A:760:LEU:O	1:A:763:LEU:HD22	0.62	1.94	4	1
1:A:793:LEU:HD21	1:A:847:ILE:HG12	0.62	1.72	4	1
1:A:806:GLU:CB	1:B:771:LEU:HD21	0.62	2.23	8	2
1:C:816:ASN:OD1	1:C:830:ILE:HD12	0.62	1.94	1	2
1:B:702:LEU:HD13	1:B:703:SER:N	0.62	2.09	7	4
1:C:816:ASN:O	1:C:820:ILE:HD12	0.62	1.94	5	2
1:C:826:THR:O	1:C:829:VAL:HG12	0.62	1.94	8	3
1:C:675:ILE:HG22	1:C:679:LEU:CD1	0.62	2.25	4	1
1:A:747:ARG:NH1	1:A:754:ALA:HB2	0.62	2.09	7	1
1:A:806:GLU:HB3	1:B:771:LEU:HD11	0.62	1.72	13	1
1:A:797:TRP:CD1	1:A:847:ILE:HD11	0.62	2.29	3	1
1:B:806:GLU:CD	1:C:771:LEU:HD21	0.62	2.14	12	1
1:C:708:VAL:HG12	1:C:741:ASP:OD2	0.62	1.94	1	1
1:C:748:LEU:HD13	1:C:748:LEU:O	0.62	1.92	11	5
1:B:795:TYR:HB3	1:C:756:ILE:HD13	0.62	1.71	6	1
1:A:770:ARG:NH1	1:A:777:ILE:HD13	0.62	2.10	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:835:GLY:O	1:B:839:ALA:HB3	0.62	1.94	4	7
1:C:685:PHE:HA	1:C:688:ILE:HD12	0.62	1.71	13	2
1:A:669:LEU:CD2	1:A:676:THR:HG23	0.62	2.24	8	1
1:B:669:LEU:CD2	1:B:676:THR:HG23	0.62	2.25	9	1
1:B:826:THR:O	1:B:830:ILE:HD12	0.62	1.94	15	1
1:A:752:SER:O	1:A:755:LEU:HD12	0.61	1.95	8	1
1:B:800:LEU:HA	1:B:803:TRP:CH2	0.61	2.30	9	1
1:A:781:ILE:HD13	1:B:746:ILE:HG13	0.61	1.72	12	2
1:C:697:ILE:HD13	1:C:697:ILE:O	0.61	1.95	5	1
1:B:663:LEU:HD23	1:B:663:LEU:O	0.61	1.94	10	1
1:C:819:ALA:HB1	1:C:826:THR:OG1	0.61	1.96	10	2
1:A:819:ALA:HB1	1:A:826:THR:OG1	0.61	1.94	12	1
1:B:808:LYS:O	1:B:812:VAL:HG22	0.61	1.96	7	3
1:A:696:ARG:HE	1:C:693:ILE:HD11	0.61	1.56	14	3
1:A:686:ILE:CG2	1:B:686:ILE:HD12	0.61	2.25	9	1
1:B:771:LEU:H	1:B:771:LEU:HD13	0.61	1.55	3	7
1:B:775:LEU:H	1:B:775:LEU:HD13	0.61	1.56	1	3
1:A:714:PRO:HB2	1:C:748:LEU:HD23	0.61	1.71	10	1
1:A:708:VAL:HG21	1:B:714:PRO:HD3	0.61	1.70	2	2
1:C:682:ILE:HD12	1:C:683:ARG:N	0.61	2.10	10	2
1:C:695:LEU:O	1:C:698:VAL:HG13	0.61	1.96	10	1
1:B:819:ALA:HB1	1:B:826:THR:HB	0.61	1.72	2	5
1:B:828:ARG:O	1:B:832:VAL:HG23	0.61	1.96	12	5
1:B:774:LEU:HD23	1:B:775:LEU:N	0.61	2.10	3	1
1:A:816:ASN:CA	1:A:830:ILE:HD11	0.61	2.26	13	3
1:B:704:LEU:HD21	1:C:714:PRO:O	0.61	1.95	1	1
1:A:840:ILE:HD13	1:A:840:ILE:O	0.61	1.94	2	2
1:B:750:ASN:O	1:B:753:LEU:HD13	0.61	1.96	6	1
1:B:854:ILE:HD13	1:B:854:ILE:O	0.60	1.96	10	1
1:A:796:TRP:HE1	1:B:756:ILE:HD13	0.60	1.57	1	1
1:B:685:PHE:O	1:B:689:VAL:HG23	0.60	1.95	12	2
1:B:759:ASP:O	1:B:763:LEU:HD12	0.60	1.95	4	2
1:B:746:ILE:O	1:B:749:VAL:HG22	0.60	1.96	12	3
1:C:756:ILE:O	1:C:756:ILE:HD13	0.60	1.95	15	1
1:B:704:LEU:HD11	1:C:712:TYR:O	0.60	1.96	9	1
1:A:776:LEU:HD13	1:A:776:LEU:N	0.60	2.11	10	1
1:A:781:ILE:HG22	1:B:746:ILE:HG21	0.60	1.73	15	1
1:B:748:LEU:O	1:B:748:LEU:HD13	0.60	1.96	11	1
1:A:764:SER:OG	1:A:771:LEU:HD22	0.60	1.96	13	1
1:A:785:LEU:HD22	1:B:750:ASN:ND2	0.60	2.12	5	1
1:B:663:LEU:O	1:B:667:ALA:HB3	0.60	1.96	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:715:LEU:HD22	1:C:715:LEU:O	0.60	1.96	2	2
1:C:829:VAL:O	1:C:833:VAL:HG22	0.60	1.96	14	3
1:A:785:LEU:HD13	1:B:749:VAL:HB	0.60	1.74	5	1
1:B:753:LEU:HD12	1:B:754:ALA:N	0.60	2.12	10	2
1:B:820:ILE:O	1:B:822:VAL:HG22	0.60	1.97	12	1
1:A:781:ILE:CG2	1:B:746:ILE:HG21	0.60	2.26	15	5
1:A:697:ILE:O	1:A:697:ILE:HD13	0.60	1.97	10	2
1:A:816:ASN:HA	1:A:830:ILE:HD11	0.60	1.70	12	2
1:B:812:VAL:HG11	1:B:834:GLN:NE2	0.60	2.11	10	1
1:B:768:TYR:O	1:B:771:LEU:HD13	0.60	1.96	12	1
1:B:847:ILE:H	1:B:847:ILE:HD13	0.60	1.57	12	1
1:C:693:ILE:HD12	1:C:693:ILE:O	0.60	1.97	4	6
1:C:812:VAL:HG12	1:C:834:GLN:CD	0.60	2.17	8	1
1:B:781:ILE:HG21	1:C:746:ILE:CG2	0.59	2.27	2	2
1:C:763:LEU:O	1:C:774:LEU:HD22	0.59	1.97	6	1
1:A:793:LEU:HD12	1:A:797:TRP:NE1	0.59	2.11	11	2
1:A:753:LEU:HD23	1:C:791:GLU:CB	0.59	2.27	2	3
1:A:754:ALA:HB1	1:B:715:LEU:HB3	0.59	1.73	7	1
1:A:765:LEU:HD12	1:A:770:ARG:NH2	0.59	2.13	1	1
1:A:678:TRP:O	1:A:682:ILE:HG23	0.59	1.96	13	2
1:A:793:LEU:HD12	1:A:847:ILE:HD11	0.59	1.75	7	2
1:C:771:LEU:HD23	1:C:772:ARG:CD	0.59	2.26	11	1
1:C:771:LEU:HD13	1:C:772:ARG:N	0.59	2.12	4	1
1:A:785:LEU:HD21	1:B:746:ILE:HG22	0.59	1.73	5	1
1:A:830:ILE:HD13	1:A:831:GLU:N	0.59	2.12	7	1
1:B:799:LEU:HD22	1:C:756:ILE:HD12	0.59	1.75	8	1
1:C:812:VAL:HG12	1:C:834:GLN:NE2	0.59	2.13	8	1
1:C:715:LEU:C	1:C:715:LEU:HD22	0.59	2.18	9	1
1:A:756:ILE:HG21	1:C:795:TYR:HB3	0.59	1.75	6	3
1:B:694:GLY:O	1:B:697:ILE:HG22	0.59	1.98	5	4
1:B:793:LEU:O	1:B:793:LEU:HD23	0.59	1.98	6	2
1:A:828:ARG:O	1:A:832:VAL:HG22	0.59	1.98	11	2
1:B:760:LEU:C	1:B:760:LEU:HD13	0.59	2.19	3	3
1:A:704:LEU:HD11	1:B:707:ARG:CB	0.58	2.27	2	2
1:A:758:ASP:HB3	1:B:715:LEU:HD11	0.58	1.75	12	1
1:B:840:ILE:HD13	1:B:840:ILE:O	0.58	1.97	2	2
1:C:821:ALA:O	1:C:822:VAL:HG13	0.58	1.97	2	1
1:A:765:LEU:HD13	1:A:766:PHE:N	0.58	2.13	4	1
1:A:799:LEU:HD23	1:A:800:LEU:N	0.58	2.13	11	1
1:A:753:LEU:HD13	1:A:754:ALA:H	0.58	1.58	6	1
1:A:753:LEU:O	1:A:756:ILE:HG22	0.58	1.98	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:791:GLU:O	1:B:794:LYS:HG3	0.58	1.99	6	9
1:B:796:TRP:HE1	1:C:756:ILE:HD11	0.58	1.59	2	1
1:B:702:LEU:O	1:B:702:LEU:HD13	0.58	1.99	4	1
1:B:682:ILE:HD13	1:B:682:ILE:C	0.58	2.18	13	1
1:A:686:ILE:HG21	1:B:686:ILE:CD1	0.58	2.28	9	2
1:B:799:LEU:HD13	1:C:756:ILE:HD11	0.58	1.76	5	1
1:B:799:LEU:O	1:B:803:TRP:CD2	0.58	2.57	13	3
1:B:693:ILE:HD11	1:C:692:LEU:HD23	0.58	1.75	8	3
1:A:663:LEU:HD13	1:A:664:ASP:N	0.58	2.14	14	2
1:A:750:ASN:CG	1:C:785:LEU:HD22	0.58	2.19	9	2
1:C:793:LEU:HD22	1:C:793:LEU:O	0.58	1.99	10	1
1:C:793:LEU:HD21	1:C:797:TRP:NE1	0.58	2.14	10	1
1:A:796:TRP:CD1	1:B:756:ILE:HD13	0.58	2.34	10	2
1:B:793:LEU:HD11	1:B:847:ILE:HG13	0.58	1.74	12	1
1:A:754:ALA:HB1	1:B:715:LEU:O	0.57	1.99	1	2
1:C:774:LEU:HD13	1:C:774:LEU:O	0.57	1.99	14	2
1:C:791:GLU:O	1:C:794:LYS:HG3	0.57	1.99	5	2
1:B:702:LEU:HD13	1:B:702:LEU:C	0.57	2.20	7	1
1:B:669:LEU:HD11	1:B:675:ILE:CG2	0.57	2.28	9	1
1:A:774:LEU:O	1:A:778:VAL:HG23	0.57	1.99	15	1
1:C:708:VAL:HG11	1:C:744:ARG:NH1	0.57	2.13	1	1
1:B:829:VAL:O	1:B:833:VAL:HG23	0.57	1.99	4	4
1:B:855:LEU:HD13	1:B:855:LEU:O	0.57	2.00	14	2
1:A:763:LEU:HD13	1:A:764:SER:H	0.57	1.60	2	1
1:B:855:LEU:HD13	1:B:856:LEU:N	0.57	2.13	2	2
1:C:775:LEU:O	1:C:775:LEU:HD22	0.57	1.99	14	2
1:B:667:ALA:CB	1:C:660:LEU:HD11	0.57	2.30	2	1
1:B:768:TYR:O	1:B:771:LEU:HD22	0.57	1.99	14	1
1:A:763:LEU:HD22	1:A:764:SER:H	0.57	1.60	7	2
1:A:821:ALA:O	1:A:822:VAL:HG13	0.57	2.00	5	1
1:B:829:VAL:O	1:B:833:VAL:HG22	0.57	1.99	7	2
1:C:695:LEU:HD22	1:C:695:LEU:O	0.57	2.00	10	1
1:B:764:SER:OG	1:B:771:LEU:HD12	0.57	1.99	12	2
1:B:816:ASN:ND2	1:B:830:ILE:HD12	0.57	2.13	8	1
1:A:686:ILE:HG12	1:B:686:ILE:HD12	0.57	1.75	8	2
1:C:702:LEU:C	1:C:702:LEU:HD13	0.57	2.19	10	7
1:A:781:ILE:HD13	1:B:746:ILE:HG12	0.57	1.74	3	2
1:A:819:ALA:HB1	1:A:826:THR:HB	0.57	1.76	7	5
1:A:790:TRP:CZ2	1:A:793:LEU:HD23	0.57	2.35	11	2
1:B:808:LYS:O	1:B:812:VAL:HG23	0.57	2.00	11	4
1:C:760:LEU:O	1:C:760:LEU:HD23	0.57	2.00	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:683:ARG:HG3	1:C:684:ILE:HD12	0.57	1.77	7	1
1:C:826:THR:O	1:C:830:ILE:HD12	0.57	1.99	8	1
1:A:750:ASN:CG	1:C:785:LEU:HD23	0.57	2.19	12	2
1:B:812:VAL:HG21	1:B:834:GLN:OE1	0.57	2.00	11	1
1:A:760:LEU:HD13	1:A:761:ARG:H	0.57	1.60	12	1
1:C:819:ALA:O	1:C:826:THR:HG21	0.56	2.00	7	2
1:B:693:ILE:HG12	1:C:692:LEU:HD21	0.56	1.77	14	1
1:A:754:ALA:HB2	1:B:715:LEU:HD11	0.56	1.77	4	1
1:A:771:LEU:C	1:A:771:LEU:HD13	0.56	2.20	7	1
1:C:774:LEU:O	1:C:778:VAL:HG23	0.56	2.00	13	1
1:A:715:LEU:HD12	1:C:751:GLY:O	0.56	1.99	6	1
1:C:828:ARG:O	1:C:832:VAL:HG12	0.56	2.00	11	2
1:B:793:LEU:HD11	1:B:847:ILE:CG1	0.56	2.30	12	1
1:A:753:LEU:HD23	1:C:791:GLU:HG3	0.56	1.76	14	1
1:B:765:LEU:HD23	1:B:774:LEU:HD11	0.56	1.77	15	1
1:B:763:LEU:H	1:B:763:LEU:HD13	0.56	1.61	5	4
1:C:764:SER:CB	1:C:771:LEU:HD12	0.56	2.30	13	1
1:C:830:ILE:HD13	1:C:830:ILE:O	0.56	2.01	7	4
1:A:808:LYS:O	1:A:812:VAL:HG22	0.56	2.01	2	4
1:A:714:PRO:HG3	1:C:705:VAL:HG22	0.56	1.76	1	2
1:B:761:ARG:O	1:B:765:LEU:HD22	0.56	2.01	7	1
1:A:785:LEU:HD23	1:B:750:ASN:CG	0.56	2.21	1	1
1:A:704:LEU:O	1:A:708:VAL:HG23	0.56	2.01	2	1
1:C:797:TRP:CG	1:C:847:ILE:HD12	0.56	2.36	3	3
1:B:821:ALA:O	1:B:822:VAL:HG13	0.56	2.01	4	1
1:C:660:LEU:C	1:C:661:LEU:HD23	0.56	2.21	4	1
1:A:781:ILE:HG23	1:B:746:ILE:CG2	0.56	2.31	13	1
1:B:751:GLY:HA2	1:C:715:LEU:HD11	0.56	1.77	2	1
1:C:771:LEU:HD23	1:C:772:ARG:CZ	0.56	2.31	2	1
1:C:663:LEU:C	1:C:663:LEU:HD22	0.56	2.22	15	2
1:A:760:LEU:HD11	1:C:799:LEU:HB2	0.56	1.76	6	1
1:A:781:ILE:HG23	1:B:746:ILE:HG23	0.56	1.77	7	2
1:A:830:ILE:O	1:A:830:ILE:HD13	0.56	2.00	8	1
1:C:819:ALA:CB	1:C:826:THR:HG21	0.56	2.23	14	1
1:A:771:LEU:HD22	1:A:771:LEU:N	0.55	2.16	4	7
1:A:819:ALA:HB1	1:A:826:THR:HG22	0.55	1.77	9	1
1:B:812:VAL:HG11	1:B:834:GLN:OE1	0.55	2.02	14	1
1:C:763:LEU:O	1:C:774:LEU:HD13	0.55	2.00	9	2
1:A:704:LEU:HD21	1:B:707:ARG:HA	0.55	1.78	8	1
1:A:819:ALA:HB3	1:A:827:ASP:OD1	0.55	2.01	11	1
1:A:771:LEU:HD22	1:A:772:ARG:H	0.55	1.62	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:756:ILE:HD13	1:C:795:TYR:CB	0.55	2.31	10	1
1:A:793:LEU:HD11	1:A:847:ILE:HG13	0.55	1.77	4	1
1:A:816:ASN:HB2	1:A:830:ILE:HD11	0.55	1.76	3	2
1:B:771:LEU:HD23	1:B:772:ARG:HD3	0.55	1.79	8	1
1:C:850:GLY:O	1:C:854:ILE:HG23	0.55	2.02	8	1
1:A:705:VAL:HG11	1:A:745:SER:HB2	0.55	1.79	12	1
1:B:793:LEU:HD12	1:B:793:LEU:O	0.55	2.01	14	1
1:B:754:ALA:HB3	1:C:715:LEU:O	0.55	2.01	15	1
1:A:795:TYR:CB	1:B:756:ILE:HG21	0.55	2.32	1	1
1:A:764:SER:HB3	1:A:771:LEU:HD12	0.55	1.78	14	3
1:B:819:ALA:O	1:B:826:THR:HG21	0.55	2.02	9	2
1:B:806:GLU:HG3	1:C:771:LEU:HD21	0.55	1.77	15	1
1:C:771:LEU:HD23	1:C:772:ARG:NE	0.55	2.16	2	1
1:C:809:ASN:O	1:C:812:VAL:HG22	0.55	2.02	8	1
1:C:771:LEU:O	1:C:774:LEU:HD23	0.55	2.01	10	1
1:A:693:ILE:HD12	1:A:693:ILE:O	0.55	2.02	15	1
1:A:774:LEU:HD13	1:A:777:ILE:HD11	0.54	1.79	8	1
1:A:692:LEU:HD12	1:A:693:ILE:N	0.54	2.17	13	1
1:C:790:TRP:CZ2	1:C:793:LEU:HD23	0.54	2.37	1	1
1:B:771:LEU:HD22	1:B:771:LEU:C	0.54	2.22	2	1
1:B:745:SER:O	1:B:748:LEU:HD23	0.54	2.02	8	1
1:B:781:ILE:HG21	1:C:746:ILE:HG21	0.54	1.78	2	3
1:A:795:TYR:CZ	1:A:796:TRP:NE1	0.54	2.76	2	7
1:C:793:LEU:HD23	1:C:847:ILE:HD11	0.54	1.78	7	1
1:C:695:LEU:O	1:C:698:VAL:HG12	0.54	2.03	13	1
1:C:675:ILE:HG22	1:C:679:LEU:HD12	0.54	1.79	4	1
1:A:693:ILE:HD11	1:B:696:ARG:HE	0.54	1.61	15	3
1:A:763:LEU:O	1:A:774:LEU:HD22	0.54	2.03	3	5
1:A:679:LEU:O	1:A:682:ILE:HG22	0.54	2.03	3	1
1:C:695:LEU:O	1:C:695:LEU:HD23	0.54	2.03	1	4
1:A:742:ARG:HH11	1:A:746:ILE:HD11	0.54	1.63	6	1
1:B:715:LEU:C	1:B:715:LEU:HD13	0.54	2.23	9	1
1:A:753:LEU:O	1:A:756:ILE:HD12	0.54	2.01	11	1
1:C:771:LEU:HD23	1:C:772:ARG:HD2	0.54	1.79	11	1
1:B:693:ILE:CG1	1:C:692:LEU:HD21	0.54	2.33	14	1
1:A:686:ILE:HD11	1:C:686:ILE:CG2	0.54	2.33	2	3
1:A:764:SER:OG	1:A:771:LEU:HD12	0.54	2.02	2	2
1:A:695:LEU:C	1:A:695:LEU:HD23	0.54	2.23	3	2
1:A:856:LEU:HD13	1:A:856:LEU:N	0.54	2.18	5	1
1:B:785:LEU:HD23	1:C:750:ASN:CG	0.54	2.23	15	2
1:C:827:ASP:HA	1:C:830:ILE:HD11	0.54	1.79	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:771:LEU:HD23	1:B:772:ARG:H	0.54	1.61	14	2
1:C:820:ILE:HD13	1:C:826:THR:HG22	0.54	1.79	14	1
1:A:760:LEU:C	1:A:760:LEU:HD13	0.54	2.23	10	5
1:B:682:ILE:HD12	1:B:683:ARG:H	0.54	1.61	11	2
1:B:799:LEU:O	1:B:803:TRP:CE3	0.54	2.61	4	3
1:A:695:LEU:HD23	1:A:695:LEU:O	0.54	2.03	2	7
1:C:702:LEU:O	1:C:702:LEU:HD13	0.54	2.03	4	1
1:C:793:LEU:HD13	1:C:794:LYS:N	0.54	2.18	10	1
1:A:845:ARG:O	1:A:847:ILE:HD13	0.54	2.03	1	1
1:C:771:LEU:HD22	1:C:771:LEU:N	0.54	2.17	11	8
1:A:802:TYR:CE1	1:B:760:LEU:HD11	0.54	2.38	7	1
1:C:819:ALA:HB1	1:C:826:THR:HG23	0.54	1.80	11	1
1:A:704:LEU:HD11	1:B:707:ARG:CG	0.53	2.33	6	2
1:C:753:LEU:C	1:C:753:LEU:HD22	0.53	2.23	6	4
1:B:686:ILE:CG2	1:C:686:ILE:HD11	0.53	2.32	2	2
1:B:695:LEU:HD23	1:B:695:LEU:O	0.53	2.04	2	2
1:B:796:TRP:NE1	1:C:756:ILE:HD11	0.53	2.18	2	1
1:A:669:LEU:HD23	1:A:676:THR:HG23	0.53	1.80	8	1
1:B:669:LEU:HD23	1:B:676:THR:HG23	0.53	1.79	12	4
1:C:768:TYR:CG	1:C:771:LEU:HD11	0.53	2.38	13	1
1:A:774:LEU:HD13	1:A:774:LEU:O	0.53	2.03	13	2
1:B:710:GLN:O	1:B:715:LEU:HD23	0.53	2.03	4	1
1:A:694:GLY:O	1:A:697:ILE:HG22	0.53	2.04	11	6
1:C:705:VAL:HG21	1:C:748:LEU:CD1	0.53	2.33	7	1
1:A:693:ILE:C	1:A:693:ILE:HD13	0.53	2.24	2	4
1:A:785:LEU:HD21	1:B:750:ASN:ND2	0.53	2.18	11	2
1:B:693:ILE:CD1	1:C:692:LEU:HD23	0.53	2.34	13	2
1:B:812:VAL:HG11	1:B:834:GLN:HE21	0.53	1.61	10	1
1:C:775:LEU:HD22	1:C:775:LEU:C	0.53	2.23	11	2
1:B:797:TRP:CD1	1:B:847:ILE:HD11	0.53	2.38	12	1
1:A:790:TRP:CH2	1:A:851:LEU:HD22	0.53	2.38	13	1
1:C:771:LEU:HD22	1:C:771:LEU:H	0.53	1.63	11	2
1:A:770:ARG:O	1:A:773:ASP:N	0.53	2.42	13	2
1:C:790:TRP:CH2	1:C:793:LEU:HD13	0.53	2.37	7	1
1:A:707:ARG:HA	1:C:704:LEU:HD13	0.53	1.81	10	2
1:A:820:ILE:O	1:A:822:VAL:HG22	0.53	2.03	14	1
1:A:763:LEU:O	1:A:774:LEU:HD13	0.53	2.04	6	1
1:A:693:ILE:HG22	1:C:693:ILE:HD13	0.53	1.80	11	1
1:A:704:LEU:O	1:A:708:VAL:HG22	0.53	2.03	14	1
1:C:756:ILE:HD13	1:C:756:ILE:C	0.53	2.24	15	1
1:B:675:ILE:HD11	1:B:679:LEU:HD12	0.53	1.78	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:715:LEU:O	1:B:716:SER:C	0.53	2.48	4	1
1:B:803:TRP:CZ2	1:C:760:LEU:HD22	0.53	2.39	4	1
1:A:760:LEU:HD21	1:C:803:TRP:CH2	0.53	2.38	5	1
1:C:771:LEU:HD22	1:C:772:ARG:H	0.53	1.61	10	1
1:B:830:ILE:HD12	1:B:831:GLU:N	0.53	2.18	11	1
1:C:663:LEU:HD23	1:C:663:LEU:O	0.53	2.03	11	1
1:C:807:LEU:O	1:C:807:LEU:HD13	0.53	2.03	12	2
1:A:803:TRP:N	1:A:803:TRP:CE3	0.53	2.77	4	13
1:C:820:ILE:HD11	1:C:827:ASP:HB2	0.53	1.78	1	1
1:A:689:VAL:O	1:A:692:LEU:HD22	0.53	2.04	8	1
1:B:675:ILE:HD12	1:B:675:ILE:O	0.53	2.04	7	2
1:B:819:ALA:HB1	1:B:826:THR:CG2	0.53	2.34	15	2
1:B:697:ILE:HD11	1:C:696:ARG:HD2	0.53	1.81	7	1
1:B:753:LEU:HD22	1:B:753:LEU:O	0.53	2.04	7	3
1:A:675:ILE:HD12	1:A:678:TRP:CE3	0.52	2.38	1	2
1:B:803:TRP:N	1:B:803:TRP:CE3	0.52	2.77	15	11
1:C:836:ALA:O	1:C:840:ILE:HG23	0.52	2.04	8	2
1:B:743:ASP:HA	1:B:746:ILE:HD12	0.52	1.80	7	1
1:A:675:ILE:CD1	1:A:679:LEU:HD23	0.52	2.34	8	1
1:A:748:LEU:HD23	1:A:748:LEU:O	0.52	2.04	11	2
1:A:710:GLN:CG	1:A:715:LEU:HD22	0.52	2.34	9	1
1:A:763:LEU:HD22	1:A:763:LEU:C	0.52	2.24	2	1
1:A:663:LEU:HD22	1:A:663:LEU:C	0.52	2.25	6	4
1:B:667:ALA:CA	1:C:660:LEU:HD11	0.52	2.34	2	1
1:A:754:ALA:HB3	1:B:715:LEU:HD21	0.52	1.81	9	1
1:A:820:ILE:HD12	1:A:827:ASP:OD1	0.52	2.04	10	1
1:A:696:ARG:HD3	1:C:693:ILE:HD11	0.52	1.82	15	1
1:A:771:LEU:HD11	1:A:772:ARG:NH2	0.52	2.19	3	1
1:A:763:LEU:HD13	1:A:763:LEU:N	0.52	2.20	4	1
1:B:816:ASN:O	1:B:820:ILE:HD12	0.52	2.05	4	1
1:A:693:ILE:HD13	1:B:696:ARG:HE	0.52	1.64	8	1
1:A:747:ARG:HG3	1:C:785:LEU:HD21	0.52	1.81	12	1
1:B:806:GLU:CB	1:C:771:LEU:HD21	0.52	2.34	10	1
1:A:791:GLU:O	1:A:794:LYS:HD2	0.52	2.05	1	1
1:B:771:LEU:N	1:B:771:LEU:HD22	0.52	2.20	8	6
1:C:779:THR:O	1:C:782:VAL:HG12	0.52	2.04	3	1
1:A:707:ARG:HB3	1:C:704:LEU:HD11	0.52	1.81	4	1
1:B:771:LEU:N	1:B:771:LEU:HD13	0.52	2.19	6	1
1:B:781:ILE:HD13	1:C:746:ILE:HG23	0.52	1.82	6	1
1:B:822:VAL:CG1	1:B:826:THR:HG22	0.52	2.34	8	1
1:B:686:ILE:CG2	1:C:686:ILE:HD12	0.52	2.35	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:756:ILE:HG21	1:C:795:TYR:CB	0.52	2.34	1	2
1:C:675:ILE:HG23	1:C:678:TRP:CZ2	0.52	2.40	4	1
1:B:771:LEU:HD13	1:B:771:LEU:N	0.52	2.19	7	3
1:C:803:TRP:N	1:C:803:TRP:CE3	0.52	2.78	3	15
1:B:781:ILE:HD12	1:C:746:ILE:HG21	0.52	1.79	3	1
1:B:781:ILE:HD12	1:C:746:ILE:CG2	0.52	2.35	3	1
1:C:745:SER:O	1:C:748:LEU:HD12	0.52	2.04	4	1
1:A:760:LEU:HD22	1:A:760:LEU:O	0.52	2.03	13	5
1:A:713:SER:O	1:A:714:PRO:C	0.52	2.49	11	5
1:C:794:LYS:HD3	1:C:795:TYR:N	0.52	2.19	6	1
1:C:678:TRP:CD1	1:C:682:ILE:HG21	0.52	2.40	11	1
1:A:697:ILE:HD13	1:A:698:VAL:H	0.52	1.65	4	3
1:A:795:TYR:CD1	1:B:756:ILE:HG23	0.52	2.40	11	1
1:A:803:TRP:N	1:A:803:TRP:HE3	0.51	2.04	1	7
1:C:753:LEU:HD12	1:C:754:ALA:N	0.51	2.19	1	1
1:B:819:ALA:HB3	1:B:830:ILE:HD11	0.51	1.82	15	1
1:B:667:ALA:HB2	1:C:660:LEU:CD1	0.51	2.35	2	1
1:A:836:ALA:O	1:A:840:ILE:HG23	0.51	2.06	9	2
1:C:695:LEU:HD13	1:C:696:ARG:HD2	0.51	1.81	10	1
1:C:826:THR:O	1:C:830:ILE:HG22	0.51	2.05	12	1
1:C:777:ILE:O	1:C:781:ILE:HG22	0.51	2.05	15	1
1:B:803:TRP:N	1:B:803:TRP:HE3	0.51	2.03	13	5
1:A:808:LYS:O	1:A:812:VAL:HG23	0.51	2.05	15	4
1:B:795:TYR:O	1:B:799:LEU:HD12	0.51	2.04	13	1
1:B:704:LEU:HD22	1:C:710:GLN:HG3	0.51	1.83	1	1
1:B:814:LEU:O	1:B:818:THR:HG22	0.51	2.05	1	1
1:A:760:LEU:HA	1:A:763:LEU:HD22	0.51	1.81	5	1
1:B:828:ARG:O	1:B:832:VAL:HG22	0.51	2.05	7	3
1:C:819:ALA:CB	1:C:830:ILE:HD11	0.51	2.34	8	1
1:A:756:ILE:HG21	1:C:795:TYR:CD2	0.51	2.41	12	1
1:A:791:GLU:HG3	1:B:753:LEU:HD13	0.51	1.82	1	1
1:A:763:LEU:HD13	1:A:764:SER:N	0.51	2.21	2	1
1:C:785:LEU:HD23	1:C:788:ARG:HD3	0.51	1.83	3	1
1:A:754:ALA:HB1	1:B:715:LEU:CB	0.51	2.35	7	1
1:A:826:THR:O	1:A:830:ILE:HG22	0.51	2.06	1	1
1:C:781:ILE:HG22	1:C:785:LEU:HD11	0.51	1.83	3	1
1:C:840:ILE:HD13	1:C:840:ILE:O	0.51	2.05	3	2
1:C:702:LEU:HD13	1:C:703:SER:N	0.51	2.20	5	3
1:A:793:LEU:HD13	1:A:847:ILE:HD12	0.51	1.83	6	1
1:A:816:ASN:CG	1:A:830:ILE:HD11	0.51	2.26	7	1
1:B:763:LEU:HD22	1:B:763:LEU:C	0.51	2.26	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:819:ALA:HB3	1:B:827:ASP:HB3	0.51	1.83	1	1
1:B:799:LEU:CD2	1:C:756:ILE:HD12	0.51	2.36	8	1
1:A:693:ILE:HD12	1:B:692:LEU:HD23	0.51	1.82	7	1
1:A:692:LEU:H	1:A:692:LEU:HD13	0.51	1.66	8	1
1:A:806:GLU:HB3	1:B:771:LEU:HD21	0.51	1.83	11	2
1:C:748:LEU:HD22	1:C:748:LEU:C	0.51	2.27	8	1
1:A:826:THR:O	1:A:829:VAL:HG12	0.51	2.06	10	1
1:A:796:TRP:HA	1:A:799:LEU:HD22	0.51	1.82	11	1
1:A:693:ILE:HD13	1:B:696:ARG:NE	0.50	2.20	8	1
1:C:793:LEU:HD13	1:C:793:LEU:C	0.50	2.26	10	1
1:C:843:ILE:H	1:C:843:ILE:HD13	0.50	1.65	7	1
1:A:750:ASN:O	1:A:753:LEU:HD23	0.50	2.07	10	1
1:A:756:ILE:H	1:A:756:ILE:HD12	0.50	1.65	2	1
1:A:771:LEU:HD23	1:A:771:LEU:H	0.50	1.65	13	1
1:C:759:ASP:O	1:C:763:LEU:HD22	0.50	2.05	13	1
1:A:828:ARG:O	1:A:832:VAL:HG12	0.50	2.07	3	5
1:A:760:LEU:HD11	1:C:803:TRP:CZ2	0.50	2.42	3	1
1:B:697:ILE:HD11	1:C:696:ARG:HB3	0.50	1.83	3	1
1:C:797:TRP:CD1	1:C:847:ILE:HD12	0.50	2.42	4	3
1:A:785:LEU:HD13	1:B:749:VAL:CB	0.50	2.36	5	1
1:C:778:VAL:O	1:C:781:ILE:HG22	0.50	2.07	12	1
1:A:754:ALA:HB3	1:B:715:LEU:HD22	0.50	1.81	14	2
1:B:675:ILE:HD12	1:B:678:TRP:CZ3	0.50	2.41	2	1
1:A:781:ILE:CG2	1:B:746:ILE:HG23	0.50	2.32	4	1
1:B:704:LEU:HD13	1:C:707:ARG:HA	0.50	1.82	4	1
1:A:669:LEU:HD23	1:A:670:TRP:CZ3	0.50	2.41	5	1
1:A:753:LEU:C	1:A:753:LEU:HD12	0.50	2.27	7	3
1:B:778:VAL:HA	1:B:781:ILE:HD11	0.50	1.83	1	1
1:A:760:LEU:HD21	1:C:803:TRP:CZ2	0.50	2.42	5	2
1:A:693:ILE:HD11	1:B:696:ARG:HG3	0.50	1.83	6	1
1:B:663:LEU:HD13	1:B:663:LEU:O	0.50	2.07	7	1
1:C:774:LEU:HD22	1:C:774:LEU:C	0.50	2.27	12	1
1:A:816:ASN:O	1:A:820:ILE:HD13	0.50	2.07	3	1
1:C:796:TRP:HA	1:C:799:LEU:HD22	0.50	1.84	3	1
1:A:746:ILE:HG12	1:C:781:ILE:HD13	0.50	1.84	4	1
1:C:790:TRP:CZ3	1:C:792:ALA:HB3	0.50	2.42	7	1
1:A:682:ILE:C	1:A:682:ILE:HD13	0.50	2.27	9	1
1:B:751:GLY:O	1:C:715:LEU:HD21	0.50	2.06	9	1
1:A:742:ARG:CZ	1:C:765:LEU:HD11	0.50	2.36	11	1
1:C:698:VAL:HG23	1:C:699:PHE:HD2	0.50	1.66	12	1
1:A:764:SER:CB	1:A:771:LEU:HD12	0.50	2.37	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:799:LEU:HD13	1:B:756:ILE:HD12	0.49	1.84	3	1
1:C:835:GLY:O	1:C:839:ALA:HB3	0.49	2.07	5	1
1:B:672:TRP:HB3	1:B:675:ILE:HG23	0.49	1.83	14	1
1:A:697:ILE:HD13	1:A:698:VAL:N	0.49	2.22	3	3
1:B:775:LEU:H	1:B:775:LEU:HD22	0.49	1.66	6	1
1:C:742:ARG:O	1:C:746:ILE:HD13	0.49	2.06	6	2
1:A:759:ASP:O	1:A:763:LEU:HD22	0.49	2.07	8	1
1:B:748:LEU:HD23	1:C:714:PRO:CB	0.49	2.37	10	1
1:A:750:ASN:ND2	1:C:781:ILE:HD11	0.49	2.22	11	1
1:B:826:THR:O	1:B:829:VAL:HG22	0.49	2.08	15	1
1:A:795:TYR:CE1	1:A:796:TRP:CD1	0.49	3.01	7	5
1:A:703:SER:OG	1:C:700:ALA:HB1	0.49	2.07	6	1
1:C:847:ILE:HD12	1:C:848:ARG:N	0.49	2.23	7	1
1:C:697:ILE:HD12	1:C:698:VAL:N	0.49	2.22	8	1
1:A:793:LEU:HD13	1:A:847:ILE:CG1	0.49	2.38	2	1
1:B:686:ILE:HG23	1:C:686:ILE:CD1	0.49	2.37	3	1
1:B:715:LEU:C	1:B:715:LEU:HD22	0.49	2.27	15	1
1:A:756:ILE:HD12	1:A:756:ILE:N	0.49	2.23	6	3
1:C:856:LEU:HD22	1:C:856:LEU:C	0.49	2.28	7	1
1:A:708:VAL:HG12	1:A:741:ASP:CG	0.49	2.28	8	1
1:B:843:ILE:H	1:B:843:ILE:HD13	0.49	1.66	12	1
1:B:695:LEU:HD21	1:B:699:PHE:CE2	0.49	2.42	1	1
1:C:685:PHE:O	1:C:689:VAL:HG23	0.49	2.07	2	2
1:A:708:VAL:HG11	1:B:713:SER:HA	0.49	1.83	3	1
1:A:791:GLU:HB3	1:B:753:LEU:HD23	0.49	1.85	7	2
1:A:793:LEU:CD1	1:A:847:ILE:HD11	0.49	2.38	7	1
1:B:694:GLY:HA2	1:B:697:ILE:HD13	0.49	1.84	7	1
1:C:793:LEU:HD12	1:C:848:ARG:CB	0.49	2.38	10	1
1:C:715:LEU:HD22	1:C:715:LEU:C	0.49	2.27	2	1
1:C:748:LEU:C	1:C:748:LEU:HD22	0.49	2.28	4	1
1:A:799:LEU:O	1:A:803:TRP:CD2	0.49	2.66	13	2
1:A:830:ILE:HD13	1:A:831:GLU:H	0.49	1.67	7	1
1:B:797:TRP:CD2	1:B:847:ILE:HD11	0.49	2.43	12	1
1:A:854:ILE:H	1:A:854:ILE:HD13	0.49	1.67	2	1
1:C:828:ARG:O	1:C:832:VAL:HG22	0.49	2.08	4	4
1:A:785:LEU:C	1:A:785:LEU:HD13	0.49	2.28	12	1
1:A:830:ILE:HD12	1:A:830:ILE:O	0.49	2.07	15	1
1:A:757:TRP:CH2	1:B:715:LEU:HD13	0.49	2.43	4	1
1:C:799:LEU:HD23	1:C:800:LEU:HG	0.49	1.84	4	1
1:A:756:ILE:O	1:A:760:LEU:HB3	0.49	2.06	15	4
1:A:785:LEU:HD11	1:B:746:ILE:HG23	0.49	1.85	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:819:ALA:HB1	1:C:826:THR:HB	0.49	1.85	13	4
1:A:792:ALA:HA	1:A:795:TYR:CE2	0.49	2.42	6	1
1:B:760:LEU:HD12	1:B:760:LEU:C	0.49	2.27	8	1
1:C:750:ASN:N	1:C:750:ASN:HD22	0.49	2.06	14	1
1:A:693:ILE:HD11	1:B:696:ARG:CD	0.48	2.38	1	1
1:B:843:ILE:O	1:B:843:ILE:HG23	0.48	2.08	1	5
1:B:820:ILE:O	1:B:822:VAL:N	0.48	2.46	4	1
1:B:781:ILE:HD13	1:C:746:ILE:CG2	0.48	2.38	6	1
1:A:785:LEU:HD13	1:A:785:LEU:C	0.48	2.29	14	1
1:A:702:LEU:C	1:A:702:LEU:HD13	0.48	2.28	15	1
1:C:672:TRP:O	1:C:674:ASP:N	0.48	2.46	15	1
1:A:695:LEU:HD22	1:A:696:ARG:NH1	0.48	2.23	3	1
1:C:803:TRP:N	1:C:803:TRP:HE3	0.48	2.07	7	3
1:B:764:SER:HB2	1:B:771:LEU:HD12	0.48	1.84	10	1
1:B:830:ILE:HD13	1:B:830:ILE:O	0.48	2.08	8	1
1:B:815:LEU:CD2	1:B:830:ILE:HD13	0.48	2.38	11	1
1:B:836:ALA:O	1:B:840:ILE:HD13	0.48	2.09	11	1
1:B:843:ILE:HD13	1:B:843:ILE:N	0.48	2.23	12	1
1:C:830:ILE:HG22	1:C:834:GLN:NE2	0.48	2.22	13	1
1:C:799:LEU:HD23	1:C:800:LEU:H	0.48	1.68	3	1
1:A:820:ILE:HD11	1:A:827:ASP:HB3	0.48	1.84	6	1
1:C:683:ARG:O	1:C:687:ILE:HD12	0.48	2.08	10	1
1:B:771:LEU:HD23	1:B:771:LEU:N	0.48	2.23	15	2
1:B:791:GLU:OE2	1:C:753:LEU:HD13	0.48	2.08	15	1
1:B:763:LEU:C	1:B:763:LEU:HD22	0.48	2.29	4	1
1:A:704:LEU:HD12	1:B:712:TYR:O	0.48	2.08	5	1
1:A:795:TYR:CD2	1:B:753:LEU:HA	0.48	2.43	6	1
1:B:803:TRP:CH2	1:C:768:TYR:CZ	0.48	3.02	7	1
1:B:672:TRP:N	1:B:672:TRP:CD1	0.48	2.81	8	2
1:C:760:LEU:C	1:C:760:LEU:HD13	0.48	2.29	15	1
1:C:694:GLY:O	1:C:697:ILE:HG22	0.48	2.08	2	1
1:A:768:TYR:C	1:A:770:ARG:H	0.48	2.11	13	3
1:A:675:ILE:HD11	1:A:678:TRP:CE3	0.48	2.44	12	1
1:A:820:ILE:HD11	1:A:827:ASP:OD2	0.48	2.09	14	1
1:B:779:THR:O	1:B:782:VAL:HG12	0.48	2.09	1	1
1:B:742:ARG:O	1:B:746:ILE:HD12	0.48	2.09	5	1
1:A:771:LEU:HD12	1:A:772:ARG:CZ	0.48	2.38	7	1
1:A:771:LEU:HD23	1:A:771:LEU:N	0.48	2.23	13	1
1:A:760:LEU:CD2	1:A:763:LEU:HD21	0.48	2.38	14	1
1:B:685:PHE:HA	1:B:688:ILE:HD12	0.48	1.85	2	1
1:C:828:ARG:O	1:C:832:VAL:HG13	0.48	2.09	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:660:LEU:HD12	1:C:661:LEU:H	0.48	1.69	14	1
1:A:771:LEU:HD22	1:A:771:LEU:H	0.48	1.69	4	2
1:C:781:ILE:O	1:C:781:ILE:HD13	0.48	2.08	9	1
1:B:715:LEU:HD12	1:B:715:LEU:C	0.48	2.29	4	1
1:B:753:LEU:HD22	1:B:753:LEU:C	0.48	2.28	6	2
1:B:771:LEU:HD23	1:B:772:ARG:HD2	0.48	1.85	10	1
1:A:753:LEU:HD22	1:A:753:LEU:O	0.47	2.09	1	2
1:A:750:ASN:HD21	1:C:785:LEU:HD23	0.47	1.69	15	2
1:A:843:ILE:N	1:A:843:ILE:HD12	0.47	2.24	3	1
1:A:696:ARG:HG3	1:C:693:ILE:HD11	0.47	1.86	12	2
1:C:816:ASN:O	1:C:820:ILE:HD13	0.47	2.09	4	1
1:B:768:TYR:HD1	1:B:771:LEU:HD11	0.47	1.69	10	1
1:C:763:LEU:HD22	1:C:763:LEU:C	0.47	2.28	10	1
1:A:791:GLU:CB	1:B:753:LEU:HD22	0.47	2.39	12	1
1:B:697:ILE:HD11	1:C:699:PHE:CE1	0.47	2.44	1	1
1:C:830:ILE:HD13	1:C:830:ILE:C	0.47	2.30	7	2
1:B:686:ILE:HG23	1:C:686:ILE:HD11	0.47	1.84	3	1
1:A:785:LEU:HD13	1:B:749:VAL:CG2	0.47	2.38	5	1
1:A:692:LEU:HD23	1:C:693:ILE:CD1	0.47	2.38	6	1
1:A:799:LEU:HD13	1:B:756:ILE:HG22	0.47	1.84	9	1
1:B:785:LEU:HD21	1:C:747:ARG:NH1	0.47	2.24	15	1
1:B:803:TRP:CE3	1:B:803:TRP:N	0.47	2.83	4	3
1:B:742:ARG:O	1:B:746:ILE:HD13	0.47	2.09	3	1
1:B:808:LYS:O	1:B:812:VAL:HG12	0.47	2.09	14	3
1:A:792:ALA:O	1:A:795:TYR:CD2	0.47	2.67	14	4
1:B:669:LEU:C	1:B:669:LEU:HD12	0.47	2.30	8	1
1:B:797:TRP:CE2	1:B:847:ILE:HD11	0.47	2.44	10	1
1:B:815:LEU:HD21	1:B:830:ILE:HD13	0.47	1.85	11	1
1:B:820:ILE:HD11	1:B:827:ASP:HB2	0.47	1.86	11	1
1:A:774:LEU:HD21	1:B:742:ARG:NH2	0.47	2.24	13	1
1:B:705:VAL:HG12	1:B:709:ARG:NH2	0.47	2.24	13	1
1:A:796:TRP:NE1	1:B:756:ILE:HD13	0.47	2.23	1	1
1:A:851:LEU:HD13	1:A:851:LEU:O	0.47	2.08	4	1
1:B:806:GLU:OE2	1:C:771:LEU:HD21	0.47	2.09	4	1
1:A:793:LEU:HD12	1:A:797:TRP:HE1	0.47	1.67	11	1
1:B:675:ILE:HD12	1:B:678:TRP:CE3	0.47	2.45	2	2
1:B:855:LEU:HD23	1:B:855:LEU:O	0.47	2.09	1	1
1:A:663:LEU:HD13	1:A:663:LEU:C	0.47	2.29	14	2
1:B:771:LEU:HD13	1:B:771:LEU:H	0.47	1.68	6	1
1:C:799:LEU:O	1:C:803:TRP:CE3	0.47	2.68	7	1
1:B:854:ILE:O	1:B:854:ILE:HG22	0.47	2.09	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:793:LEU:HD12	1:B:797:TRP:NE1	0.47	2.25	3	1
1:C:808:LYS:O	1:C:812:VAL:HG23	0.47	2.09	4	5
1:B:768:TYR:CD1	1:B:771:LEU:HD11	0.47	2.43	10	1
1:A:774:LEU:HD13	1:A:774:LEU:C	0.47	2.30	4	3
1:B:785:LEU:HD21	1:C:750:ASN:ND2	0.47	2.24	2	1
1:A:742:ARG:O	1:A:746:ILE:HD12	0.47	2.10	6	1
1:B:700:ALA:HB1	1:C:703:SER:OG	0.47	2.10	10	1
1:C:775:LEU:HD22	1:C:775:LEU:O	0.47	2.09	11	1
1:A:705:VAL:HG11	1:A:745:SER:CB	0.47	2.39	12	1
1:A:847:ILE:HG23	1:A:848:ARG:N	0.47	2.25	12	1
1:C:663:LEU:HD13	1:C:663:LEU:H	0.47	1.69	12	1
1:B:660:LEU:N	1:B:660:LEU:HD12	0.47	2.25	13	1
1:A:753:LEU:HA	1:C:791:GLU:OE2	0.47	2.09	14	1
1:A:770:ARG:O	1:A:774:LEU:N	0.47	2.48	11	5
1:A:715:LEU:HD12	1:C:751:GLY:HA3	0.47	1.87	2	1
1:B:687:ILE:HD12	1:B:687:ILE:H	0.47	1.69	2	1
1:B:754:ALA:HB1	1:C:715:LEU:HB3	0.47	1.87	3	1
1:C:808:LYS:O	1:C:812:VAL:HG12	0.47	2.09	11	2
1:A:760:LEU:HD22	1:A:760:LEU:C	0.47	2.30	13	1
1:A:753:LEU:HD13	1:A:753:LEU:C	0.47	2.30	15	1
1:A:765:LEU:HD12	1:A:770:ARG:HH21	0.47	1.68	1	1
1:C:829:VAL:O	1:C:833:VAL:HG12	0.47	2.09	1	1
1:A:781:ILE:HG21	1:B:746:ILE:HG21	0.47	1.87	8	2
1:B:710:GLN:CD	1:B:715:LEU:HD21	0.47	2.30	3	1
1:A:746:ILE:CG2	1:C:781:ILE:HG21	0.47	2.40	5	3
1:A:750:ASN:HD21	1:C:785:LEU:HD13	0.47	1.69	6	1
1:B:705:VAL:CG2	1:B:748:LEU:HD13	0.47	2.40	6	1
1:C:793:LEU:HD12	1:C:848:ARG:HB2	0.47	1.87	10	1
1:A:836:ALA:O	1:A:840:ILE:HD13	0.47	2.09	11	1
1:B:794:LYS:HD3	1:B:795:TYR:N	0.47	2.25	2	5
1:C:790:TRP:C	1:C:792:ALA:N	0.47	2.68	5	5
1:A:791:GLU:O	1:A:795:TYR:CD2	0.47	2.68	6	1
1:C:750:ASN:O	1:C:753:LEU:HD12	0.47	2.10	7	1
1:A:663:LEU:HD13	1:B:660:LEU:CB	0.47	2.40	8	1
1:A:707:ARG:NH2	1:A:712:TYR:CZ	0.47	2.83	11	1
1:A:669:LEU:HD12	1:A:676:THR:HG23	0.46	1.86	1	1
1:B:793:LEU:C	1:B:793:LEU:HD13	0.46	2.30	12	2
1:C:847:ILE:H	1:C:847:ILE:HD13	0.46	1.69	9	2
1:B:847:ILE:C	1:B:847:ILE:HD13	0.46	2.30	15	1
1:B:796:TRP:CD1	1:C:756:ILE:HD11	0.46	2.45	3	1
1:C:832:VAL:O	1:C:836:ALA:HB2	0.46	2.10	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:820:ILE:HD12	1:A:820:ILE:N	0.46	2.25	12	3
1:A:755:LEU:HD22	1:A:755:LEU:C	0.46	2.30	8	1
1:A:790:TRP:CE2	1:A:793:LEU:HD23	0.46	2.45	15	2
1:A:707:ARG:HB3	1:C:704:LEU:HD21	0.46	1.86	12	2
1:A:802:TYR:CD1	1:B:768:TYR:CZ	0.46	3.03	14	1
1:B:799:LEU:HD13	1:C:756:ILE:HG23	0.46	1.87	2	1
1:C:687:ILE:H	1:C:687:ILE:HD12	0.46	1.70	13	1
1:A:771:LEU:H	1:A:771:LEU:CD1	0.46	2.22	15	1
1:A:678:TRP:CD1	1:A:682:ILE:HD13	0.46	2.45	2	2
1:B:822:VAL:HG12	1:B:826:THR:CG2	0.46	2.38	8	1
1:B:760:LEU:HD22	1:B:760:LEU:C	0.46	2.30	12	4
1:B:679:LEU:HD13	1:B:679:LEU:O	0.46	2.10	5	1
1:A:692:LEU:HD23	1:C:693:ILE:HD11	0.46	1.87	6	1
1:B:828:ARG:O	1:B:832:VAL:HG13	0.46	2.11	10	3
1:B:684:ILE:HD12	1:B:684:ILE:N	0.46	2.25	8	3
1:C:826:THR:O	1:C:829:VAL:HG22	0.46	2.10	11	1
1:A:771:LEU:HD13	1:A:771:LEU:N	0.46	2.23	15	2
1:C:790:TRP:CE3	1:C:793:LEU:HD12	0.46	2.46	5	1
1:A:763:LEU:HB2	1:A:774:LEU:HD22	0.46	1.88	7	1
1:C:843:ILE:HD13	1:C:843:ILE:O	0.46	2.10	13	1
1:A:779:THR:O	1:A:782:VAL:HG12	0.46	2.10	2	1
1:C:856:LEU:HD22	1:C:856:LEU:O	0.46	2.11	7	1
1:A:819:ALA:HB3	1:A:827:ASP:CG	0.46	2.31	10	1
1:B:669:LEU:HD12	1:B:676:THR:HG23	0.46	1.86	1	1
1:A:847:ILE:HD13	1:A:847:ILE:H	0.46	1.70	3	1
1:C:764:SER:O	1:C:765:LEU:O	0.46	2.33	7	1
1:B:843:ILE:HD13	1:B:844:PRO:N	0.46	2.26	11	1
1:A:707:ARG:CG	1:C:704:LEU:HD11	0.46	2.40	1	1
1:A:790:TRP:C	1:A:792:ALA:N	0.46	2.67	2	13
1:C:663:LEU:HD13	1:C:664:ASP:H	0.46	1.71	2	1
1:A:693:ILE:HG13	1:B:693:ILE:HG22	0.46	1.88	5	1
1:A:700:ALA:HB1	1:B:703:SER:OG	0.46	2.11	6	1
1:A:753:LEU:HD22	1:C:788:ARG:O	0.46	2.10	8	1
1:C:705:VAL:HG22	1:C:748:LEU:HD11	0.46	1.87	9	1
1:C:822:VAL:HG22	1:C:823:GLY:N	0.46	2.26	12	1
1:A:843:ILE:O	1:A:843:ILE:HG23	0.46	2.11	14	1
1:B:774:LEU:O	1:B:777:ILE:HG13	0.46	2.11	14	1
1:C:819:ALA:HB3	1:C:826:THR:CG2	0.46	2.24	14	1
1:A:847:ILE:HD13	1:A:847:ILE:N	0.46	2.26	1	1
1:A:781:ILE:HG21	1:B:746:ILE:HG22	0.46	1.87	2	1
1:C:675:ILE:HD12	1:C:678:TRP:CE3	0.46	2.45	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:686:ILE:CD1	1:C:686:ILE:HG21	0.46	2.41	5	1
1:C:661:LEU:HD22	1:C:661:LEU:N	0.46	2.26	6	1
1:C:790:TRP:CH2	1:C:851:LEU:HD22	0.46	2.46	6	1
1:B:830:ILE:HD13	1:B:830:ILE:C	0.46	2.30	8	1
1:B:705:VAL:HG22	1:C:714:PRO:HG3	0.46	1.87	10	1
1:C:799:LEU:HD22	1:C:803:TRP:CE2	0.46	2.44	11	1
1:A:796:TRP:CD1	1:A:799:LEU:HD12	0.46	2.45	15	1
1:C:662:GLU:O	1:C:663:LEU:HD12	0.46	2.10	15	1
1:A:803:TRP:CE3	1:A:803:TRP:N	0.45	2.84	3	2
1:B:667:ALA:HB2	1:C:660:LEU:CD2	0.45	2.41	5	1
1:B:750:ASN:ND2	1:B:750:ASN:H	0.45	2.09	6	3
1:B:812:VAL:HG21	1:B:834:GLN:HG3	0.45	1.87	8	1
1:C:819:ALA:HB1	1:C:826:THR:CB	0.45	2.41	8	1
1:C:763:LEU:C	1:C:774:LEU:HD13	0.45	2.31	9	1
1:A:829:VAL:O	1:A:833:VAL:HG12	0.45	2.11	15	1
1:C:778:VAL:HA	1:C:781:ILE:HD12	0.45	1.87	4	1
1:A:693:ILE:O	1:A:693:ILE:HD13	0.45	2.12	5	2
1:B:775:LEU:HD13	1:B:776:LEU:N	0.45	2.26	11	1
1:B:711:GLY:O	1:B:713:SER:N	0.45	2.48	12	1
1:A:714:PRO:CG	1:C:705:VAL:HG22	0.45	2.41	1	2
1:C:713:SER:O	1:C:714:PRO:C	0.45	2.54	2	5
1:B:675:ILE:HD13	1:B:675:ILE:C	0.45	2.32	8	1
1:A:777:ILE:O	1:A:781:ILE:HD12	0.45	2.11	9	1
1:B:792:ALA:HA	1:B:795:TYR:CZ	0.45	2.47	11	1
1:C:822:VAL:HG13	1:C:823:GLY:H	0.45	1.71	12	1
1:A:702:LEU:HD13	1:A:706:ASN:OD1	0.45	2.12	1	1
1:B:771:LEU:HA	1:B:774:LEU:HD23	0.45	1.88	2	1
1:A:795:TYR:CZ	1:A:796:TRP:CD1	0.45	3.05	5	2
1:B:834:GLN:HG3	1:B:835:GLY:N	0.45	2.26	5	1
1:C:705:VAL:HG21	1:C:748:LEU:HD22	0.45	1.88	5	1
1:A:756:ILE:HG23	1:C:799:LEU:CD2	0.45	2.41	12	1
1:A:689:VAL:O	1:A:692:LEU:HD11	0.45	2.10	13	1
1:A:833:VAL:HG23	1:A:834:GLN:NE2	0.45	2.27	6	1
1:C:785:LEU:HD12	1:C:786:GLY:N	0.45	2.27	6	1
1:B:697:ILE:HD12	1:B:697:ILE:N	0.45	2.26	7	1
1:B:753:LEU:O	1:B:756:ILE:HG22	0.45	2.12	15	2
1:A:693:ILE:HG21	1:B:693:ILE:HG22	0.45	1.87	11	2
1:A:791:GLU:OE2	1:B:753:LEU:HD13	0.45	2.10	12	2
1:B:820:ILE:HD11	1:B:827:ASP:CB	0.45	2.41	11	1
1:A:683:ARG:O	1:A:687:ILE:HD12	0.45	2.11	13	1
1:B:678:TRP:CD1	1:B:678:TRP:C	0.45	2.90	12	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:816:ASN:HA	1:A:830:ILE:HG21	0.45	1.89	8	1
1:A:778:VAL:O	1:A:782:VAL:HG23	0.45	2.11	9	1
1:C:760:LEU:HD22	1:C:760:LEU:C	0.45	2.31	1	1
1:A:851:LEU:C	1:A:851:LEU:HD13	0.45	2.32	15	3
1:A:750:ASN:CG	1:C:785:LEU:HD21	0.45	2.32	4	1
1:A:744:ARG:O	1:A:747:ARG:HB2	0.45	2.12	9	1
1:B:791:GLU:HB3	1:C:753:LEU:HD23	0.45	1.89	9	1
1:B:762:SER:O	1:B:765:LEU:HD23	0.45	2.11	14	1
1:A:678:TRP:C	1:A:678:TRP:CD1	0.45	2.90	9	2
1:A:705:VAL:HG21	1:A:748:LEU:CD1	0.45	2.40	10	1
1:A:828:ARG:O	1:A:832:VAL:HG23	0.45	2.12	9	2
1:B:760:LEU:HD13	1:B:760:LEU:C	0.45	2.32	1	1
1:B:744:ARG:O	1:B:747:ARG:HB2	0.45	2.11	3	1
1:A:791:GLU:HG2	1:B:753:LEU:HD23	0.45	1.89	10	1
1:B:791:GLU:OE1	1:C:753:LEU:HD23	0.45	2.12	11	1
1:A:686:ILE:CG1	1:B:686:ILE:HD11	0.45	2.42	12	1
1:B:704:LEU:HD13	1:C:707:ARG:HB2	0.45	1.89	13	1
1:C:776:LEU:O	1:C:776:LEU:HD23	0.45	2.11	14	2
1:C:678:TRP:C	1:C:678:TRP:CD1	0.45	2.91	7	1
1:A:756:ILE:HG23	1:C:799:LEU:HD21	0.45	1.89	12	1
1:A:692:LEU:HD12	1:A:693:ILE:H	0.45	1.71	13	1
1:C:843:ILE:N	1:C:844:PRO:CD	0.45	2.80	13	2
1:B:753:LEU:HD13	1:B:753:LEU:C	0.44	2.32	7	2
1:A:819:ALA:O	1:A:822:VAL:HG22	0.44	2.12	11	1
1:B:771:LEU:HD22	1:B:771:LEU:H	0.44	1.72	1	1
1:B:663:LEU:C	1:B:663:LEU:HD13	0.44	2.33	2	1
1:C:695:LEU:C	1:C:695:LEU:HD23	0.44	2.32	6	1
1:A:777:ILE:HD12	1:A:778:VAL:N	0.44	2.28	8	1
1:B:771:LEU:HD23	1:B:772:ARG:CD	0.44	2.42	10	1
1:B:803:TRP:CE3	1:C:768:TYR:CZ	0.44	3.05	13	1
1:A:760:LEU:HD23	1:C:799:LEU:CD2	0.44	2.41	1	1
1:A:790:TRP:CE3	1:A:790:TRP:HA	0.44	2.47	5	2
1:B:855:LEU:HD13	1:B:855:LEU:C	0.44	2.33	2	1
1:C:829:VAL:O	1:C:833:VAL:HG23	0.44	2.12	4	2
1:A:663:LEU:HD11	1:B:660:LEU:HB2	0.44	1.88	5	1
1:A:750:ASN:ND2	1:C:785:LEU:HD13	0.44	2.26	6	1
1:A:771:LEU:C	1:A:771:LEU:CD1	0.44	2.86	7	1
1:A:795:TYR:CE2	1:A:796:TRP:CD1	0.44	3.06	14	2
1:B:704:LEU:HD13	1:B:704:LEU:O	0.44	2.13	9	1
1:C:771:LEU:HD13	1:C:771:LEU:N	0.44	2.26	10	1
1:B:704:LEU:HD21	1:C:707:ARG:HA	0.44	1.90	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:756:ILE:O	1:B:760:LEU:HB3	0.44	2.12	11	2
1:C:816:ASN:OD1	1:C:830:ILE:HG21	0.44	2.13	3	1
1:B:693:ILE:HD13	1:C:696:ARG:NE	0.44	2.26	12	1
1:A:669:LEU:HD22	1:A:669:LEU:N	0.44	2.27	3	1
1:C:763:LEU:HD23	1:C:763:LEU:C	0.44	2.33	3	2
1:A:795:TYR:HA	1:B:756:ILE:HD13	0.44	1.88	5	1
1:C:705:VAL:HG21	1:C:748:LEU:HD12	0.44	1.88	7	1
1:A:693:ILE:HD11	1:B:696:ARG:CZ	0.44	2.41	4	1
1:B:775:LEU:C	1:B:775:LEU:HD13	0.44	2.33	4	1
1:B:699:PHE:CD2	1:B:702:LEU:HD23	0.44	2.47	12	1
1:A:741:ASP:O	1:A:745:SER:N	0.44	2.50	3	2
1:A:755:LEU:HD13	1:A:755:LEU:C	0.44	2.32	8	1
1:B:816:ASN:OD1	1:B:830:ILE:HD11	0.44	2.12	1	1
1:B:790:TRP:C	1:B:792:ALA:N	0.44	2.71	14	7
1:B:713:SER:O	1:B:714:PRO:C	0.44	2.57	4	6
1:C:756:ILE:O	1:C:760:LEU:HG	0.44	2.13	4	1
1:B:763:LEU:O	1:B:774:LEU:CB	0.44	2.66	14	2
1:B:806:GLU:HG3	1:C:771:LEU:HD11	0.44	1.90	5	1
1:C:765:LEU:HD12	1:C:765:LEU:C	0.44	2.32	7	1
1:C:682:ILE:HD13	1:C:683:ARG:H	0.44	1.71	8	1
1:A:747:ARG:NE	1:C:785:LEU:HD21	0.44	2.27	9	1
1:A:820:ILE:HD12	1:A:827:ASP:CG	0.44	2.32	10	1
1:C:793:LEU:O	1:C:797:TRP:CD1	0.44	2.71	12	1
1:B:819:ALA:CB	1:B:830:ILE:HD11	0.44	2.42	15	1
1:A:712:TYR:O	1:C:704:LEU:HD11	0.44	2.13	3	2
1:B:774:LEU:O	1:B:778:VAL:HG23	0.44	2.12	3	1
1:A:826:THR:O	1:A:830:ILE:HD12	0.44	2.12	5	1
1:B:771:LEU:H	1:B:771:LEU:HD22	0.44	1.73	10	2
1:C:822:VAL:HG12	1:C:822:VAL:O	0.44	2.12	10	1
1:A:771:LEU:O	1:A:774:LEU:HD23	0.44	2.13	12	1
1:B:756:ILE:C	1:B:756:ILE:HD13	0.44	2.33	13	1
1:A:753:LEU:C	1:A:753:LEU:CD2	0.43	2.85	6	2
1:C:673:PHE:O	1:C:674:ASP:CB	0.43	2.66	2	1
1:B:797:TRP:CD1	1:B:847:ILE:HG21	0.43	2.48	3	1
1:A:795:TYR:CD1	1:B:756:ILE:HD13	0.43	2.48	6	1
1:B:754:ALA:HB1	1:C:715:LEU:O	0.43	2.13	6	1
1:A:760:LEU:HD23	1:A:763:LEU:HD21	0.43	1.89	7	1
1:B:796:TRP:CD1	1:C:756:ILE:HD13	0.43	2.48	7	1
1:B:710:GLN:OE1	1:B:715:LEU:HD11	0.43	2.13	8	1
1:A:715:LEU:O	1:C:754:ALA:HB1	0.43	2.13	9	1
1:B:663:LEU:C	1:B:663:LEU:HD12	0.43	2.33	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:769:HIS:N	1:B:771:LEU:HD22	0.43	2.28	11	1
1:C:703:SER:O	1:C:706:ASN:ND2	0.43	2.52	11	1
1:B:803:TRP:CE2	1:C:768:TYR:OH	0.43	2.65	13	1
1:A:679:LEU:HD21	1:C:683:ARG:HH12	0.43	1.73	15	1
1:A:686:ILE:CG2	1:B:686:ILE:HD11	0.43	2.43	15	1
1:B:688:ILE:HD12	1:B:688:ILE:N	0.43	2.28	10	3
1:B:774:LEU:C	1:B:774:LEU:HD13	0.43	2.33	4	1
1:C:799:LEU:O	1:C:803:TRP:CE2	0.43	2.71	5	1
1:C:695:LEU:HD23	1:C:695:LEU:O	0.43	2.13	6	1
1:C:790:TRP:O	1:C:790:TRP:CD1	0.43	2.71	6	1
1:C:749:VAL:HG23	1:C:750:ASN:N	0.43	2.29	8	1
1:A:753:LEU:HA	1:C:791:GLU:CD	0.43	2.34	14	1
1:A:771:LEU:HD21	1:C:806:GLU:HG2	0.43	1.89	15	1
1:A:678:TRP:CD1	1:A:678:TRP:C	0.43	2.91	11	6
1:B:702:LEU:C	1:B:702:LEU:CD1	0.43	2.87	10	2
1:B:774:LEU:HD13	1:B:774:LEU:O	0.43	2.13	10	1
1:B:855:LEU:C	1:B:855:LEU:HD12	0.43	2.33	11	1
1:C:822:VAL:HG22	1:C:822:VAL:O	0.43	2.12	11	1
1:B:768:TYR:O	1:B:771:LEU:CD1	0.43	2.66	12	1
1:A:663:LEU:O	1:A:663:LEU:HD23	0.43	2.14	15	1
1:A:830:ILE:HG23	1:A:831:GLU:N	0.43	2.29	1	1
1:A:693:ILE:HD13	1:A:693:ILE:C	0.43	2.34	3	1
1:B:707:ARG:NH1	1:C:712:TYR:O	0.43	2.52	7	1
1:B:847:ILE:HD11	1:B:851:LEU:CD1	0.43	2.44	7	1
1:B:768:TYR:O	1:B:769:HIS:CG	0.43	2.71	8	1
1:B:836:ALA:O	1:B:840:ILE:HD12	0.43	2.13	8	2
1:C:778:VAL:O	1:C:782:VAL:HG23	0.43	2.13	15	1
1:A:747:ARG:O	1:A:750:ASN:N	0.43	2.52	4	2
1:B:785:LEU:HD23	1:C:750:ASN:CB	0.43	2.43	10	1
1:C:742:ARG:O	1:C:746:ILE:HD12	0.43	2.14	12	1
1:C:851:LEU:O	1:C:851:LEU:HD13	0.43	2.14	12	1
1:B:771:LEU:HD23	1:B:771:LEU:H	0.43	1.73	13	1
1:A:704:LEU:N	1:A:704:LEU:HD22	0.43	2.28	14	1
1:A:756:ILE:O	1:A:760:LEU:CD1	0.43	2.67	4	1
1:B:803:TRP:HH2	1:C:760:LEU:HD22	0.43	1.69	4	1
1:C:702:LEU:HD13	1:C:702:LEU:C	0.43	2.33	4	2
1:B:812:VAL:HG12	1:B:816:ASN:OD1	0.43	2.13	8	1
1:B:748:LEU:C	1:B:748:LEU:HD12	0.43	2.34	9	1
1:C:851:LEU:HD13	1:C:851:LEU:C	0.43	2.34	12	1
1:A:771:LEU:HD21	1:C:806:GLU:HB2	0.43	1.90	14	1
1:B:760:LEU:C	1:B:760:LEU:HD23	0.43	2.34	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:775:LEU:C	1:C:775:LEU:HD13	0.43	2.34	15	1
1:C:797:TRP:HE1	1:C:847:ILE:HD13	0.43	1.74	2	1
1:A:747:ARG:O	1:A:750:ASN:HB2	0.43	2.12	4	1
1:A:822:VAL:CG2	1:A:826:THR:HG21	0.43	2.44	5	1
1:B:763:LEU:HD22	1:B:764:SER:H	0.43	1.73	7	1
1:A:832:VAL:HG23	1:A:833:VAL:N	0.43	2.28	11	2
1:A:847:ILE:HD12	1:A:848:ARG:N	0.43	2.28	11	2
1:B:750:ASN:HD22	1:B:750:ASN:N	0.43	2.12	11	1
1:B:669:LEU:HD22	1:B:679:LEU:HD22	0.43	1.90	13	1
1:B:812:VAL:HG22	1:B:816:ASN:OD1	0.43	2.14	14	1
1:C:660:LEU:HD12	1:C:661:LEU:N	0.43	2.29	14	1
1:B:704:LEU:HD11	1:C:707:ARG:HB3	0.43	1.89	2	1
1:C:689:VAL:O	1:C:693:ILE:HG23	0.43	2.14	3	1
1:C:763:LEU:HD23	1:C:764:SER:N	0.43	2.29	13	3
1:B:850:GLY:O	1:B:854:ILE:HD12	0.43	2.14	4	1
1:B:799:LEU:HD12	1:C:756:ILE:HD12	0.43	1.91	6	1
1:B:662:GLU:O	1:B:663:LEU:CB	0.43	2.67	7	1
1:A:795:TYR:HB2	1:B:756:ILE:HB	0.43	1.91	8	1
1:B:797:TRP:HE1	1:B:847:ILE:HG21	0.43	1.74	9	1
1:A:795:TYR:OH	1:B:755:LEU:HD23	0.43	2.13	11	1
1:A:704:LEU:HD11	1:B:707:ARG:HG2	0.43	1.90	12	1
1:C:748:LEU:C	1:C:748:LEU:HD13	0.43	2.34	12	1
1:B:803:TRP:CZ3	1:C:768:TYR:CE1	0.43	3.06	15	1
1:C:799:LEU:O	1:C:803:TRP:CD2	0.43	2.71	8	2
1:B:774:LEU:O	1:B:777:ILE:HD12	0.43	2.14	11	1
1:B:843:ILE:HD13	1:B:843:ILE:C	0.43	2.34	11	1
1:A:776:LEU:HD12	1:A:777:ILE:N	0.43	2.29	13	1
1:A:696:ARG:NE	1:C:693:ILE:HD11	0.43	2.29	1	1
1:A:790:TRP:CD1	1:A:793:LEU:HD23	0.43	2.49	2	1
1:A:781:ILE:O	1:A:785:LEU:HG	0.43	2.14	5	1
1:B:747:ARG:HA	1:B:750:ASN:HD21	0.43	1.74	6	1
1:A:715:LEU:HD12	1:A:715:LEU:N	0.43	2.29	11	1
1:A:776:LEU:O	1:A:779:THR:HG22	0.43	2.14	11	1
1:A:795:TYR:CZ	1:A:796:TRP:CE2	0.43	3.07	14	1
1:B:833:VAL:HG23	1:B:834:GLN:N	0.43	2.29	15	1
1:A:663:LEU:C	1:A:663:LEU:HD23	0.42	2.35	13	2
1:A:830:ILE:C	1:A:830:ILE:HD12	0.42	2.34	10	2
1:C:797:TRP:CB	1:C:847:ILE:HD12	0.42	2.44	3	1
1:A:763:LEU:HD23	1:A:763:LEU:C	0.42	2.35	6	2
1:B:704:LEU:HD12	1:C:714:PRO:HA	0.42	1.91	9	1
1:A:768:TYR:CZ	1:C:802:TYR:CD2	0.42	3.06	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:819:ALA:HB1	1:A:826:THR:CB	0.42	2.44	12	1
1:C:756:ILE:H	1:C:756:ILE:HD13	0.42	1.74	12	1
1:B:704:LEU:HD13	1:C:707:ARG:CB	0.42	2.44	13	1
1:C:675:ILE:HD11	1:C:678:TRP:CE3	0.42	2.49	15	1
1:A:746:ILE:O	1:A:749:VAL:HG23	0.42	2.13	14	2
1:C:670:TRP:N	1:C:670:TRP:CD1	0.42	2.87	3	1
1:B:791:GLU:HG2	1:C:753:LEU:HD13	0.42	1.92	5	1
1:C:770:ARG:O	1:C:774:LEU:N	0.42	2.52	12	1
1:B:771:LEU:HD21	1:B:772:ARG:HE	0.42	1.74	14	1
1:A:774:LEU:HD21	1:B:742:ARG:CZ	0.42	2.44	1	1
1:A:793:LEU:HD11	1:A:848:ARG:HB2	0.42	1.89	2	1
1:B:771:LEU:HD13	1:B:772:ARG:H	0.42	1.74	2	1
1:C:775:LEU:O	1:C:778:VAL:HG12	0.42	2.14	2	1
1:C:661:LEU:HD23	1:C:661:LEU:N	0.42	2.30	4	1
1:A:747:ARG:O	1:A:751:GLY:N	0.42	2.52	7	1
1:C:755:LEU:C	1:C:755:LEU:HD23	0.42	2.34	7	1
1:C:843:ILE:HD13	1:C:843:ILE:N	0.42	2.28	7	1
1:A:760:LEU:HD23	1:A:760:LEU:C	0.42	2.34	8	1
1:A:750:ASN:HB3	1:C:785:LEU:HD23	0.42	1.90	11	1
1:B:677:ASN:O	1:B:681:TYR:CZ	0.42	2.72	11	1
1:C:791:GLU:O	1:C:794:LYS:HD2	0.42	2.15	12	1
1:C:830:ILE:HG23	1:C:831:GLU:N	0.42	2.29	12	1
1:B:695:LEU:HD23	1:B:695:LEU:C	0.42	2.35	14	1
1:C:660:LEU:HD12	1:C:660:LEU:O	0.42	2.15	1	1
1:C:833:VAL:HG23	1:C:834:GLN:N	0.42	2.29	12	6
1:A:793:LEU:HD21	1:A:847:ILE:CG1	0.42	2.41	4	1
1:A:812:VAL:HG13	1:A:834:GLN:OE1	0.42	2.15	5	1
1:A:705:VAL:O	1:A:708:VAL:HG23	0.42	2.15	7	1
1:A:816:ASN:CB	1:A:830:ILE:HD11	0.42	2.44	7	1
1:A:675:ILE:HD12	1:A:679:LEU:HD21	0.42	1.90	9	1
1:C:855:LEU:HD12	1:C:855:LEU:C	0.42	2.35	9	1
1:C:753:LEU:O	1:C:756:ILE:HG22	0.42	2.15	14	1
1:C:771:LEU:C	1:C:771:LEU:HD12	0.42	2.34	14	1
1:C:688:ILE:HD12	1:C:688:ILE:N	0.42	2.29	1	1
1:A:803:TRP:CH2	1:B:768:TYR:CZ	0.42	3.06	3	1
1:B:830:ILE:HG23	1:B:831:GLU:N	0.42	2.29	10	4
1:A:757:TRP:CD1	1:A:757:TRP:C	0.42	2.92	4	1
1:C:771:LEU:C	1:C:771:LEU:HD22	0.42	2.35	4	1
1:C:820:ILE:HD13	1:C:820:ILE:N	0.42	2.30	6	1
1:A:751:GLY:HA2	1:B:715:LEU:HD11	0.42	1.90	9	1
1:C:748:LEU:HD13	1:C:748:LEU:C	0.42	2.35	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:688:ILE:HD12	1:A:688:ILE:H	0.42	1.74	2	1
1:B:799:LEU:HD23	1:B:800:LEU:H	0.42	1.72	2	1
1:C:840:ILE:HA	1:C:843:ILE:HD11	0.42	1.90	2	1
1:A:822:VAL:HG13	1:A:823:GLY:N	0.42	2.29	13	1
1:B:765:LEU:C	1:B:765:LEU:HD12	0.42	2.35	1	1
1:C:781:ILE:HG22	1:C:785:LEU:CD1	0.42	2.45	3	1
1:A:748:LEU:C	1:A:748:LEU:HD13	0.42	2.34	6	1
1:A:795:TYR:CE1	1:B:756:ILE:HD13	0.42	2.50	6	1
1:B:708:VAL:HG12	1:B:741:ASP:HB2	0.42	1.92	10	1
1:B:821:ALA:O	1:B:822:VAL:HG22	0.42	2.15	10	1
1:C:764:SER:HB3	1:C:771:LEU:HD12	0.42	1.91	13	1
1:A:760:LEU:HD22	1:A:763:LEU:HD21	0.42	1.90	14	1
1:A:771:LEU:H	1:A:771:LEU:HD22	0.42	1.75	14	1
1:C:832:VAL:HG23	1:C:833:VAL:N	0.42	2.30	14	2
1:A:785:LEU:C	1:A:785:LEU:HD12	0.42	2.35	4	1
1:B:749:VAL:HG23	1:B:750:ASN:N	0.42	2.30	6	1
1:C:708:VAL:HG12	1:C:741:ASP:HB2	0.42	1.91	9	1
1:A:704:LEU:HD12	1:B:710:GLN:OE1	0.42	2.15	10	1
1:B:795:TYR:O	1:B:799:LEU:CD2	0.42	2.68	10	1
1:B:775:LEU:HD13	1:B:775:LEU:C	0.42	2.35	11	1
1:A:747:ARG:HA	1:A:750:ASN:HD21	0.42	1.74	14	1
1:A:843:ILE:HD13	1:A:844:PRO:N	0.42	2.30	15	1
1:A:714:PRO:HB3	1:C:748:LEU:HD13	0.42	1.92	1	1
1:B:775:LEU:O	1:B:778:VAL:HG12	0.42	2.15	2	1
1:A:753:LEU:O	1:A:756:ILE:HG12	0.42	2.15	4	1
1:A:756:ILE:O	1:A:760:LEU:CD2	0.42	2.68	4	1
1:B:841:ARG:O	1:B:842:HIS:C	0.42	2.58	4	1
1:B:808:LYS:O	1:B:812:VAL:HG13	0.42	2.14	6	1
1:C:695:LEU:HD23	1:C:695:LEU:C	0.42	2.35	8	1
1:B:774:LEU:O	1:B:777:ILE:HG23	0.42	2.15	11	1
1:A:796:TRP:CD1	1:A:799:LEU:HD21	0.42	2.49	12	1
1:B:777:ILE:HD13	1:B:777:ILE:C	0.42	2.34	12	1
1:A:771:LEU:HD21	1:C:806:GLU:OE1	0.42	2.14	13	1
1:A:754:ALA:CB	1:B:715:LEU:HD22	0.42	2.45	14	1
1:B:778:VAL:HG23	1:C:746:ILE:HD11	0.42	1.92	2	1
1:A:753:LEU:HD13	1:C:791:GLU:HB3	0.42	1.91	8	1
1:C:760:LEU:C	1:C:760:LEU:HD23	0.42	2.35	8	1
1:B:748:LEU:HD23	1:C:714:PRO:HB3	0.42	1.91	10	1
1:A:753:LEU:HD12	1:A:754:ALA:N	0.42	2.30	12	1
1:A:829:VAL:O	1:A:833:VAL:HG23	0.41	2.15	2	1
1:A:785:LEU:HD21	1:B:746:ILE:CG2	0.41	2.45	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:806:GLU:HG3	1:B:771:LEU:HD21	0.41	1.91	5	1
1:C:715:LEU:HD23	1:C:715:LEU:O	0.41	2.14	5	1
1:C:822:VAL:HG23	1:C:823:GLY:N	0.41	2.30	8	1
1:B:672:TRP:CD1	1:B:672:TRP:N	0.41	2.88	12	2
1:A:748:LEU:HD23	1:A:748:LEU:C	0.41	2.35	11	1
1:A:760:LEU:C	1:A:760:LEU:HD22	0.41	2.35	12	1
1:A:791:GLU:HB2	1:B:753:LEU:HD22	0.41	1.92	12	1
1:A:746:ILE:HD12	1:A:746:ILE:N	0.41	2.29	3	2
1:B:820:ILE:HD12	1:B:820:ILE:N	0.41	2.30	7	2
1:C:750:ASN:ND2	1:C:750:ASN:H	0.41	2.13	3	1
1:C:822:VAL:HG13	1:C:822:VAL:O	0.41	2.15	4	1
1:A:795:TYR:O	1:B:756:ILE:HG21	0.41	2.15	5	2
1:A:764:SER:HB3	1:A:771:LEU:HD23	0.41	1.92	7	1
1:B:819:ALA:O	1:B:822:VAL:HG22	0.41	2.15	9	1
1:C:699:PHE:HA	1:C:702:LEU:HB3	0.41	1.92	9	2
1:B:748:LEU:C	1:B:748:LEU:HD23	0.41	2.35	14	1
1:A:812:VAL:HG23	1:A:813:SER:N	0.41	2.30	2	4
1:A:806:GLU:HG3	1:B:771:LEU:HD11	0.41	1.92	5	1
1:A:775:LEU:HD22	1:A:775:LEU:N	0.41	2.29	6	1
1:C:826:THR:O	1:C:830:ILE:HD13	0.41	2.15	6	1
1:A:710:GLN:HG2	1:A:715:LEU:HD22	0.41	1.90	9	1
1:A:696:ARG:HD2	1:C:697:ILE:HG22	0.41	1.91	10	1
1:B:675:ILE:HD12	1:B:675:ILE:C	0.41	2.34	12	1
1:C:702:LEU:HD22	1:C:702:LEU:C	0.41	2.36	12	1
1:C:774:LEU:HD13	1:C:774:LEU:C	0.41	2.35	12	1
1:A:814:LEU:O	1:A:814:LEU:HD13	0.41	2.15	15	1
1:C:710:GLN:OE1	1:C:715:LEU:HD22	0.41	2.16	1	1
1:B:796:TRP:HA	1:B:799:LEU:HD22	0.41	1.91	2	1
1:A:808:LYS:HE3	1:A:839:ALA:HB2	0.41	1.92	4	1
1:B:712:TYR:CG	1:B:713:SER:N	0.41	2.88	14	2
1:C:690:GLY:O	1:C:693:ILE:HG23	0.41	2.15	8	2
1:A:795:TYR:CD1	1:A:795:TYR:C	0.41	2.94	11	1
1:B:855:LEU:HD22	1:B:855:LEU:C	0.41	2.34	12	1
1:A:707:ARG:NH2	1:C:707:ARG:CZ	0.41	2.83	15	1
1:C:682:ILE:HD13	1:C:682:ILE:N	0.41	2.30	15	1
1:B:826:THR:O	1:B:829:VAL:HG12	0.41	2.15	4	1
1:A:708:VAL:HG21	1:B:714:PRO:HD2	0.41	1.93	5	1
1:B:686:ILE:HD12	1:B:686:ILE:N	0.41	2.30	6	1
1:C:745:SER:O	1:C:748:LEU:HD22	0.41	2.15	6	1
1:A:686:ILE:HG21	1:B:686:ILE:HD11	0.41	1.92	7	1
1:A:661:LEU:HD12	1:C:666:TRP:CG	0.41	2.50	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:820:ILE:N	1:C:820:ILE:HD12	0.41	2.30	11	1
1:A:704:LEU:HD21	1:B:707:ARG:HB2	0.41	1.92	6	1
1:A:714:PRO:O	1:C:704:LEU:HD21	0.41	2.16	3	1
1:A:771:LEU:HD12	1:A:771:LEU:C	0.41	2.36	3	1
1:A:795:TYR:CD2	1:B:753:LEU:O	0.41	2.74	3	1
1:A:803:TRP:CZ2	1:B:760:LEU:HD11	0.41	2.50	3	1
1:B:768:TYR:C	1:B:770:ARG:H	0.41	2.18	5	1
1:C:743:ASP:O	1:C:746:ILE:HG22	0.41	2.15	5	1
1:C:836:ALA:O	1:C:840:ILE:HD12	0.41	2.15	7	1
1:B:794:LYS:CD	1:B:795:TYR:N	0.41	2.84	8	1
1:A:661:LEU:HD12	1:C:666:TRP:CD2	0.41	2.51	11	1
1:C:854:ILE:HD13	1:C:854:ILE:O	0.41	2.16	12	1
1:A:663:LEU:HD23	1:B:660:LEU:O	0.41	2.16	14	1
1:C:699:PHE:O	1:C:702:LEU:HB3	0.41	2.16	1	2
1:A:707:ARG:HB2	1:C:704:LEU:HD21	0.41	1.93	2	1
1:A:756:ILE:O	1:A:760:LEU:CB	0.41	2.68	2	1
1:B:763:LEU:HD23	1:B:763:LEU:C	0.41	2.36	6	2
1:C:816:ASN:OD1	1:C:816:ASN:N	0.41	2.53	3	1
1:B:821:ALA:C	1:B:822:VAL:HG22	0.41	2.36	4	1
1:A:792:ALA:O	1:A:795:TYR:HD2	0.41	1.98	10	3
1:A:816:ASN:O	1:A:827:ASP:OD2	0.41	2.38	10	1
1:B:847:ILE:HD13	1:B:847:ILE:N	0.41	2.30	14	1
1:A:677:ASN:O	1:A:681:TYR:CZ	0.41	2.74	2	1
1:C:715:LEU:HD13	1:C:715:LEU:C	0.41	2.35	2	1
1:A:760:LEU:HD11	1:C:803:TRP:CH2	0.41	2.49	3	1
1:B:781:ILE:HD12	1:C:746:ILE:CB	0.41	2.45	3	1
1:B:814:LEU:HD13	1:B:814:LEU:C	0.41	2.36	4	1
1:B:847:ILE:HG23	1:B:848:ARG:N	0.41	2.31	9	2
1:C:678:TRP:CD1	1:C:678:TRP:C	0.41	2.94	4	1
1:A:742:ARG:NH2	1:C:774:LEU:HD21	0.41	2.31	5	1
1:B:667:ALA:HB2	1:C:660:LEU:HD22	0.41	1.91	5	1
1:A:747:ARG:O	1:A:747:ARG:CD	0.41	2.69	7	1
1:A:774:LEU:HD23	1:A:774:LEU:C	0.41	2.36	9	1
1:A:851:LEU:HD22	1:A:854:ILE:HD11	0.41	1.92	9	1
1:C:750:ASN:H	1:C:750:ASN:ND2	0.41	2.14	9	1
1:B:760:LEU:O	1:B:763:LEU:HD13	0.41	2.16	10	1
1:B:753:LEU:HD12	1:B:753:LEU:H	0.41	1.76	11	1
1:B:775:LEU:HD22	1:B:775:LEU:C	0.41	2.36	11	1
1:C:704:LEU:O	1:C:707:ARG:HB3	0.41	2.16	12	1
1:B:803:TRP:CE3	1:C:768:TYR:CE2	0.41	3.09	13	1
1:A:660:LEU:N	1:A:660:LEU:HD22	0.41	2.31	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:776:LEU:HD12	1:B:777:ILE:N	0.41	2.31	14	1
1:A:746:ILE:HG22	1:C:785:LEU:HD22	0.41	1.92	1	1
1:C:768:TYR:O	1:C:769:HIS:CB	0.41	2.69	2	1
1:A:753:LEU:HD22	1:C:791:GLU:HB2	0.41	1.92	3	1
1:A:675:ILE:HD13	1:A:675:ILE:C	0.41	2.36	5	2
1:C:774:LEU:O	1:C:777:ILE:HG22	0.41	2.15	6	1
1:A:806:GLU:OE2	1:B:771:LEU:HD21	0.41	2.16	11	1
1:B:845:ARG:O	1:B:846:ARG:C	0.41	2.59	11	1
1:A:815:LEU:O	1:A:819:ALA:HB2	0.41	2.16	14	1
1:A:779:THR:O	1:A:782:VAL:HG22	0.41	2.15	15	1
1:A:746:ILE:HG21	1:C:781:ILE:HG21	0.40	1.93	9	2
1:C:679:LEU:HD23	1:C:679:LEU:O	0.40	2.16	1	1
1:A:756:ILE:HD12	1:A:756:ILE:H	0.40	1.76	6	1
1:A:760:LEU:HD21	1:C:799:LEU:HD12	0.40	1.93	7	1
1:B:765:LEU:HD13	1:B:774:LEU:HD11	0.40	1.92	9	1
1:C:698:VAL:HG23	1:C:699:PHE:CD2	0.40	2.49	12	1
1:B:821:ALA:O	1:B:822:VAL:CB	0.40	2.70	13	1
1:A:814:LEU:O	1:A:818:THR:HG22	0.40	2.16	2	1
1:A:760:LEU:HG	1:C:799:LEU:HD12	0.40	1.92	3	1
1:B:781:ILE:CD1	1:C:746:ILE:HG21	0.40	2.45	3	1
1:A:660:LEU:HG	1:C:667:ALA:HB2	0.40	1.91	7	1
1:B:799:LEU:HD21	1:C:760:LEU:HD12	0.40	1.93	7	1
1:A:808:LYS:O	1:A:812:VAL:HG12	0.40	2.16	8	1
1:B:758:ASP:O	1:B:761:ARG:CZ	0.40	2.69	10	1
1:A:693:ILE:HD11	1:B:692:LEU:HD23	0.40	1.93	11	1
1:A:754:ALA:HB3	1:B:715:LEU:CD2	0.40	2.47	15	1
1:A:793:LEU:HD12	1:A:797:TRP:CE2	0.40	2.51	15	1
1:A:836:ALA:O	1:A:840:ILE:HG22	0.40	2.17	15	1
1:B:755:LEU:CA	1:C:715:LEU:HD11	0.40	2.46	1	1
1:C:760:LEU:HD13	1:C:761:ARG:N	0.40	2.31	1	1
1:C:812:VAL:HG12	1:C:816:ASN:ND2	0.40	2.30	1	1
1:A:750:ASN:ND2	1:A:750:ASN:N	0.40	2.69	5	1
1:B:683:ARG:NH1	1:C:679:LEU:HD11	0.40	2.31	5	1
1:C:782:VAL:HA	1:C:785:LEU:HD11	0.40	1.93	6	1
1:A:803:TRP:O	1:A:806:GLU:HG3	0.40	2.15	7	1
1:B:822:VAL:HG23	1:B:823:GLY:N	0.40	2.32	9	1
1:C:847:ILE:HG13	1:C:848:ARG:H	0.40	1.76	10	1
1:C:843:ILE:H	1:C:844:PRO:CD	0.40	2.29	11	1
1:B:816:ASN:ND2	1:B:820:ILE:HD11	0.40	2.31	15	1
1:B:830:ILE:HD12	1:B:830:ILE:C	0.40	2.37	1	1
1:C:706:ASN:O	1:C:710:GLN:N	0.40	2.54	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:808:LYS:NZ	1:B:834:GLN:O	0.40	2.54	11	1
1:B:842:HIS:HB3	1:B:843:ILE:HD13	0.40	1.93	12	1
1:A:763:LEU:O	1:A:774:LEU:CB	0.40	2.70	15	1
1:A:678:TRP:CD1	1:A:679:LEU:N	0.40	2.90	2	1
1:A:694:GLY:O	1:A:697:ILE:HG13	0.40	2.16	6	1
1:C:790:TRP:CH2	1:C:793:LEU:HD22	0.40	2.51	6	1
1:C:802:TYR:HB3	1:C:803:TRP:CZ3	0.40	2.52	6	1
1:C:682:ILE:HD13	1:C:683:ARG:N	0.40	2.31	8	1
1:B:795:TYR:O	1:B:799:LEU:HD23	0.40	2.16	10	1
1:C:746:ILE:O	1:C:749:VAL:HG23	0.40	2.16	10	1
1:C:663:LEU:HD22	1:C:664:ASP:N	0.40	2.30	12	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	171/197 (87%)	154±2 (90±1%)	10±2 (6±1%)	7±2 (4±1%)	5	32
1	B	171/197 (87%)	152±2 (89±1%)	10±2 (6±1%)	8±2 (5±1%)	4	26
1	C	171/197 (87%)	154±2 (90±1%)	10±2 (6±1%)	7±3 (4±2%)	5	31
All	All	7695/8865 (87%)	6905 (90%)	459 (6%)	331 (4%)	5	29

All 68 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	714	PRO	15
1	C	714	PRO	15
1	B	714	PRO	14
1	C	712	TYR	11
1	A	741	ASP	9
1	B	673	PHE	9
1	C	673	PHE	9
1	B	765	LEU	8

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Mol	Chain	Res	Type	Models (Total)
1	C	767	SER	8
1	C	843	ILE	8
1	B	846	ARG	8
1	A	825	GLY	7
1	C	661	LEU	7
1	B	824	GLU	7
1	B	842	HIS	7
1	B	844	PRO	7
1	C	769	HIS	7
1	A	673	PHE	6
1	A	768	TYR	6
1	C	765	LEU	6
1	C	822	VAL	6
1	A	661	LEU	6
1	B	712	TYR	6
1	B	661	LEU	5
1	C	766	PHE	5
1	A	822	VAL	5
1	B	674	ASP	5
1	B	766	PHE	5
1	B	825	GLY	5
1	A	712	TYR	5
1	A	769	HIS	5
1	A	846	ARG	5
1	B	767	SER	5
1	B	822	VAL	5
1	A	765	LEU	4
1	B	663	LEU	4
1	B	769	HIS	4
1	C	674	ASP	4
1	C	821	ALA	4
1	A	821	ALA	4
1	B	662	GLU	4
1	B	768	TYR	4
1	B	821	ALA	4
1	A	662	GLU	4
1	C	824	GLU	4
1	A	824	GLU	4
1	A	674	ASP	3
1	A	843	ILE	3
1	A	767	SER	2
1	B	845	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	B	843	ILE	2
1	C	846	ARG	2
1	A	766	PHE	2
1	B	823	GLY	2
1	A	844	PRO	2
1	A	845	ARG	2
1	C	823	GLY	2
1	C	768	TYR	2
1	B	741	ASP	1
1	C	662	GLU	1
1	B	715	LEU	1
1	B	711	GLY	1
1	A	823	GLY	1
1	C	844	PRO	1
1	A	715	LEU	1
1	C	825	GLY	1
1	C	663	LEU	1
1	C	715	LEU	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	155/173 (90%)	116±6 (75±4%)	39±6 (25±4%)	2	25
1	B	155/173 (90%)	117±6 (76±4%)	38±6 (24±4%)	2	26
1	C	155/173 (90%)	115±5 (74±3%)	40±5 (26±3%)	2	23
All	All	6975/7785 (90%)	5231 (75%)	1744 (25%)	2	25

All 409 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	803	TRP	15
1	B	803	TRP	15
1	C	771	LEU	15
1	C	794	LYS	15
1	C	803	TRP	15

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Mol	Chain	Res	Type	Models (Total)
1	B	794	LYS	14
1	A	744	ARG	13
1	A	771	LEU	13
1	B	771	LEU	13
1	A	678	TRP	12
1	A	763	LEU	12
1	A	794	LYS	12
1	B	744	ARG	12
1	C	761	ARG	12
1	C	795	TYR	12
1	A	715	LEU	11
1	A	795	TYR	11
1	B	834	GLN	11
1	C	678	TRP	11
1	A	693	ILE	11
1	A	780	ARG	11
1	B	678	TRP	11
1	C	799	LEU	11
1	A	753	LEU	10
1	A	770	ARG	10
1	B	763	LEU	10
1	B	772	ARG	10
1	C	693	ILE	10
1	C	744	ARG	10
1	C	757	TRP	10
1	C	774	LEU	10
1	C	775	LEU	10
1	A	830	ILE	10
1	B	675	ILE	10
1	C	696	ARG	10
1	C	715	LEU	10
1	A	679	LEU	10
1	A	772	ARG	9
1	A	838	ARG	9
1	B	702	LEU	9
1	B	715	LEU	9
1	B	774	LEU	9
1	B	795	TYR	9
1	B	802	TYR	9
1	C	680	TRP	9
1	B	799	LEU	9
1	A	697	ILE	8

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Mol	Chain	Res	Type	Models (Total)
1	A	712	TYR	8
1	C	675	ILE	8
1	C	707	ARG	8
1	C	758	ASP	8
1	C	780	ARG	8
1	C	838	ARG	8
1	C	847	ILE	8
1	A	692	LEU	8
1	B	693	ILE	8
1	C	663	LEU	8
1	C	764	SER	8
1	C	772	ARG	8
1	A	747	ARG	8
1	A	663	LEU	7
1	A	674	ASP	7
1	A	675	ILE	7
1	A	806	GLU	7
1	A	814	LEU	7
1	A	834	GLN	7
1	A	847	ILE	7
1	B	707	ARG	7
1	C	756	ILE	7
1	C	856	LEU	7
1	A	758	ASP	7
1	A	760	LEU	7
1	A	790	TRP	7
1	B	765	LEU	7
1	B	770	ARG	7
1	C	673	PHE	7
1	C	713	SER	7
1	C	748	LEU	7
1	A	765	LEU	7
1	B	805	GLN	7
1	B	847	ILE	7
1	A	662	GLU	6
1	A	757	TRP	6
1	B	674	ASP	6
1	B	708	VAL	6
1	B	760	LEU	6
1	B	767	SER	6
1	B	785	LEU	6
1	B	800	LEU	6

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Mol	Chain	Res	Type	Models (Total)
1	C	660	LEU	6
1	C	770	ARG	6
1	C	830	ILE	6
1	C	855	LEU	6
1	A	704	LEU	6
1	B	698	VAL	6
1	B	756	ILE	6
1	B	758	ASP	6
1	C	765	LEU	6
1	A	742	ARG	6
1	B	685	PHE	6
1	C	750	ASN	6
1	B	742	ARG	6
1	A	761	ARG	6
1	A	797	TRP	6
1	B	780	ARG	6
1	C	702	LEU	6
1	B	753	LEU	6
1	A	684	ILE	5
1	A	696	ARG	5
1	A	755	LEU	5
1	A	766	PHE	5
1	A	788	ARG	5
1	B	696	ARG	5
1	B	713	SER	5
1	B	775	LEU	5
1	B	781	ILE	5
1	B	830	ILE	5
1	B	846	ARG	5
1	C	682	ILE	5
1	C	697	ILE	5
1	C	706	ASN	5
1	C	760	LEU	5
1	C	802	TYR	5
1	C	841	ARG	5
1	C	846	ARG	5
1	C	848	ARG	5
1	A	660	LEU	5
1	A	785	LEU	5
1	A	799	LEU	5
1	A	856	LEU	5
1	B	679	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	B	757	TRP	5
1	B	801	GLN	5
1	B	855	LEU	5
1	B	856	LEU	5
1	C	763	LEU	5
1	C	779	THR	5
1	A	739	GLU	5
1	A	828	ARG	5
1	B	755	LEU	5
1	B	773	ASP	5
1	A	793	LEU	5
1	B	837	SER	5
1	C	791	GLU	5
1	B	745	SER	5
1	B	750	ASN	5
1	C	753	LEU	5
1	C	787	ARG	5
1	B	672	TRP	5
1	C	747	ARG	5
1	A	710	GLN	4
1	A	741	ASP	4
1	A	805	GLN	4
1	B	743	ASP	4
1	B	791	GLU	4
1	B	824	GLU	4
1	B	845	ARG	4
1	B	852	GLU	4
1	C	661	LEU	4
1	C	679	LEU	4
1	C	686	ILE	4
1	C	692	LEU	4
1	C	740	ARG	4
1	C	766	PHE	4
1	C	784	LEU	4
1	C	793	LEU	4
1	C	805	GLN	4
1	C	824	GLU	4
1	A	764	SER	4
1	A	774	LEU	4
1	A	776	LEU	4
1	A	854	ILE	4
1	B	673	PHE	4

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Mol	Chain	Res	Type	Models (Total)
1	B	692	LEU	4
1	B	739	GLU	4
1	B	814	LEU	4
1	C	676	THR	4
1	C	704	LEU	4
1	A	673	PHE	4
1	A	852	GLU	4
1	B	853	ARG	4
1	C	800	LEU	4
1	C	845	ARG	4
1	A	703	SER	4
1	A	746	ILE	4
1	B	746	ILE	4
1	C	716	SER	4
1	C	785	LEU	4
1	C	834	GLN	4
1	A	707	ARG	4
1	A	750	ASN	4
1	B	766	PHE	4
1	B	816	ASN	4
1	C	849	GLN	4
1	A	845	ARG	4
1	B	790	TRP	4
1	B	806	GLU	4
1	C	710	GLN	4
1	A	669	LEU	3
1	A	808	LYS	3
1	A	841	ARG	3
1	B	704	LEU	3
1	B	793	LEU	3
1	B	809	ASN	3
1	C	662	GLU	3
1	C	746	ILE	3
1	C	768	TYR	3
1	C	782	VAL	3
1	C	801	GLN	3
1	C	852	GLU	3
1	A	713	SER	3
1	A	752	SER	3
1	A	775	LEU	3
1	B	677	ASN	3
1	B	686	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	B	706	ASN	3
1	B	778	VAL	3
1	C	683	ARG	3
1	A	827	ASP	3
1	B	697	ILE	3
1	B	807	LEU	3
1	B	827	ASP	3
1	C	767	SER	3
1	C	816	ASN	3
1	C	826	THR	3
1	A	702	LEU	3
1	A	851	LEU	3
1	B	682	ILE	3
1	B	748	LEU	3
1	B	788	ARG	3
1	B	826	THR	3
1	C	709	ARG	3
1	C	806	GLU	3
1	A	665	LYS	3
1	A	791	GLU	3
1	A	800	LEU	3
1	A	843	ILE	3
1	B	661	LEU	3
1	B	662	GLU	3
1	B	663	LEU	3
1	B	740	ARG	3
1	B	761	ARG	3
1	B	764	SER	3
1	B	787	ARG	3
1	B	848	ARG	3
1	C	671	ASN	3
1	C	703	SER	3
1	C	762	SER	3
1	C	809	ASN	3
1	A	787	ARG	3
1	A	846	ARG	3
1	C	714	PRO	3
1	C	752	SER	3
1	C	843	ILE	3
1	A	807	LEU	3
1	A	815	LEU	3
1	B	660	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	C	743	ASP	3
1	C	790	TRP	3
1	A	769	HIS	3
1	A	677	ASN	3
1	B	777	ILE	3
1	A	767	SER	2
1	A	773	ASP	2
1	A	802	TYR	2
1	A	824	GLU	2
1	A	840	ILE	2
1	B	812	VAL	2
1	C	674	ASP	2
1	C	712	TYR	2
1	C	853	ARG	2
1	A	701	VAL	2
1	A	748	LEU	2
1	A	782	VAL	2
1	A	822	VAL	2
1	B	712	TYR	2
1	B	769	HIS	2
1	B	840	ILE	2
1	C	742	ARG	2
1	C	755	LEU	2
1	C	773	ASP	2
1	C	827	ASP	2
1	A	685	PHE	2
1	A	848	ARG	2
1	A	849	GLN	2
1	B	776	LEU	2
1	C	759	ASP	2
1	C	776	LEU	2
1	C	820	ILE	2
1	C	840	ILE	2
1	A	683	ARG	2
1	A	691	SER	2
1	A	743	ASP	2
1	B	701	VAL	2
1	B	808	LYS	2
1	B	838	ARG	2
1	C	769	HIS	2
1	C	851	LEU	2
1	A	768	TYR	2

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Mol	Chain	Res	Type	Models (Total)
1	B	669	LEU	2
1	B	762	SER	2
1	B	798	ASN	2
1	C	808	LYS	2
1	C	813	SER	2
1	A	664	ASP	2
1	A	676	THR	2
1	A	709	ARG	2
1	B	683	ARG	2
1	B	747	ARG	2
1	B	797	TRP	2
1	B	854	ILE	2
1	A	716	SER	2
1	A	777	ILE	2
1	B	699	PHE	2
1	C	691	SER	2
1	C	854	ILE	2
1	A	689	VAL	2
1	A	779	THR	2
1	A	801	GLN	2
1	B	842	HIS	2
1	C	664	ASP	2
1	C	739	GLU	2
1	B	710	GLN	2
1	B	783	GLU	2
1	B	784	LEU	2
1	C	781	ILE	2
1	A	809	ASN	2
1	B	815	LEU	2
1	B	828	ARG	2
1	C	705	VAL	2
1	A	855	LEU	2
1	B	843	ILE	2
1	A	671	ASN	2
1	A	708	VAL	2
1	C	807	LEU	2
1	B	841	ARG	2
1	A	820	ILE	1
1	B	671	ASN	1
1	C	684	ILE	1
1	A	810	SER	1
1	A	816	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	B	670	TRP	1
1	B	810	SER	1
1	C	669	LEU	1
1	C	822	VAL	1
1	A	714	PRO	1
1	A	781	ILE	1
1	C	670	TRP	1
1	C	677	ASN	1
1	C	699	PHE	1
1	C	708	VAL	1
1	C	783	GLU	1
1	B	714	PRO	1
1	B	752	SER	1
1	B	822	VAL	1
1	C	665	LYS	1
1	C	741	ASP	1
1	A	670	TRP	1
1	A	740	ARG	1
1	B	695	LEU	1
1	C	745	SER	1
1	C	804	SER	1
1	A	672	TRP	1
1	A	831	GLU	1
1	C	668	SER	1
1	C	831	GLU	1
1	A	661	LEU	1
1	B	691	SER	1
1	C	701	VAL	1
1	A	682	ILE	1
1	A	804	SER	1
1	B	782	VAL	1
1	C	815	LEU	1
1	B	716	SER	1
1	B	749	VAL	1
1	B	818	THR	1
1	B	851	LEU	1
1	C	695	LEU	1
1	C	778	VAL	1
1	C	788	ARG	1
1	C	797	TRP	1
1	C	810	SER	1
1	A	680	TRP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	698	VAL	1
1	A	699	PHE	1
1	A	783	GLU	1
1	B	668	SER	1
1	B	688	ILE	1
1	C	672	TRP	1
1	C	698	VAL	1
1	A	686	ILE	1
1	B	680	TRP	1
1	C	818	THR	1
1	A	668	SER	1
1	A	706	ASN	1
1	B	676	THR	1
1	B	684	ILE	1
1	B	813	SER	1
1	C	842	HIS	1
1	A	842	HIS	1
1	A	853	ARG	1
1	B	831	GLU	1
1	A	688	ILE	1
1	A	756	ILE	1
1	A	762	SER	1
1	A	826	THR	1
1	A	837	SER	1
1	B	664	ASP	1
1	B	804	SER	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no monosaccharides 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 8% for the well-defined parts and 8% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *HIV1\_gp41\_MPER-TMD-CT\_chemical\_shifts.tab*

#### 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	657
Number of shifts mapped to atoms	622
Number of unparsed shifts	0
Number of shifts with mapping errors	35
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 35 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	717	PHE	H	8.05	0.01	1
1	A	717	PHE	C	175.43	0.05	1
1	A	717	PHE	CA	57.49	0.05	1
1	A	717	PHE	N	120.86	0.03	1
1	A	718	GLN	H	8.13	0.01	1
1	A	718	GLN	C	175.94	0.05	1
1	A	718	GLN	CA	55.56	0.05	1
1	A	718	GLN	N	120.21	0.03	1
1	A	719	THR	H	8.03	0.01	1
1	A	719	THR	CA	61.81	0.05	1
1	A	719	THR	N	114.2	0.03	1
1	A	720	HIS	C	174.75	0.05	1
1	A	720	HIS	CA	55.7	0.05	1
1	A	721	LEU	H	8.02	0.01	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	721	LEU	CA	52.47	0.05	1
1	A	721	LEU	N	123.97	0.03	1
1	A	722	PRO	C	176.74	0.05	1
1	A	722	PRO	CA	62.54	0.05	1
1	A	723	THR	H	8.15	0.01	1
1	A	723	THR	CA	59.45	0.05	1
1	A	723	THR	N	116.61	0.03	1
1	A	724	PRO	C	177.1	0.05	1
1	A	724	PRO	CA	62.91	0.05	1
1	A	725	ARG	H	8.45	0.01	1
1	A	725	ARG	C	177.14	0.05	1
1	A	725	ARG	CA	55.87	0.05	1
1	A	725	ARG	N	121.18	0.03	1
1	A	737	GLY	H	8.48	0.01	1
1	A	737	GLY	C	174.84	0.05	1
1	A	737	GLY	CA	45.06	0.05	1
1	A	737	GLY	N	110.12	0.03	1
1	A	738	GLY	H	8.32	0.01	1
1	A	738	GLY	C	174.61	0.05	1
1	A	738	GLY	CA	44.88	0.05	1
1	A	738	GLY	N	108.9	0.03	1

### 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
$^{13}\text{C}_\alpha$	171	$-0.04 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	158	$-0.28 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	164	$0.90 \pm 0.26$	Should be applied

### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 8%, i.e. 622 atoms were assigned a chemical shift out of a possible 7980. 0 out of 132 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	622/2643 (24%)	156/1074 (15%)	310/1050 (30%)	156/519 (30%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Sidechain	0/4674 (0%)	0/3063 (0%)	0/1377 (0%)	0/234 (0%)
Aromatic	0/663 (0%)	0/324 (0%)	0/297 (0%)	0/42 (0%)
Overall	622/7980 (8%)	156/4461 (3%)	310/2724 (11%)	156/795 (20%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 622 atoms were assigned a chemical shift out of a possible 7980. 0 out of 132 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	622/2643 (24%)	156/1074 (15%)	310/1050 (30%)	156/519 (30%)
Sidechain	0/4674 (0%)	0/3063 (0%)	0/1377 (0%)	0/234 (0%)
Aromatic	0/663 (0%)	0/324 (0%)	0/297 (0%)	0/42 (0%)
Overall	622/7980 (8%)	156/4461 (3%)	310/2724 (11%)	156/795 (20%)

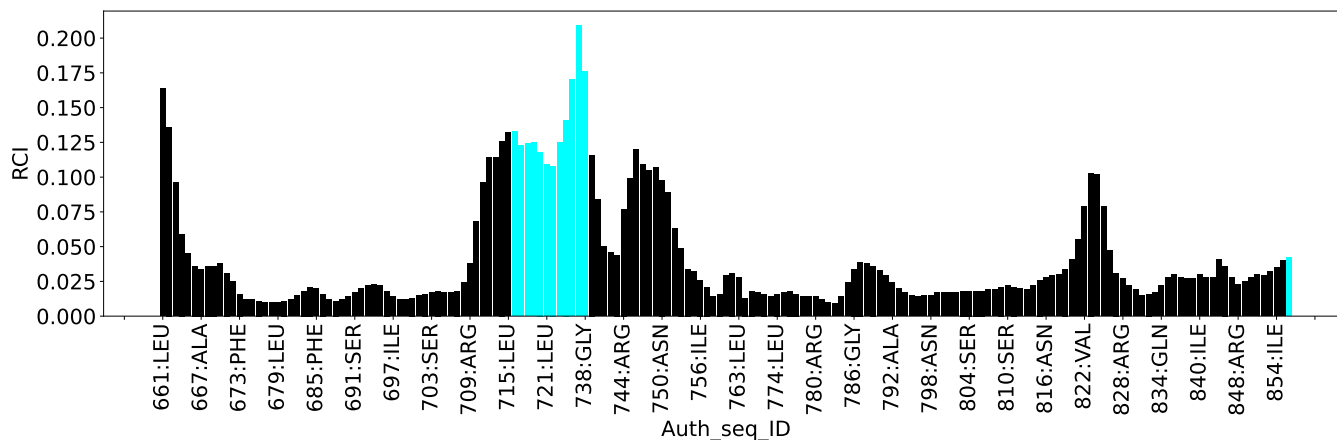
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1746
Intra-residue ( $ i-j =0$ )	191
Sequential ( $ i-j =1$ )	522
Medium range ( $ i-j >1$ and $ i-j <5$ )	532
Long range ( $ i-j \geq 5$ )	131
Inter-chain	112
Hydrogen bond restraints	258
Disulfide bond restraints	0
Total dihedral-angle restraints	298
Number of unmapped restraints	38
Number of restraints per residue	3.5
Number of long range restraints per residue <sup>1</sup>	0.2

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

### 8.2 Residual restraint violations

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

#### 8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	125.6	0.2
0.2-0.5 (Medium)	115.5	0.5
>0.5 (Large)	143.6	56.95

### 8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	42.2	7.2
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis

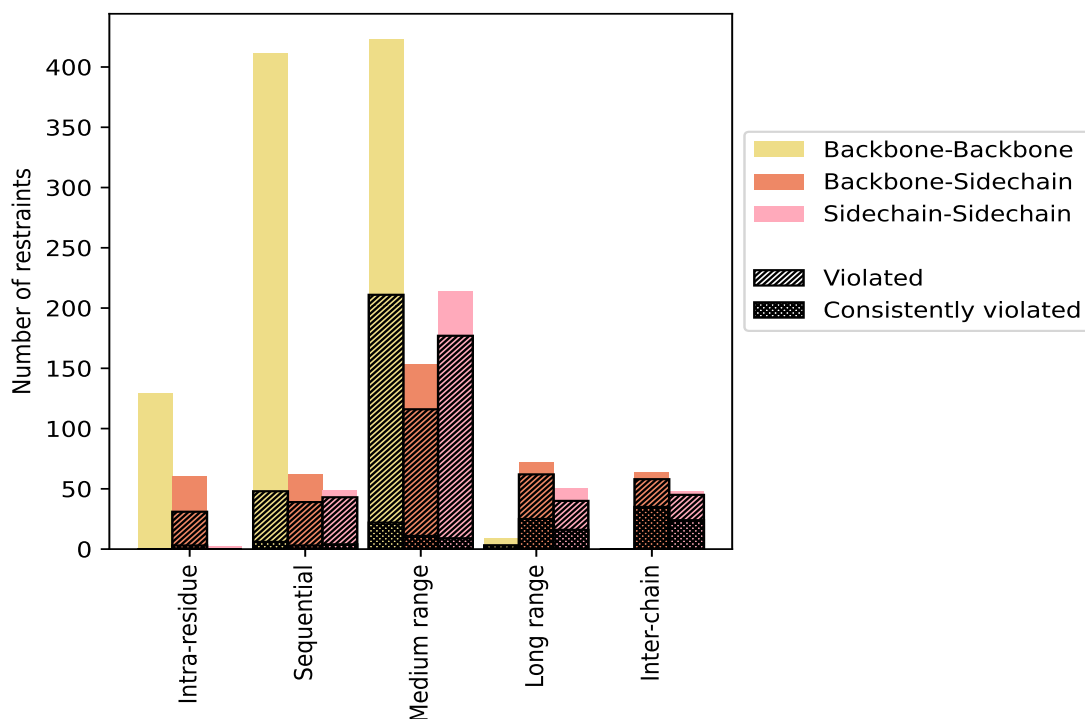
### 9.1 Summary of distance violations

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

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>191</b>	<b>10.9</b>	<b>31</b>	<b>16.2</b>	<b>1.8</b>	<b>3</b>	<b>1.6</b>	<b>0.2</b>
Backbone-Backbone	129	7.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	60	3.4	31	51.7	1.8	3	5.0	0.2
Sidechain-Sidechain	2	0.1	0	0.0	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>522</b>	<b>29.9</b>	<b>130</b>	<b>24.9</b>	<b>7.4</b>	<b>13</b>	<b>2.5</b>	<b>0.7</b>
Backbone-Backbone	411	23.5	48	11.7	2.7	6	1.5	0.3
Backbone-Sidechain	62	3.6	39	62.9	2.2	3	4.8	0.2
Sidechain-Sidechain	49	2.8	43	87.8	2.5	4	8.2	0.2
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>532</b>	<b>30.5</b>	<b>387</b>	<b>72.7</b>	<b>22.2</b>	<b>36</b>	<b>6.8</b>	<b>2.1</b>
Backbone-Backbone	165	9.5	94	57.0	5.4	16	9.7	0.9
Backbone-Sidechain	153	8.8	116	75.8	6.6	11	7.2	0.6
Sidechain-Sidechain	214	12.3	177	82.7	10.1	9	4.2	0.5
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>131</b>	<b>7.5</b>	<b>105</b>	<b>80.2</b>	<b>6.0</b>	<b>44</b>	<b>33.6</b>	<b>2.5</b>
Backbone-Backbone	9	0.5	3	33.3	0.2	3	33.3	0.2
Backbone-Sidechain	72	4.1	62	86.1	3.6	25	34.7	1.4
Sidechain-Sidechain	50	2.9	40	80.0	2.3	16	32.0	0.9
<b>Inter-chain</b>	<b>112</b>	<b>6.4</b>	<b>103</b>	<b>92.0</b>	<b>5.9</b>	<b>59</b>	<b>52.7</b>	<b>3.4</b>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	64	3.7	58	90.6	3.3	35	54.7	2.0
Sidechain-Sidechain	48	2.7	45	93.8	2.6	24	50.0	1.4
<b>Hydrogen bond</b>	<b>258</b>	<b>14.8</b>	<b>117</b>	<b>45.3</b>	<b>6.7</b>	<b>6</b>	<b>2.3</b>	<b>0.3</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>1746</b>	<b>100.0</b>	<b>873</b>	<b>50.0</b>	<b>50.0</b>	<b>161</b>	<b>9.2</b>	<b>9.2</b>
Backbone-Backbone	972	55.7	262	27.0	15.0	31	3.2	1.8
Backbone-Sidechain	411	23.5	306	74.5	17.5	77	18.7	4.4
Sidechain-Sidechain	363	20.8	305	84.0	17.5	53	14.6	3.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	9	51	181	62	76	379	4.89	56.95	10.28	0.34
2	11	40	159	68	74	352	5.23	54.31	10.53	0.36
3	10	49	190	59	76	384	4.81	55.51	10.2	0.34
4	9	36	175	62	81	363	5.01	56.86	10.42	0.32
5	15	46	167	68	77	373	4.86	55.88	10.23	0.33
6	15	62	189	63	77	406	4.5	55.56	9.9	0.33
7	10	49	196	64	75	394	4.62	54.51	9.99	0.33
8	12	45	202	62	78	399	4.63	56.35	10.04	0.3
9	11	45	169	68	78	371	4.98	53.78	10.28	0.33
10	14	46	187	68	85	400	4.59	55.73	9.96	0.32
11	14	46	197	61	73	391	4.69	54.48	10.01	0.31

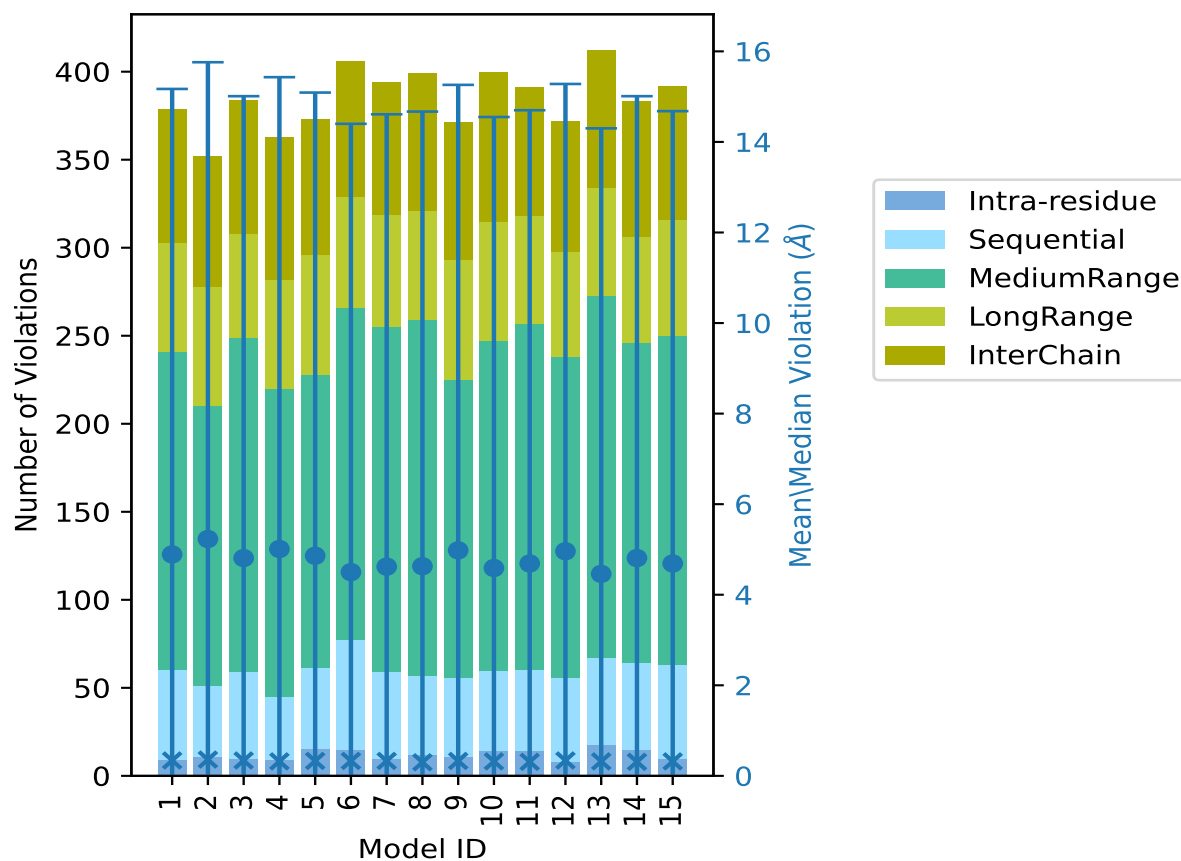
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
12	8	48	182	60	74	372	4.96	55.54	10.32	0.34
13	18	49	206	61	78	412	4.46	55.28	9.84	0.32
14	15	49	182	60	77	383	4.81	54.55	10.2	0.31
15	10	53	187	66	76	392	4.69	56.0	9.99	0.32

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

### 9.3 Distance violation statistics for the ensemble [i](#)

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

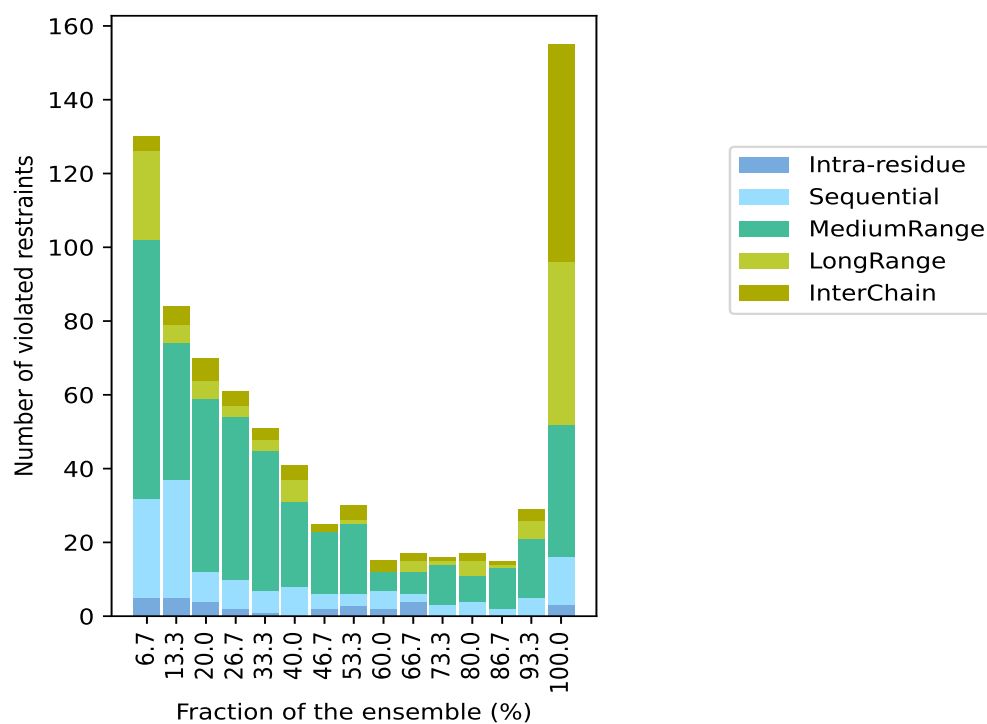
for a given fraction of the ensemble. In total, 732(IR:160, SQ:392, MR:145, LR:26, IC:9) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
5	27	70	24	4	130	1	6.7
5	32	37	5	5	84	2	13.3
4	8	47	5	6	70	3	20.0
2	8	44	3	4	61	4	26.7
1	6	38	3	3	51	5	33.3
0	8	23	6	4	41	6	40.0
2	4	17	0	2	25	7	46.7
3	3	19	1	4	30	8	53.3
2	5	5	0	3	15	9	60.0
4	2	6	3	2	17	10	66.7
0	3	11	1	1	16	11	73.3
0	4	7	4	2	17	12	80.0
0	2	11	1	1	15	13	86.7
0	5	16	5	3	29	14	93.3
3	13	36	44	59	155	15	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations



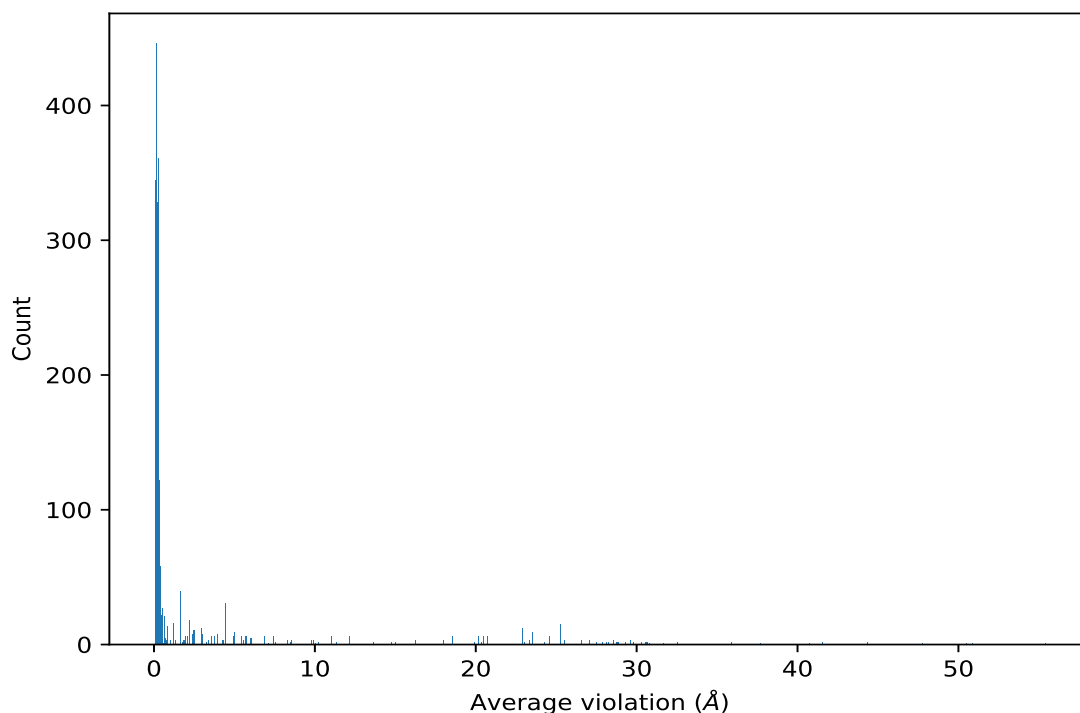
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

### 9.4.1 Histogram : Distribution of mean distance violations [i](#)

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



#### 9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,181)	1:B:806:GLU:H	1:A:772:ARG:HE	15	55.42	0.91	55.54
(2,178)	1:B:806:GLU:H	1:A:771:LEU:HG	15	50.87	0.91	50.41
(2,182)	1:A:806:GLU:H	1:A:772:ARG:HE	15	50.52	0.88	50.68
(2,179)	1:A:806:GLU:H	1:A:771:LEU:HG	15	47.76	0.56	47.6
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB2	15	44.31	0.6	44.38
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB3	15	44.31	0.6	44.38
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB2	15	41.56	0.56	41.55
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB3	15	41.56	0.56	41.55
(2,175)	1:B:803:TRP:HE1	1:A:764:SER:HG	15	40.79	1.03	40.8
(2,176)	1:A:803:TRP:HE1	1:A:764:SER:HG	15	37.7	0.93	37.76
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB2	15	35.91	0.64	35.98
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB3	15	35.91	0.64	35.98
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB2	15	32.52	0.8	32.43
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB3	15	32.52	0.8	32.43
(2,133)	1:A:756:ILE:H	1:A:796:TRP:HE1	15	31.69	0.64	31.53
(2,134)	1:A:756:ILE:H	1:B:796:TRP:HE1	15	30.82	0.77	31.01

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG12	15	30.7	0.43	30.75
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG13	15	30.7	0.43	30.75
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB2	15	30.62	0.58	30.7
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB3	15	30.62	0.58	30.7
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG12	15	30.56	0.48	30.46
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG13	15	30.56	0.48	30.46
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD2	15	30.33	0.54	30.35
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD3	15	30.33	0.54	30.35
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB2	15	29.8	0.49	29.8
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB3	15	29.8	0.49	29.8
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG21	15	29.65	0.51	29.55
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG22	15	29.65	0.51	29.55
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG23	15	29.65	0.51	29.55
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG12	15	29.3	0.43	29.32
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG13	15	29.3	0.43	29.32
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD2	15	28.89	0.56	28.77
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD3	15	28.89	0.56	28.77
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB2	15	28.83	0.53	28.85
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB3	15	28.83	0.53	28.85
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD2	15	28.77	0.48	28.79
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD3	15	28.77	0.48	28.79
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG21	15	28.59	0.43	28.53
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG22	15	28.59	0.43	28.53
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG23	15	28.59	0.43	28.53
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB2	15	28.28	0.82	28.13
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB3	15	28.28	0.82	28.13
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD1	15	28.14	0.54	28.18
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD2	15	28.14	0.54	28.18
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG12	15	27.9	0.39	28.0
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG13	15	27.9	0.39	28.0
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD1	15	27.51	0.69	27.61
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD2	15	27.51	0.69	27.61
(2,113)	1:A:781:ILE:HD11	1:A:743:ASP:HA	15	27.09	0.85	27.04
(2,113)	1:A:781:ILE:HD12	1:A:743:ASP:HA	15	27.09	0.85	27.04
(2,113)	1:A:781:ILE:HD13	1:A:743:ASP:HA	15	27.09	0.85	27.04
(2,125)	1:A:785:LEU:HD21	1:A:749:VAL:HB	15	26.58	1.04	26.72
(2,125)	1:A:785:LEU:HD22	1:A:749:VAL:HB	15	26.58	1.04	26.72
(2,125)	1:A:785:LEU:HD23	1:A:749:VAL:HB	15	26.58	1.04	26.72
(2,124)	1:B:785:LEU:HD21	1:A:749:VAL:HB	15	25.52	0.76	25.62
(2,124)	1:B:785:LEU:HD22	1:A:749:VAL:HB	15	25.52	0.76	25.62
(2,124)	1:B:785:LEU:HD23	1:A:749:VAL:HB	15	25.52	0.76	25.62
(2,112)	1:B:781:ILE:HD11	1:A:743:ASP:HA	15	25.28	0.83	25.3

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,112)	1:B:781:ILE:HD12	1:A:743:ASP:HA	15	25.28	0.83	25.3
(2,112)	1:B:781:ILE:HD13	1:A:743:ASP:HA	15	25.28	0.83	25.3
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD11	15	25.27	0.61	25.15
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD12	15	25.27	0.61	25.15
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD13	15	25.27	0.61	25.15
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD21	15	25.27	0.61	25.15
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD22	15	25.27	0.61	25.15
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD23	15	25.27	0.61	25.15
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD2	15	25.26	0.56	25.49
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD3	15	25.26	0.56	25.49
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD2	15	25.26	0.56	25.49
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD3	15	25.26	0.56	25.49
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD2	15	25.26	0.56	25.49
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD3	15	25.26	0.56	25.49
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD11	15	24.59	0.5	24.45
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD12	15	24.59	0.5	24.45
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD13	15	24.59	0.5	24.45
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD21	15	24.59	0.5	24.45
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD22	15	24.59	0.5	24.45
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD23	15	24.59	0.5	24.45
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD2	15	24.29	0.54	24.23
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD3	15	24.29	0.54	24.23
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD21	15	23.53	0.96	23.43
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD22	15	23.53	0.96	23.43
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD23	15	23.53	0.96	23.43
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG12	15	23.5	0.9	23.48
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG13	15	23.5	0.9	23.48
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG12	15	23.5	0.9	23.48
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG13	15	23.5	0.9	23.48
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG12	15	23.5	0.9	23.48
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG13	15	23.5	0.9	23.48
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD21	15	23.3	0.63	23.09
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD22	15	23.3	0.63	23.09
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD23	15	23.3	0.63	23.09
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB2	15	23.01	0.63	22.95
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB3	15	23.01	0.63	22.95
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG12	15	22.89	0.73	23.04
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG13	15	22.89	0.73	23.04
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG12	15	22.89	0.73	23.04
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG13	15	22.89	0.73	23.04
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG12	15	22.89	0.73	23.04
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG13	15	22.89	0.73	23.04

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD2	15	22.86	0.6	23.1
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD3	15	22.86	0.6	23.1
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD2	15	22.86	0.6	23.1
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD3	15	22.86	0.6	23.1
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD2	15	22.86	0.6	23.1
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD3	15	22.86	0.6	23.1
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB2	15	20.74	0.65	20.65
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB3	15	20.74	0.65	20.65
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB2	15	20.74	0.65	20.65
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB3	15	20.74	0.65	20.65
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB2	15	20.74	0.65	20.65
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB3	15	20.74	0.65	20.65
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD2	15	20.49	1.37	20.56
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD3	15	20.49	1.37	20.56
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD2	15	20.49	1.37	20.56
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD3	15	20.49	1.37	20.56
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD2	15	20.49	1.37	20.56
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD3	15	20.49	1.37	20.56
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB2	15	20.35	0.55	20.3
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB3	15	20.35	0.55	20.3
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD2	15	20.19	0.49	20.22
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD3	15	20.19	0.49	20.22
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD2	15	20.19	0.49	20.22
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD3	15	20.19	0.49	20.22
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD2	15	20.19	0.49	20.22
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD3	15	20.19	0.49	20.22
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD2	15	19.92	0.72	19.82
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD3	15	19.92	0.72	19.82
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB2	15	18.54	0.94	18.4
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB3	15	18.54	0.94	18.4
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB2	15	18.54	0.94	18.4
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB3	15	18.54	0.94	18.4
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB2	15	18.54	0.94	18.4
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB3	15	18.54	0.94	18.4
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD21	15	17.96	0.71	18.02
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD22	15	17.96	0.71	18.02
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD23	15	17.96	0.71	18.02
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD21	15	16.26	0.51	16.48
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD22	15	16.26	0.51	16.48
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD23	15	16.26	0.51	16.48
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB2	15	15.0	0.36	15.05
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB3	15	15.0	0.36	15.05

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD2	15	14.77	0.62	14.76
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD3	15	14.77	0.62	14.76
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB2	15	13.68	0.59	13.79
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB3	15	13.68	0.59	13.79
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE21	15	12.14	0.9	12.24
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE22	15	12.14	0.9	12.24
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE21	15	12.14	0.9	12.24
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE22	15	12.14	0.9	12.24
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE21	15	12.14	0.9	12.24
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE22	15	12.14	0.9	12.24
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD2	15	11.33	0.45	11.39
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD3	15	11.33	0.45	11.39
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE21	15	11.02	0.84	10.76
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE22	15	11.02	0.84	10.76
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE21	15	11.02	0.84	10.76
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE22	15	11.02	0.84	10.76
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE21	15	11.02	0.84	10.76
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE22	15	11.02	0.84	10.76
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB2	15	10.22	0.61	10.45
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB3	15	10.22	0.61	10.45
(2,21)	1:A:678:TRP:HE1	1:B:683:ARG:HE	15	10.04	1.32	9.98
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD11	15	9.92	1.22	10.34
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD12	15	9.92	1.22	10.34
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD13	15	9.92	1.22	10.34
(2,79)	1:B:708:VAL:HG21	1:A:714:PRO:HA	15	9.75	0.78	9.49
(2,79)	1:B:708:VAL:HG22	1:A:714:PRO:HA	15	9.75	0.78	9.49
(2,79)	1:B:708:VAL:HG23	1:A:714:PRO:HA	15	9.75	0.78	9.49
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG21	15	8.51	0.72	8.48
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG22	15	8.51	0.72	8.48
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG23	15	8.51	0.72	8.48
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB2	15	8.48	0.51	8.41
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB3	15	8.48	0.51	8.41
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD11	15	8.34	0.62	8.57
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD12	15	8.34	0.62	8.57
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD13	15	8.34	0.62	8.57
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB2	15	7.57	0.78	7.59
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB3	15	7.57	0.78	7.59
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD2	15	7.44	0.52	7.39
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD3	15	7.44	0.52	7.39
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD2	15	7.44	0.52	7.39
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD3	15	7.44	0.52	7.39
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD2	15	7.44	0.52	7.39

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD3	15	7.44	0.52	7.39
(2,20)	1:A:678:TRP:HE1	1:A:683:ARG:HE	15	7.11	0.31	7.12
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB2	15	6.89	0.53	6.86
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB3	15	6.89	0.53	6.86
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB2	15	6.89	0.53	6.86
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB3	15	6.89	0.53	6.86
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB2	15	6.89	0.53	6.86
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB3	15	6.89	0.53	6.86
(2,39)	1:A:692:LEU:HD21	1:B:694:GLY:H	15	6.1	0.64	6.15
(2,39)	1:A:692:LEU:HD22	1:B:694:GLY:H	15	6.1	0.64	6.15
(2,39)	1:A:692:LEU:HD23	1:B:694:GLY:H	15	6.1	0.64	6.15
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA2	15	6.09	0.69	6.28
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA3	15	6.09	0.69	6.28
(2,80)	1:A:708:VAL:HG21	1:A:714:PRO:HA	15	5.98	0.53	5.76
(2,80)	1:A:708:VAL:HG22	1:A:714:PRO:HA	15	5.98	0.53	5.76
(2,80)	1:A:708:VAL:HG23	1:A:714:PRO:HA	15	5.98	0.53	5.76
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD2	15	5.98	0.35	5.98
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD3	15	5.98	0.35	5.98
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB2	15	5.8	1.31	6.33
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB3	15	5.8	1.31	6.33
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB2	15	5.8	1.31	6.33
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB3	15	5.8	1.31	6.33
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB2	15	5.8	1.31	6.33
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB3	15	5.8	1.31	6.33
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD2	15	5.67	0.38	5.58
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD3	15	5.67	0.38	5.58
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD2	15	5.67	0.38	5.58
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD3	15	5.67	0.38	5.58
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD2	15	5.67	0.38	5.58
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD3	15	5.67	0.38	5.58
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD21	15	5.6	0.64	5.65
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD22	15	5.6	0.64	5.65
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD23	15	5.6	0.64	5.65
(2,2)	1:A:661:LEU:HD11	1:A:680:TRP:HE1	15	5.4	1.05	5.6
(2,2)	1:A:661:LEU:HD12	1:A:680:TRP:HE1	15	5.4	1.05	5.6
(2,2)	1:A:661:LEU:HD13	1:A:680:TRP:HE1	15	5.4	1.05	5.6
(2,2)	1:A:661:LEU:HD21	1:A:680:TRP:HE1	15	5.4	1.05	5.6
(2,2)	1:A:661:LEU:HD22	1:A:680:TRP:HE1	15	5.4	1.05	5.6
(2,2)	1:A:661:LEU:HD23	1:A:680:TRP:HE1	15	5.4	1.05	5.6
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB1	15	5.0	0.62	4.97
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB2	15	5.0	0.62	4.97
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB3	15	5.0	0.62	4.97

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB1	15	5.0	0.62	4.97
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB2	15	5.0	0.62	4.97
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB3	15	5.0	0.62	4.97
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB1	15	5.0	0.62	4.97
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB2	15	5.0	0.62	4.97
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB3	15	5.0	0.62	4.97
(2,3)	1:A:661:LEU:HD11	1:B:680:TRP:HE1	15	4.9	0.84	5.03
(2,3)	1:A:661:LEU:HD12	1:B:680:TRP:HE1	15	4.9	0.84	5.03
(2,3)	1:A:661:LEU:HD13	1:B:680:TRP:HE1	15	4.9	0.84	5.03
(2,3)	1:A:661:LEU:HD21	1:B:680:TRP:HE1	15	4.9	0.84	5.03
(2,3)	1:A:661:LEU:HD22	1:B:680:TRP:HE1	15	4.9	0.84	5.03
(2,3)	1:A:661:LEU:HD23	1:B:680:TRP:HE1	15	4.9	0.84	5.03
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG21	15	4.47	0.53	4.68
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG22	15	4.47	0.53	4.68
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG23	15	4.47	0.53	4.68
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG21	15	4.47	0.53	4.68
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG22	15	4.47	0.53	4.68
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG23	15	4.47	0.53	4.68
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG21	15	4.47	0.53	4.68
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG22	15	4.47	0.53	4.68
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG23	15	4.47	0.53	4.68
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH21	15	4.46	0.8	4.23
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH22	15	4.46	0.8	4.23
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH21	15	4.46	0.8	4.23
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH22	15	4.46	0.8	4.23
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH21	15	4.46	0.8	4.23
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH22	15	4.46	0.8	4.23
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG21	15	4.33	0.4	4.47
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG22	15	4.33	0.4	4.47
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG23	15	4.33	0.4	4.47
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD11	15	4.28	0.78	4.54
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD12	15	4.28	0.78	4.54
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD13	15	4.28	0.78	4.54
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB2	15	3.76	0.49	3.73
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB3	15	3.76	0.49	3.73
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB2	15	3.76	0.49	3.73
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB3	15	3.76	0.49	3.73
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB2	15	3.76	0.49	3.73
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB3	15	3.76	0.49	3.73
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE1	15	3.56	0.59	3.38
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE2	15	3.56	0.59	3.38
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE1	15	3.56	0.59	3.38

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE2	15	3.56	0.59	3.38
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE1	15	3.56	0.59	3.38
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE2	15	3.56	0.59	3.38
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD11	15	3.39	0.76	3.63
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD12	15	3.39	0.76	3.63
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD13	15	3.39	0.76	3.63
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB2	15	3.29	0.68	3.38
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB3	15	3.29	0.68	3.38
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD1	15	3.04	1.24	2.76
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD2	15	3.04	1.24	2.76
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD1	15	3.04	1.24	2.76
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD2	15	3.04	1.24	2.76
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD1	15	3.04	1.24	2.76
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD2	15	3.04	1.24	2.76
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD1	15	3.04	1.24	2.76
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD2	15	3.04	1.24	2.76
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD1	15	2.97	0.41	2.92
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD2	15	2.97	0.41	2.92
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD1	15	2.97	0.41	2.92
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD2	15	2.97	0.41	2.92
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD1	15	2.97	0.41	2.92
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD2	15	2.97	0.41	2.92
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB2	15	2.96	0.48	2.97
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB3	15	2.96	0.48	2.97
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB2	15	2.96	0.48	2.97
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB3	15	2.96	0.48	2.97
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB2	15	2.96	0.48	2.97
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB3	15	2.96	0.48	2.97
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH21	15	2.92	1.01	2.92
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH22	15	2.92	1.01	2.92
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH21	15	2.92	1.01	2.92
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH22	15	2.92	1.01	2.92
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH21	15	2.92	1.01	2.92
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH22	15	2.92	1.01	2.92
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD11	15	2.53	0.57	2.42
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD12	15	2.53	0.57	2.42
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD13	15	2.53	0.57	2.42
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD1	15	2.51	1.04	2.46
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD2	15	2.51	1.04	2.46
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD1	15	2.51	1.04	2.46
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD2	15	2.51	1.04	2.46
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD1	15	2.51	1.04	2.46

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD2	15	2.51	1.04	2.46
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD1	15	2.51	1.04	2.46
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD2	15	2.51	1.04	2.46
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB1	15	2.49	0.43	2.48
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB2	15	2.49	0.43	2.48
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB3	15	2.49	0.43	2.48
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB1	15	2.49	0.43	2.48
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB2	15	2.49	0.43	2.48
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB3	15	2.49	0.43	2.48
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB1	15	2.49	0.43	2.48
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB2	15	2.49	0.43	2.48
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB3	15	2.49	0.43	2.48
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG11	15	2.42	1.11	1.98
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG12	15	2.42	1.11	1.98
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG13	15	2.42	1.11	1.98
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB2	15	2.2	0.79	2.47
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB3	15	2.2	0.79	2.47
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB2	15	1.98	0.67	1.71
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB3	15	1.98	0.67	1.71
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB2	15	1.98	0.67	1.71
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB3	15	1.98	0.67	1.71
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB2	15	1.98	0.67	1.71
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB3	15	1.98	0.67	1.71
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG21	15	1.88	1.03	2.0
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG22	15	1.88	1.03	2.0
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG23	15	1.88	1.03	2.0
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA2	15	1.79	0.43	1.71
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA3	15	1.79	0.43	1.71
(2,15)	1:A:666:TRP:HE1	1:B:666:TRP:HD1	15	1.0	0.19	1.07
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD2	15	0.82	0.25	0.75
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD3	15	0.82	0.25	0.75
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	15	0.82	0.09	0.81
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	15	0.82	0.09	0.81
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	15	0.82	0.09	0.81
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	15	0.82	0.09	0.81
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	15	0.82	0.09	0.81
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	15	0.82	0.09	0.81
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB1	15	0.76	0.1	0.78
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB2	15	0.76	0.1	0.78
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB3	15	0.76	0.1	0.78
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB2	15	0.73	0.12	0.76
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB3	15	0.73	0.12	0.76

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1047)	1:A:802:TYR:H	1:A:803:TRP:HH2	15	0.72	0.17	0.71
(2,1472)	1:A:802:TYR:H	1:A:803:TRP:HH2	15	0.72	0.17	0.71
(2,622)	1:B:802:TYR:H	1:B:803:TRP:HH2	15	0.71	0.18	0.74
(2,1045)	1:A:802:TYR:H	1:A:802:TYR:HB3	15	0.63	0.1	0.65
(2,1470)	1:A:802:TYR:H	1:A:802:TYR:HB3	15	0.63	0.1	0.65
(2,536)	1:B:774:LEU:H	1:B:764:SER:HA	15	0.56	0.15	0.56
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG21	15	0.54	0.22	0.56
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG22	15	0.54	0.22	0.56
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG23	15	0.54	0.22	0.56
(2,620)	1:B:802:TYR:H	1:B:802:TYR:HB3	15	0.54	0.13	0.57
(2,888)	1:A:746:ILE:H	1:A:742:ARG:HA	15	0.54	0.12	0.53
(2,1313)	1:A:746:ILE:H	1:A:742:ARG:HA	15	0.54	0.12	0.53
(2,439)	1:B:710:GLN:H	1:B:708:VAL:HA	15	0.51	0.18	0.53
(2,961)	1:A:774:LEU:H	1:A:764:SER:HA	15	0.5	0.13	0.48
(2,1386)	1:A:774:LEU:H	1:A:764:SER:HA	15	0.5	0.13	0.48
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD2	15	0.48	0.18	0.42
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD3	15	0.48	0.18	0.42
(2,614)	1:B:793:LEU:H	1:B:790:TRP:HE3	15	0.47	0.13	0.45
(2,853)	1:A:708:VAL:HG11	1:A:705:VAL:HA	15	0.47	0.14	0.47
(2,853)	1:A:708:VAL:HG12	1:A:705:VAL:HA	15	0.47	0.14	0.47
(2,853)	1:A:708:VAL:HG13	1:A:705:VAL:HA	15	0.47	0.14	0.47
(2,1278)	1:A:708:VAL:HG11	1:A:705:VAL:HA	15	0.47	0.14	0.47
(2,1278)	1:A:708:VAL:HG12	1:A:705:VAL:HA	15	0.47	0.14	0.47
(2,1278)	1:A:708:VAL:HG13	1:A:705:VAL:HA	15	0.47	0.14	0.47
(2,1039)	1:A:793:LEU:H	1:A:790:TRP:HE3	15	0.45	0.1	0.43
(2,1464)	1:A:793:LEU:H	1:A:790:TRP:HE3	15	0.45	0.1	0.43
(2,463)	1:B:746:ILE:H	1:B:742:ARG:HA	15	0.44	0.12	0.45
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG12	15	0.43	0.2	0.37
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG13	15	0.43	0.2	0.37
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG12	15	0.43	0.2	0.37
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG13	15	0.43	0.2	0.37
(1,1)	1:B:790:TRP:O	1:B:794:LYS:H	15	0.4	0.07	0.4
(1,87)	1:B:790:TRP:O	1:B:794:LYS:H	15	0.4	0.07	0.4
(1,173)	1:B:790:TRP:O	1:B:794:LYS:H	15	0.4	0.07	0.4
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE1	15	0.4	0.19	0.39
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE2	15	0.4	0.19	0.39
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE1	15	0.4	0.19	0.39
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE2	15	0.4	0.19	0.39
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE1	15	0.4	0.19	0.39
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE2	15	0.4	0.19	0.39
(2,826)	1:A:705:VAL:HG11	1:A:702:LEU:HA	15	0.4	0.04	0.41
(2,826)	1:A:705:VAL:HG12	1:A:702:LEU:HA	15	0.4	0.04	0.41

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,826)	1:A:705:VAL:HG13	1:A:702:LEU:HA	15	0.4	0.04	0.41
(2,1251)	1:A:705:VAL:HG11	1:A:702:LEU:HA	15	0.4	0.04	0.41
(2,1251)	1:A:705:VAL:HG12	1:A:702:LEU:HA	15	0.4	0.04	0.41
(2,1251)	1:A:705:VAL:HG13	1:A:702:LEU:HA	15	0.4	0.04	0.41
(2,432)	1:B:709:ARG:H	1:B:707:ARG:H	15	0.39	0.09	0.41
(2,984)	1:A:778:VAL:H	1:A:775:LEU:HA	15	0.39	0.11	0.4
(2,1409)	1:A:778:VAL:H	1:A:775:LEU:HA	15	0.39	0.11	0.4
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD2	15	0.38	0.14	0.38
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD3	15	0.38	0.14	0.38
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD2	15	0.38	0.14	0.38
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD3	15	0.38	0.14	0.38
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD2	15	0.38	0.14	0.38
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD3	15	0.38	0.14	0.38
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG12	15	0.37	0.1	0.38
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG13	15	0.37	0.1	0.38
(2,965)	1:A:775:LEU:H	1:A:772:ARG:HA	15	0.37	0.09	0.35
(2,1390)	1:A:775:LEU:H	1:A:772:ARG:HA	15	0.37	0.09	0.35
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB2	15	0.36	0.1	0.37
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB3	15	0.36	0.1	0.37
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB2	15	0.36	0.1	0.37
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB3	15	0.36	0.1	0.37
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB2	15	0.36	0.1	0.37
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB3	15	0.36	0.1	0.37
(2,857)	1:A:709:ARG:H	1:A:707:ARG:H	15	0.36	0.08	0.35
(2,1282)	1:A:709:ARG:H	1:A:707:ARG:H	15	0.36	0.08	0.35
(2,401)	1:B:705:VAL:HG11	1:B:702:LEU:HA	15	0.35	0.07	0.36
(2,401)	1:B:705:VAL:HG12	1:B:702:LEU:HA	15	0.35	0.07	0.36
(2,401)	1:B:705:VAL:HG13	1:B:702:LEU:HA	15	0.35	0.07	0.36
(2,540)	1:B:775:LEU:H	1:B:772:ARG:HA	15	0.34	0.13	0.33
(1,2)	1:B:790:TRP:O	1:B:794:LYS:N	15	0.33	0.06	0.32
(1,88)	1:B:790:TRP:O	1:B:794:LYS:N	15	0.33	0.06	0.32
(1,174)	1:B:790:TRP:O	1:B:794:LYS:N	15	0.33	0.06	0.32
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD2	15	0.31	0.08	0.28
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD3	15	0.31	0.08	0.28
(2,907)	1:A:749:VAL:H	1:A:746:ILE:HA	15	0.3	0.08	0.32
(2,1332)	1:A:749:VAL:H	1:A:746:ILE:HA	15	0.3	0.08	0.32
(2,482)	1:B:749:VAL:H	1:B:746:ILE:HA	15	0.28	0.09	0.26
(2,565)	1:B:779:THR:H	1:B:776:LEU:HA	15	0.27	0.09	0.26
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG12	15	0.24	0.11	0.22
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG13	15	0.24	0.11	0.22
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	15	0.22	0.07	0.22
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	15	0.22	0.07	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	15	0.22	0.07	0.22
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	15	0.22	0.07	0.22
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	15	0.22	0.07	0.22
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	15	0.22	0.07	0.22
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	15	0.22	0.07	0.22
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	15	0.22	0.07	0.22
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	15	0.22	0.07	0.22
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	15	0.22	0.07	0.22
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	15	0.22	0.07	0.22
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	15	0.22	0.07	0.22
(2,229)	1:B:665:LYS:H	1:B:664:ASP:HA	15	0.2	0.01	0.2
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	15	0.18	0.07	0.17
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	15	0.18	0.07	0.17
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	15	0.18	0.07	0.17
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	15	0.18	0.07	0.17
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	15	0.18	0.07	0.17
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	15	0.18	0.07	0.17
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	15	0.18	0.07	0.17
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	15	0.18	0.07	0.17
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	15	0.18	0.07	0.17
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	15	0.18	0.07	0.17
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	15	0.18	0.07	0.17
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	15	0.18	0.07	0.17
(2,788)	1:A:700:ALA:H	1:A:699:PHE:HA	15	0.18	0.01	0.18
(2,1213)	1:A:700:ALA:H	1:A:699:PHE:HA	15	0.18	0.01	0.18
(2,654)	1:A:665:LYS:H	1:A:664:ASP:HA	15	0.18	0.03	0.19
(2,1079)	1:A:665:LYS:H	1:A:664:ASP:HA	15	0.18	0.03	0.19
(2,363)	1:B:700:ALA:H	1:B:699:PHE:HA	15	0.17	0.01	0.17
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	14	4.49	1.25	4.93
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	14	4.49	1.25	4.93
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	14	4.49	1.25	4.93
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	14	4.49	1.25	4.93
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	14	4.49	1.25	4.93
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	14	4.49	1.25	4.93
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	14	4.49	1.25	4.93
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	14	4.49	1.25	4.93
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	14	4.49	1.25	4.93
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	14	4.49	1.25	4.93
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	14	4.49	1.25	4.93
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	14	4.49	1.25	4.93
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	14	4.49	1.25	4.93
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	14	4.49	1.25	4.93

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	14	4.49	1.25	4.93
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	14	4.49	1.25	4.93
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD1	14	3.93	1.81	4.56
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD2	14	3.93	1.81	4.56
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD1	14	3.93	1.81	4.56
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD2	14	3.93	1.81	4.56
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD1	14	3.93	1.81	4.56
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD2	14	3.93	1.81	4.56
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD1	14	3.93	1.81	4.56
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD2	14	3.93	1.81	4.56
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG12	14	2.45	0.7	2.63
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG13	14	2.45	0.7	2.63
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE1	14	2.06	0.6	2.12
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE2	14	2.06	0.6	2.12
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE1	14	2.06	0.6	2.12
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE2	14	2.06	0.6	2.12
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE1	14	2.06	0.6	2.12
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE2	14	2.06	0.6	2.12
(2,38)	1:A:692:LEU:HD21	1:A:694:GLY:H	14	1.84	0.21	1.9
(2,38)	1:A:692:LEU:HD22	1:A:694:GLY:H	14	1.84	0.21	1.9
(2,38)	1:A:692:LEU:HD23	1:A:694:GLY:H	14	1.84	0.21	1.9
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	14	1.7	0.82	1.69
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	14	1.7	0.82	1.69
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	14	1.7	0.82	1.69
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	14	1.7	0.82	1.69
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	14	1.7	0.82	1.69
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	14	1.7	0.82	1.69
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	14	1.7	0.82	1.69
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	14	1.7	0.82	1.69
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	14	1.7	0.82	1.69
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	14	1.7	0.82	1.69
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	14	1.7	0.82	1.69
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	14	1.7	0.82	1.69
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	14	1.7	0.82	1.69
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	14	1.7	0.82	1.69
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	14	1.7	0.82	1.69
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	14	1.7	0.82	1.69
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	14	1.7	1.08	1.48
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	14	1.7	1.08	1.48
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	14	1.7	1.08	1.48
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	14	1.7	1.08	1.48
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	14	1.7	1.08	1.48

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	14	1.7	1.08	1.48
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	14	1.7	1.08	1.48
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	14	1.7	1.08	1.48
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	14	1.7	1.08	1.48
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	14	1.7	1.08	1.48
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	14	1.7	1.08	1.48
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	14	1.7	1.08	1.48
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	14	1.7	1.08	1.48
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	14	1.7	1.08	1.48
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	14	1.7	1.08	1.48
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	14	1.7	1.08	1.48
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD21	14	1.34	0.21	1.4
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD22	14	1.34	0.21	1.4
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD23	14	1.34	0.21	1.4
(2,457)	1:B:740:ARG:H	1:B:739:GLU:HA	14	0.48	0.02	0.48
(2,180)	1:A:806:GLU:H	1:B:771:LEU:HG	14	0.44	0.18	0.43
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB2	14	0.43	0.16	0.46
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB3	14	0.43	0.16	0.46
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD2	14	0.41	0.23	0.4
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD3	14	0.41	0.23	0.4
(2,559)	1:B:778:VAL:H	1:B:775:LEU:HA	14	0.32	0.09	0.31
(2,990)	1:A:779:THR:H	1:A:776:LEU:HA	14	0.3	0.09	0.32
(2,1415)	1:A:779:THR:H	1:A:776:LEU:HA	14	0.3	0.09	0.32
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD2	14	0.29	0.09	0.3
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD3	14	0.29	0.09	0.3
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG12	14	0.29	0.1	0.29
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG13	14	0.29	0.1	0.29
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG12	14	0.29	0.1	0.29
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG13	14	0.29	0.1	0.29
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA2	14	0.27	0.11	0.22
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA3	14	0.27	0.11	0.22
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA2	14	0.27	0.11	0.22
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA3	14	0.27	0.11	0.22
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA2	14	0.27	0.11	0.22
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA3	14	0.27	0.11	0.22
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	14	0.26	0.08	0.27
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	14	0.26	0.08	0.27
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	14	0.26	0.08	0.27
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	14	0.26	0.08	0.27
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	14	0.26	0.08	0.27
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	14	0.26	0.08	0.27
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	14	0.26	0.08	0.27

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	14	0.26	0.08	0.27
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	14	0.26	0.08	0.27
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	14	0.26	0.08	0.27
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	14	0.26	0.08	0.27
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	14	0.26	0.08	0.27
(2,1006)	1:A:782:VAL:H	1:A:779:THR:HA	14	0.23	0.08	0.22
(2,1431)	1:A:782:VAL:H	1:A:779:THR:HA	14	0.23	0.08	0.22
(2,224)	1:B:664:ASP:H	1:B:663:LEU:HA	14	0.2	0.02	0.2
(1,23)	1:B:801:GLN:O	1:B:805:GLN:H	14	0.19	0.06	0.18
(1,109)	1:B:801:GLN:O	1:B:805:GLN:H	14	0.19	0.06	0.18
(1,195)	1:B:801:GLN:O	1:B:805:GLN:H	14	0.19	0.06	0.18
(2,649)	1:A:664:ASP:H	1:A:663:LEU:HA	14	0.18	0.04	0.19
(2,1074)	1:A:664:ASP:H	1:A:663:LEU:HA	14	0.18	0.04	0.19
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	13	2.2	1.03	2.42
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	13	2.2	1.03	2.42
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	13	2.2	1.03	2.42
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	13	2.2	1.03	2.42
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	13	2.2	1.03	2.42
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	13	2.2	1.03	2.42
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	13	2.2	1.03	2.42
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	13	2.2	1.03	2.42
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	13	2.2	1.03	2.42
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	13	2.2	1.03	2.42
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	13	2.2	1.03	2.42
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	13	2.2	1.03	2.42
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	13	2.2	1.03	2.42
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	13	2.2	1.03	2.42
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	13	2.2	1.03	2.42
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	13	2.2	1.03	2.42
(2,135)	1:B:756:ILE:H	1:A:796:TRP:HE1	13	0.63	0.23	0.57
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD2	13	0.41	0.16	0.35
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD3	13	0.41	0.16	0.35
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD2	13	0.41	0.16	0.35
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD3	13	0.41	0.16	0.35
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ1	13	0.32	0.11	0.33
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ2	13	0.32	0.11	0.33
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ3	13	0.32	0.11	0.33
(2,472)	1:B:746:ILE:HG21	1:B:750:ASN:HD21	13	0.28	0.08	0.26
(2,472)	1:B:746:ILE:HG22	1:B:750:ASN:HD21	13	0.28	0.08	0.26
(2,472)	1:B:746:ILE:HG23	1:B:750:ASN:HD21	13	0.28	0.08	0.26
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	13	0.27	0.09	0.24
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	13	0.27	0.09	0.24

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	13	0.27	0.09	0.24
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	13	0.27	0.09	0.24
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	13	0.27	0.09	0.24
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	13	0.27	0.09	0.24
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	13	0.27	0.09	0.24
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	13	0.27	0.09	0.24
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	13	0.27	0.09	0.24
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	13	0.27	0.09	0.24
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	13	0.27	0.09	0.24
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	13	0.27	0.09	0.24
(2,369)	1:B:701:VAL:H	1:B:698:VAL:HA	13	0.24	0.04	0.23
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB2	13	0.23	0.06	0.24
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB3	13	0.23	0.06	0.24
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB2	13	0.23	0.06	0.24
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB3	13	0.23	0.06	0.24
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB2	13	0.23	0.06	0.24
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB3	13	0.23	0.06	0.24
(2,839)	1:A:707:ARG:H	1:A:704:LEU:HA	13	0.23	0.08	0.22
(2,1264)	1:A:707:ARG:H	1:A:704:LEU:HA	13	0.23	0.08	0.22
(2,581)	1:B:782:VAL:H	1:B:779:THR:HA	13	0.22	0.07	0.2
(2,242)	1:B:667:ALA:H	1:B:664:ASP:HA	13	0.19	0.06	0.18
(2,428)	1:B:708:VAL:HG11	1:B:705:VAL:HA	12	0.42	0.17	0.42
(2,428)	1:B:708:VAL:HG12	1:B:705:VAL:HA	12	0.42	0.17	0.42
(2,428)	1:B:708:VAL:HG13	1:B:705:VAL:HA	12	0.42	0.17	0.42
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD2	12	0.42	0.2	0.44
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD3	12	0.42	0.2	0.44
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD2	12	0.42	0.2	0.44
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD3	12	0.42	0.2	0.44
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB2	12	0.31	0.14	0.34
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB3	12	0.31	0.14	0.34
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB2	12	0.31	0.14	0.34
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB3	12	0.31	0.14	0.34
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB2	12	0.31	0.14	0.34
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB3	12	0.31	0.14	0.34
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB2	12	0.31	0.14	0.34
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB3	12	0.31	0.14	0.34
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB2	12	0.31	0.14	0.34
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB3	12	0.31	0.14	0.34
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB2	12	0.31	0.14	0.34
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB3	12	0.31	0.14	0.34
(2,183)	1:A:806:GLU:H	1:B:772:ARG:HE	12	0.29	0.12	0.26
(2,864)	1:A:710:GLN:H	1:A:708:VAL:HA	12	0.28	0.14	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1289)	1:A:710:GLN:H	1:A:708:VAL:HA	12	0.28	0.14	0.22
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	12	0.28	0.15	0.22
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	12	0.28	0.15	0.22
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	12	0.28	0.15	0.22
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	12	0.28	0.15	0.22
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	12	0.28	0.15	0.22
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	12	0.28	0.15	0.22
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	12	0.28	0.15	0.22
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	12	0.28	0.15	0.22
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	12	0.28	0.15	0.22
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	12	0.28	0.15	0.22
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	12	0.28	0.15	0.22
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	12	0.28	0.15	0.22
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	12	0.26	0.12	0.24
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	12	0.26	0.12	0.24
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	12	0.26	0.12	0.24
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	12	0.26	0.12	0.24
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD11	12	0.26	0.12	0.24
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD12	12	0.26	0.12	0.24
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD13	12	0.26	0.12	0.24
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB2	12	0.24	0.1	0.23
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB3	12	0.24	0.1	0.23
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB2	12	0.24	0.1	0.23
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB3	12	0.24	0.1	0.23
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB2	12	0.24	0.1	0.23
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB3	12	0.24	0.1	0.23
(2,670)	1:A:667:ALA:H	1:A:666:TRP:HD1	12	0.21	0.06	0.22
(2,1095)	1:A:667:ALA:H	1:A:666:TRP:HD1	12	0.21	0.06	0.22
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB2	12	0.18	0.06	0.18
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB3	12	0.18	0.06	0.18
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE1	11	2.36	1.28	2.93
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE2	11	2.36	1.28	2.93
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE1	11	2.36	1.28	2.93
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE2	11	2.36	1.28	2.93
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE1	11	2.36	1.28	2.93
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE2	11	2.36	1.28	2.93
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE1	11	2.36	1.28	2.93
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE2	11	2.36	1.28	2.93
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD1	11	1.66	0.67	1.69
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD2	11	1.66	0.67	1.69
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD1	11	1.66	0.67	1.69
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD2	11	1.66	0.67	1.69

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD1	11	1.66	0.67	1.69
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD2	11	1.66	0.67	1.69
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD1	11	1.66	0.67	1.69
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD2	11	1.66	0.67	1.69
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	11	1.21	0.7	1.34
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	11	1.21	0.7	1.34
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	11	1.21	0.7	1.34
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	11	1.21	0.7	1.34
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	11	1.21	0.7	1.34
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	11	1.21	0.7	1.34
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	11	1.21	0.7	1.34
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	11	1.21	0.7	1.34
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	11	1.21	0.7	1.34
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	11	1.21	0.7	1.34
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	11	1.21	0.7	1.34
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	11	1.21	0.7	1.34
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	11	1.21	0.7	1.34
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	11	1.21	0.7	1.34
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	11	1.21	0.7	1.34
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	11	1.21	0.7	1.34
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG21	11	0.68	0.15	0.69
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG22	11	0.68	0.15	0.69
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG23	11	0.68	0.15	0.69
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG21	11	0.68	0.15	0.69
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG22	11	0.68	0.15	0.69
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG23	11	0.68	0.15	0.69
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG21	11	0.68	0.15	0.69
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG22	11	0.68	0.15	0.69
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG23	11	0.68	0.15	0.69
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	11	0.51	0.14	0.53
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	11	0.51	0.14	0.53
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	11	0.51	0.14	0.53
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	11	0.51	0.14	0.53
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	11	0.51	0.14	0.53
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	11	0.51	0.14	0.53
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	11	0.51	0.14	0.53
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	11	0.51	0.14	0.53
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	11	0.51	0.14	0.53
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	11	0.51	0.14	0.53
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	11	0.51	0.14	0.53
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	11	0.51	0.14	0.53
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD2	11	0.34	0.13	0.3

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD3	11	0.34	0.13	0.3
(2,721)	1:A:682:ILE:HD11	1:A:681:TYR:H	11	0.3	0.1	0.31
(2,721)	1:A:682:ILE:HD12	1:A:681:TYR:H	11	0.3	0.1	0.31
(2,721)	1:A:682:ILE:HD13	1:A:681:TYR:H	11	0.3	0.1	0.31
(2,1146)	1:A:682:ILE:HD11	1:A:681:TYR:H	11	0.3	0.1	0.31
(2,1146)	1:A:682:ILE:HD12	1:A:681:TYR:H	11	0.3	0.1	0.31
(2,1146)	1:A:682:ILE:HD13	1:A:681:TYR:H	11	0.3	0.1	0.31
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG12	11	0.28	0.13	0.23
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG13	11	0.28	0.13	0.23
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD11	11	0.25	0.11	0.22
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD12	11	0.25	0.11	0.22
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD13	11	0.25	0.11	0.22
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD2	11	0.22	0.06	0.2
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD3	11	0.22	0.06	0.2
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD2	11	0.22	0.06	0.2
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD3	11	0.22	0.06	0.2
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD2	11	0.22	0.06	0.2
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD3	11	0.22	0.06	0.2
(2,794)	1:A:701:VAL:H	1:A:698:VAL:HA	11	0.21	0.06	0.21
(2,1219)	1:A:701:VAL:H	1:A:698:VAL:HA	11	0.21	0.06	0.21
(1,9)	1:B:794:LYS:O	1:B:798:ASN:H	11	0.18	0.04	0.19
(1,95)	1:B:794:LYS:O	1:B:798:ASN:H	11	0.18	0.04	0.19
(1,181)	1:B:794:LYS:O	1:B:798:ASN:H	11	0.18	0.04	0.19
(2,356)	1:B:698:VAL:HG11	1:B:695:LEU:HG	11	0.16	0.03	0.17
(2,356)	1:B:698:VAL:HG12	1:B:695:LEU:HG	11	0.16	0.03	0.17
(2,356)	1:B:698:VAL:HG13	1:B:695:LEU:HG	11	0.16	0.03	0.17
(2,815)	1:A:704:LEU:H	1:A:704:LEU:HB3	10	0.52	0.17	0.54
(2,1240)	1:A:704:LEU:H	1:A:704:LEU:HB3	10	0.52	0.17	0.54
(2,764)	1:A:693:ILE:HG21	1:A:694:GLY:H	10	0.49	0.06	0.5
(2,764)	1:A:693:ILE:HG22	1:A:694:GLY:H	10	0.49	0.06	0.5
(2,764)	1:A:693:ILE:HG23	1:A:694:GLY:H	10	0.49	0.06	0.5
(2,1189)	1:A:693:ILE:HG21	1:A:694:GLY:H	10	0.49	0.06	0.5
(2,1189)	1:A:693:ILE:HG22	1:A:694:GLY:H	10	0.49	0.06	0.5
(2,1189)	1:A:693:ILE:HG23	1:A:694:GLY:H	10	0.49	0.06	0.5
(2,355)	1:B:698:VAL:HG11	1:B:695:LEU:HA	10	0.33	0.1	0.34
(2,355)	1:B:698:VAL:HG12	1:B:695:LEU:HA	10	0.33	0.1	0.34
(2,355)	1:B:698:VAL:HG13	1:B:695:LEU:HA	10	0.33	0.1	0.34
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD2	10	0.31	0.22	0.22
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD3	10	0.31	0.22	0.22
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB2	10	0.27	0.08	0.31
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB3	10	0.27	0.08	0.31
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB2	10	0.27	0.08	0.31

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB3	10	0.27	0.08	0.31
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB2	10	0.27	0.08	0.31
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB3	10	0.27	0.08	0.31
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB2	10	0.27	0.15	0.22
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB3	10	0.27	0.15	0.22
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB2	10	0.27	0.15	0.22
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB3	10	0.27	0.15	0.22
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB2	10	0.27	0.15	0.22
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB3	10	0.27	0.15	0.22
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD2	10	0.25	0.07	0.26
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD3	10	0.25	0.07	0.26
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD2	10	0.25	0.07	0.26
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD3	10	0.25	0.07	0.26
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE1	10	0.24	0.14	0.19
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE2	10	0.24	0.14	0.19
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE1	10	0.24	0.14	0.19
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE2	10	0.24	0.14	0.19
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE1	10	0.24	0.14	0.19
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE2	10	0.24	0.14	0.19
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB2	10	0.23	0.08	0.21
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB3	10	0.23	0.08	0.21
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB2	10	0.23	0.08	0.21
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB3	10	0.23	0.08	0.21
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG2	10	0.22	0.06	0.2
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG3	10	0.22	0.06	0.2
(2,522)	1:B:764:SER:H	1:B:761:ARG:HA	10	0.19	0.05	0.18
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD11	10	0.19	0.04	0.18
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD12	10	0.19	0.04	0.18
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD13	10	0.19	0.04	0.18
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD11	10	0.19	0.04	0.18
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD12	10	0.19	0.04	0.18
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD13	10	0.19	0.04	0.18
(1,19)	1:B:799:LEU:O	1:B:803:TRP:H	10	0.18	0.04	0.18
(1,105)	1:B:799:LEU:O	1:B:803:TRP:H	10	0.18	0.04	0.18
(1,191)	1:B:799:LEU:O	1:B:803:TRP:H	10	0.18	0.04	0.18
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD1	9	0.32	0.07	0.33
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD2	9	0.32	0.07	0.33
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	9	0.28	0.16	0.2
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	9	0.28	0.16	0.2
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	9	0.28	0.16	0.2
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	9	0.28	0.16	0.2
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	9	0.28	0.16	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	9	0.28	0.16	0.2
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	9	0.28	0.16	0.2
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	9	0.28	0.16	0.2
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	9	0.28	0.16	0.2
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	9	0.28	0.16	0.2
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	9	0.28	0.16	0.2
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	9	0.28	0.16	0.2
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB2	9	0.24	0.11	0.2
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB3	9	0.24	0.11	0.2
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB2	9	0.22	0.08	0.2
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB3	9	0.22	0.08	0.2
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB2	9	0.22	0.08	0.2
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB3	9	0.22	0.08	0.2
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB2	9	0.22	0.08	0.2
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB3	9	0.22	0.08	0.2
(2,1040)	1:A:796:TRP:HE1	1:A:796:TRP:H	9	0.22	0.06	0.26
(2,1465)	1:A:796:TRP:HE1	1:A:796:TRP:H	9	0.22	0.06	0.26
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB2	9	0.22	0.06	0.21
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB3	9	0.22	0.06	0.21
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB2	9	0.22	0.06	0.21
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB3	9	0.22	0.06	0.21
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB2	9	0.22	0.06	0.21
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB3	9	0.22	0.06	0.21
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG2	9	0.21	0.06	0.22
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG3	9	0.21	0.06	0.22
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG2	9	0.21	0.06	0.22
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG3	9	0.21	0.06	0.22
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE21	9	0.19	0.02	0.19
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE22	9	0.19	0.02	0.19
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE21	9	0.19	0.02	0.19
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE22	9	0.19	0.02	0.19
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD11	9	0.19	0.13	0.13
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD12	9	0.19	0.13	0.13
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD13	9	0.19	0.13	0.13
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD21	9	0.19	0.13	0.13
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD22	9	0.19	0.13	0.13
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD23	9	0.19	0.13	0.13
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD2	9	0.19	0.07	0.16
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD3	9	0.19	0.07	0.16
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD2	9	0.19	0.07	0.16
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD3	9	0.19	0.07	0.16
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD2	9	0.19	0.07	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD3	9	0.19	0.07	0.16
(2,37)	1:B:692:LEU:HD21	1:A:694:GLY:H	9	0.14	0.03	0.13
(2,37)	1:B:692:LEU:HD22	1:A:694:GLY:H	9	0.14	0.03	0.13
(2,37)	1:B:692:LEU:HD23	1:A:694:GLY:H	9	0.14	0.03	0.13
(2,444)	1:B:710:GLN:H	1:B:710:GLN:HB3	8	0.52	0.11	0.55
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG12	8	0.41	0.16	0.48
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG13	8	0.41	0.16	0.48
(2,869)	1:A:710:GLN:H	1:A:710:GLN:HB3	8	0.39	0.15	0.44
(2,1294)	1:A:710:GLN:H	1:A:710:GLN:HB3	8	0.39	0.15	0.44
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB1	8	0.36	0.14	0.35
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB2	8	0.36	0.14	0.35
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB3	8	0.36	0.14	0.35
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB1	8	0.36	0.14	0.35
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB2	8	0.36	0.14	0.35
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB3	8	0.36	0.14	0.35
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB1	8	0.36	0.14	0.35
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB2	8	0.36	0.14	0.35
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB3	8	0.36	0.14	0.35
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD11	8	0.3	0.16	0.29
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD12	8	0.3	0.16	0.29
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD13	8	0.3	0.16	0.29
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD21	8	0.3	0.16	0.29
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD22	8	0.3	0.16	0.29
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD23	8	0.3	0.16	0.29
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD2	8	0.29	0.08	0.28
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD3	8	0.29	0.08	0.28
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD2	8	0.29	0.08	0.28
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD3	8	0.29	0.08	0.28
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH21	8	0.25	0.14	0.2
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH22	8	0.25	0.14	0.2
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH21	8	0.25	0.14	0.2
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH22	8	0.25	0.14	0.2
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH21	8	0.25	0.14	0.2
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH22	8	0.25	0.14	0.2
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD11	8	0.25	0.08	0.26
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD12	8	0.25	0.08	0.26
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD13	8	0.25	0.08	0.26
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD11	8	0.24	0.09	0.21
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD12	8	0.24	0.09	0.21
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD13	8	0.24	0.09	0.21
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB2	8	0.23	0.07	0.22
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB3	8	0.23	0.07	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB2	8	0.23	0.07	0.22
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB3	8	0.23	0.07	0.22
(2,897)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	8	0.23	0.09	0.24
(2,897)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	8	0.23	0.09	0.24
(2,897)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	8	0.23	0.09	0.24
(2,1322)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	8	0.23	0.09	0.24
(2,1322)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	8	0.23	0.09	0.24
(2,1322)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	8	0.23	0.09	0.24
(2,1005)	1:A:781:ILE:HG21	1:A:778:VAL:HA	8	0.22	0.03	0.24
(2,1005)	1:A:781:ILE:HG22	1:A:778:VAL:HA	8	0.22	0.03	0.24
(2,1005)	1:A:781:ILE:HG23	1:A:778:VAL:HA	8	0.22	0.03	0.24
(2,1430)	1:A:781:ILE:HG21	1:A:778:VAL:HA	8	0.22	0.03	0.24
(2,1430)	1:A:781:ILE:HG22	1:A:778:VAL:HA	8	0.22	0.03	0.24
(2,1430)	1:A:781:ILE:HG23	1:A:778:VAL:HA	8	0.22	0.03	0.24
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD2	8	0.22	0.09	0.18
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD3	8	0.22	0.09	0.18
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD1	8	0.22	0.05	0.22
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD2	8	0.22	0.05	0.22
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD1	8	0.22	0.05	0.22
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD2	8	0.22	0.05	0.22
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD1	8	0.22	0.05	0.22
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD2	8	0.22	0.05	0.22
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB2	8	0.22	0.13	0.15
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB3	8	0.22	0.13	0.15
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	8	0.21	0.12	0.16
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	8	0.21	0.12	0.16
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	8	0.21	0.12	0.16
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	8	0.21	0.12	0.16
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	8	0.21	0.12	0.16
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	8	0.21	0.12	0.16
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	8	0.21	0.12	0.16
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	8	0.21	0.12	0.16
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	8	0.21	0.12	0.16
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	8	0.21	0.12	0.16
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	8	0.21	0.12	0.16
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	8	0.21	0.12	0.16
(2,545)	1:B:775:LEU:HD11	1:B:772:ARG:HA	8	0.2	0.07	0.18
(2,545)	1:B:775:LEU:HD12	1:B:772:ARG:HA	8	0.2	0.07	0.18
(2,545)	1:B:775:LEU:HD13	1:B:772:ARG:HA	8	0.2	0.07	0.18
(2,781)	1:A:698:VAL:HG11	1:A:695:LEU:HG	8	0.18	0.05	0.17
(2,781)	1:A:698:VAL:HG12	1:A:695:LEU:HG	8	0.18	0.05	0.17
(2,781)	1:A:698:VAL:HG13	1:A:695:LEU:HG	8	0.18	0.05	0.17

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1206)	1:A:698:VAL:HG11	1:A:695:LEU:HG	8	0.18	0.05	0.17
(2,1206)	1:A:698:VAL:HG12	1:A:695:LEU:HG	8	0.18	0.05	0.17
(2,1206)	1:A:698:VAL:HG13	1:A:695:LEU:HG	8	0.18	0.05	0.17
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB2	8	0.18	0.03	0.18
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB3	8	0.18	0.03	0.18
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD21	8	0.17	0.04	0.18
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD22	8	0.17	0.04	0.18
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD23	8	0.17	0.04	0.18
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD1	8	0.16	0.03	0.16
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD2	8	0.16	0.03	0.16
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD1	8	0.16	0.03	0.16
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD2	8	0.16	0.03	0.16
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD1	8	0.16	0.03	0.16
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD2	8	0.16	0.03	0.16
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	8	0.16	0.06	0.14
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	8	0.16	0.06	0.14
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	8	0.16	0.06	0.14
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	8	0.16	0.06	0.14
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	8	0.16	0.06	0.14
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	8	0.16	0.06	0.14
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	8	0.16	0.06	0.14
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	8	0.16	0.06	0.14
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	8	0.16	0.06	0.14
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	8	0.16	0.06	0.14
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	8	0.16	0.06	0.14
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	8	0.16	0.06	0.14
(1,20)	1:B:799:LEU:O	1:B:803:TRP:N	8	0.15	0.04	0.14
(1,106)	1:B:799:LEU:O	1:B:803:TRP:N	8	0.15	0.04	0.14
(1,192)	1:B:799:LEU:O	1:B:803:TRP:N	8	0.15	0.04	0.14
(2,778)	1:A:697:ILE:HG21	1:A:698:VAL:HA	7	0.81	0.18	0.88
(2,778)	1:A:697:ILE:HG22	1:A:698:VAL:HA	7	0.81	0.18	0.88
(2,778)	1:A:697:ILE:HG23	1:A:698:VAL:HA	7	0.81	0.18	0.88
(2,1203)	1:A:697:ILE:HG21	1:A:698:VAL:HA	7	0.81	0.18	0.88
(2,1203)	1:A:697:ILE:HG22	1:A:698:VAL:HA	7	0.81	0.18	0.88
(2,1203)	1:A:697:ILE:HG23	1:A:698:VAL:HA	7	0.81	0.18	0.88
(2,393)	1:B:704:LEU:HD11	1:B:707:ARG:HD2	7	0.33	0.12	0.32
(2,393)	1:B:704:LEU:HD11	1:B:707:ARG:HD3	7	0.33	0.12	0.32
(2,393)	1:B:704:LEU:HD12	1:B:707:ARG:HD2	7	0.33	0.12	0.32
(2,393)	1:B:704:LEU:HD12	1:B:707:ARG:HD3	7	0.33	0.12	0.32
(2,393)	1:B:704:LEU:HD13	1:B:707:ARG:HD2	7	0.33	0.12	0.32
(2,393)	1:B:704:LEU:HD13	1:B:707:ARG:HD3	7	0.33	0.12	0.32
(2,421)	1:B:707:ARG:H	1:B:707:ARG:HD2	7	0.32	0.16	0.29

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,421)	1:B:707:ARG:H	1:B:707:ARG:HD3	7	0.32	0.16	0.29
(2,983)	1:A:777:ILE:HG21	1:A:780:ARG:HD2	7	0.32	0.17	0.27
(2,983)	1:A:777:ILE:HG21	1:A:780:ARG:HD3	7	0.32	0.17	0.27
(2,983)	1:A:777:ILE:HG22	1:A:780:ARG:HD2	7	0.32	0.17	0.27
(2,983)	1:A:777:ILE:HG22	1:A:780:ARG:HD3	7	0.32	0.17	0.27
(2,983)	1:A:777:ILE:HG23	1:A:780:ARG:HD2	7	0.32	0.17	0.27
(2,983)	1:A:777:ILE:HG23	1:A:780:ARG:HD3	7	0.32	0.17	0.27
(2,1408)	1:A:777:ILE:HG21	1:A:780:ARG:HD2	7	0.32	0.17	0.27
(2,1408)	1:A:777:ILE:HG21	1:A:780:ARG:HD3	7	0.32	0.17	0.27
(2,1408)	1:A:777:ILE:HG22	1:A:780:ARG:HD2	7	0.32	0.17	0.27
(2,1408)	1:A:777:ILE:HG22	1:A:780:ARG:HD3	7	0.32	0.17	0.27
(2,1408)	1:A:777:ILE:HG23	1:A:780:ARG:HD2	7	0.32	0.17	0.27
(2,1408)	1:A:777:ILE:HG23	1:A:780:ARG:HD3	7	0.32	0.17	0.27
(2,390)	1:B:704:LEU:H	1:B:704:LEU:HB3	7	0.31	0.21	0.23
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD11	7	0.27	0.1	0.3
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD12	7	0.27	0.1	0.3
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD13	7	0.27	0.1	0.3
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD21	7	0.27	0.1	0.3
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD22	7	0.27	0.1	0.3
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD23	7	0.27	0.1	0.3
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD11	7	0.27	0.1	0.3
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD12	7	0.27	0.1	0.3
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD13	7	0.27	0.1	0.3
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD21	7	0.27	0.1	0.3
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD22	7	0.27	0.1	0.3
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD23	7	0.27	0.1	0.3
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD11	7	0.27	0.04	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD12	7	0.27	0.04	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD13	7	0.27	0.04	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD21	7	0.27	0.04	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD22	7	0.27	0.04	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD23	7	0.27	0.04	0.25
(2,473)	1:B:746:ILE:HG21	1:B:750:ASN:HD22	7	0.22	0.11	0.16
(2,473)	1:B:746:ILE:HG22	1:B:750:ASN:HD22	7	0.22	0.11	0.16
(2,473)	1:B:746:ILE:HG23	1:B:750:ASN:HD22	7	0.22	0.11	0.16
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD11	7	0.22	0.06	0.22
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD12	7	0.22	0.06	0.22
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD13	7	0.22	0.06	0.22
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD11	7	0.22	0.06	0.22
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD12	7	0.22	0.06	0.22
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD13	7	0.22	0.06	0.22
(2,93)	1:A:754:ALA:H	1:B:716:SER:HB2	7	0.21	0.09	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,93)	1:A:754:ALA:H	1:B:716:SER:HB3	7	0.21	0.09	0.18
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD11	7	0.2	0.04	0.21
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD12	7	0.2	0.04	0.21
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD13	7	0.2	0.04	0.21
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD11	7	0.2	0.04	0.21
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD12	7	0.2	0.04	0.21
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD13	7	0.2	0.04	0.21
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD11	7	0.2	0.04	0.21
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD12	7	0.2	0.04	0.21
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD13	7	0.2	0.04	0.21
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD11	7	0.18	0.08	0.14
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD12	7	0.18	0.08	0.14
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD13	7	0.18	0.08	0.14
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD11	7	0.18	0.08	0.14
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD12	7	0.18	0.08	0.14
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD13	7	0.18	0.08	0.14
(2,177)	1:A:803:TRP:HE1	1:B:764:SER:HG	7	0.17	0.04	0.17
(2,1050)	1:A:806:GLU:H	1:A:803:TRP:HB2	7	0.16	0.03	0.15
(2,1050)	1:A:806:GLU:H	1:A:803:TRP:HB3	7	0.16	0.03	0.15
(2,1475)	1:A:806:GLU:H	1:A:803:TRP:HB2	7	0.16	0.03	0.15
(2,1475)	1:A:806:GLU:H	1:A:803:TRP:HB3	7	0.16	0.03	0.15
(2,245)	1:B:667:ALA:H	1:B:666:TRP:HD1	7	0.16	0.04	0.15
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD11	7	0.16	0.03	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD12	7	0.16	0.03	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD13	7	0.16	0.03	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD21	7	0.16	0.03	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD22	7	0.16	0.03	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD23	7	0.16	0.03	0.14
(1,10)	1:B:794:LYS:O	1:B:798:ASN:N	7	0.15	0.04	0.13
(1,96)	1:B:794:LYS:O	1:B:798:ASN:N	7	0.15	0.04	0.13
(1,182)	1:B:794:LYS:O	1:B:798:ASN:N	7	0.15	0.04	0.13
(1,25)	1:B:802:TYR:O	1:B:806:GLU:H	7	0.15	0.04	0.13
(1,111)	1:B:802:TYR:O	1:B:806:GLU:H	7	0.15	0.04	0.13
(1,197)	1:B:802:TYR:O	1:B:806:GLU:H	7	0.15	0.04	0.13
(1,75)	1:B:837:SER:O	1:B:841:ARG:H	7	0.14	0.03	0.14
(1,161)	1:B:837:SER:O	1:B:841:ARG:H	7	0.14	0.03	0.14
(1,247)	1:B:837:SER:O	1:B:841:ARG:H	7	0.14	0.03	0.14
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD11	7	0.14	0.04	0.13
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD12	7	0.14	0.04	0.13
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD13	7	0.14	0.04	0.13
(2,683)	1:A:669:LEU:HD11	1:A:672:TRP:HZ3	7	0.13	0.01	0.13
(2,683)	1:A:669:LEU:HD12	1:A:672:TRP:HZ3	7	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,683)	1:A:669:LEU:HD13	1:A:672:TRP:HZ3	7	0.13	0.01	0.13
(2,683)	1:A:669:LEU:HD21	1:A:672:TRP:HZ3	7	0.13	0.01	0.13
(2,683)	1:A:669:LEU:HD22	1:A:672:TRP:HZ3	7	0.13	0.01	0.13
(2,683)	1:A:669:LEU:HD23	1:A:672:TRP:HZ3	7	0.13	0.01	0.13
(2,1108)	1:A:669:LEU:HD11	1:A:672:TRP:HZ3	7	0.13	0.01	0.13
(2,1108)	1:A:669:LEU:HD12	1:A:672:TRP:HZ3	7	0.13	0.01	0.13
(2,1108)	1:A:669:LEU:HD13	1:A:672:TRP:HZ3	7	0.13	0.01	0.13
(2,1108)	1:A:669:LEU:HD21	1:A:672:TRP:HZ3	7	0.13	0.01	0.13
(2,1108)	1:A:669:LEU:HD22	1:A:672:TRP:HZ3	7	0.13	0.01	0.13
(2,1108)	1:A:669:LEU:HD23	1:A:672:TRP:HZ3	7	0.13	0.01	0.13
(2,81)	1:A:708:VAL:HG21	1:B:714:PRO:HA	6	0.32	0.11	0.36
(2,81)	1:A:708:VAL:HG22	1:B:714:PRO:HA	6	0.32	0.11	0.36
(2,81)	1:A:708:VAL:HG23	1:B:714:PRO:HA	6	0.32	0.11	0.36
(2,782)	1:A:698:VAL:HG11	1:A:699:PHE:HD1	6	0.3	0.15	0.3
(2,782)	1:A:698:VAL:HG11	1:A:699:PHE:HD2	6	0.3	0.15	0.3
(2,782)	1:A:698:VAL:HG12	1:A:699:PHE:HD1	6	0.3	0.15	0.3
(2,782)	1:A:698:VAL:HG12	1:A:699:PHE:HD2	6	0.3	0.15	0.3
(2,782)	1:A:698:VAL:HG13	1:A:699:PHE:HD1	6	0.3	0.15	0.3
(2,782)	1:A:698:VAL:HG13	1:A:699:PHE:HD2	6	0.3	0.15	0.3
(2,1207)	1:A:698:VAL:HG11	1:A:699:PHE:HD1	6	0.3	0.15	0.3
(2,1207)	1:A:698:VAL:HG11	1:A:699:PHE:HD2	6	0.3	0.15	0.3
(2,1207)	1:A:698:VAL:HG12	1:A:699:PHE:HD1	6	0.3	0.15	0.3
(2,1207)	1:A:698:VAL:HG12	1:A:699:PHE:HD2	6	0.3	0.15	0.3
(2,1207)	1:A:698:VAL:HG13	1:A:699:PHE:HD1	6	0.3	0.15	0.3
(2,1207)	1:A:698:VAL:HG13	1:A:699:PHE:HD2	6	0.3	0.15	0.3
(2,471)	1:B:746:ILE:HD11	1:B:743:ASP:HB2	6	0.27	0.14	0.24
(2,471)	1:B:746:ILE:HD11	1:B:743:ASP:HB3	6	0.27	0.14	0.24
(2,471)	1:B:746:ILE:HD12	1:B:743:ASP:HB2	6	0.27	0.14	0.24
(2,471)	1:B:746:ILE:HD12	1:B:743:ASP:HB3	6	0.27	0.14	0.24
(2,471)	1:B:746:ILE:HD13	1:B:743:ASP:HB2	6	0.27	0.14	0.24
(2,471)	1:B:746:ILE:HD13	1:B:743:ASP:HB3	6	0.27	0.14	0.24
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD11	6	0.26	0.14	0.22
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD12	6	0.26	0.14	0.22
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD13	6	0.26	0.14	0.22
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD21	6	0.26	0.14	0.22
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD22	6	0.26	0.14	0.22
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD23	6	0.26	0.14	0.22
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD11	6	0.26	0.14	0.22
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD12	6	0.26	0.14	0.22
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD13	6	0.26	0.14	0.22
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD21	6	0.26	0.14	0.22
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD22	6	0.26	0.14	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD23	6	0.26	0.14	0.22
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG11	6	0.26	0.09	0.28
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG12	6	0.26	0.09	0.28
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG13	6	0.26	0.09	0.28
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG21	6	0.26	0.09	0.28
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG22	6	0.26	0.09	0.28
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG23	6	0.26	0.09	0.28
(2,296)	1:B:682:ILE:HD11	1:B:681:TYR:H	6	0.23	0.11	0.21
(2,296)	1:B:682:ILE:HD12	1:B:681:TYR:H	6	0.23	0.11	0.21
(2,296)	1:B:682:ILE:HD13	1:B:681:TYR:H	6	0.23	0.11	0.21
(2,575)	1:B:781:ILE:H	1:B:778:VAL:HA	6	0.23	0.06	0.25
(2,405)	1:B:705:VAL:HG21	1:B:702:LEU:HG	6	0.22	0.16	0.16
(2,405)	1:B:705:VAL:HG22	1:B:702:LEU:HG	6	0.22	0.16	0.16
(2,405)	1:B:705:VAL:HG23	1:B:702:LEU:HG	6	0.22	0.16	0.16
(2,1018)	1:A:784:LEU:H	1:A:781:ILE:HA	6	0.22	0.13	0.17
(2,1443)	1:A:784:LEU:H	1:A:781:ILE:HA	6	0.22	0.13	0.17
(2,948)	1:A:764:SER:H	1:A:771:LEU:HB2	6	0.22	0.09	0.16
(2,948)	1:A:764:SER:H	1:A:771:LEU:HB3	6	0.22	0.09	0.16
(2,1373)	1:A:764:SER:H	1:A:771:LEU:HB2	6	0.22	0.09	0.16
(2,1373)	1:A:764:SER:H	1:A:771:LEU:HB3	6	0.22	0.09	0.16
(2,142)	1:A:781:ILE:H	1:B:746:ILE:HG12	6	0.21	0.07	0.18
(2,142)	1:A:781:ILE:H	1:B:746:ILE:HG13	6	0.21	0.07	0.18
(2,558)	1:B:777:ILE:HG21	1:B:780:ARG:HD2	6	0.2	0.07	0.2
(2,558)	1:B:777:ILE:HG21	1:B:780:ARG:HD3	6	0.2	0.07	0.2
(2,558)	1:B:777:ILE:HG22	1:B:780:ARG:HD2	6	0.2	0.07	0.2
(2,558)	1:B:777:ILE:HG22	1:B:780:ARG:HD3	6	0.2	0.07	0.2
(2,558)	1:B:777:ILE:HG23	1:B:780:ARG:HD2	6	0.2	0.07	0.2
(2,558)	1:B:777:ILE:HG23	1:B:780:ARG:HD3	6	0.2	0.07	0.2
(2,185)	1:A:808:LYS:H	1:A:838:ARG:HD2	6	0.2	0.08	0.18
(2,185)	1:A:808:LYS:H	1:A:838:ARG:HD3	6	0.2	0.08	0.18
(2,186)	1:A:808:LYS:H	1:A:838:ARG:HD2	6	0.2	0.08	0.18
(2,186)	1:A:808:LYS:H	1:A:838:ARG:HD3	6	0.2	0.08	0.18
(2,1000)	1:A:781:ILE:H	1:A:778:VAL:HA	6	0.2	0.04	0.2
(2,1425)	1:A:781:ILE:H	1:A:778:VAL:HA	6	0.2	0.04	0.2
(2,939)	1:A:760:LEU:HD11	1:A:756:ILE:HG12	6	0.19	0.08	0.16
(2,939)	1:A:760:LEU:HD11	1:A:756:ILE:HG13	6	0.19	0.08	0.16
(2,939)	1:A:760:LEU:HD12	1:A:756:ILE:HG12	6	0.19	0.08	0.16
(2,939)	1:A:760:LEU:HD12	1:A:756:ILE:HG13	6	0.19	0.08	0.16
(2,939)	1:A:760:LEU:HD13	1:A:756:ILE:HG12	6	0.19	0.08	0.16
(2,939)	1:A:760:LEU:HD13	1:A:756:ILE:HG13	6	0.19	0.08	0.16
(2,1364)	1:A:760:LEU:HD11	1:A:756:ILE:HG12	6	0.19	0.08	0.16
(2,1364)	1:A:760:LEU:HD11	1:A:756:ILE:HG13	6	0.19	0.08	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1364)	1:A:760:LEU:HD12	1:A:756:ILE:HG12	6	0.19	0.08	0.16
(2,1364)	1:A:760:LEU:HD12	1:A:756:ILE:HG13	6	0.19	0.08	0.16
(2,1364)	1:A:760:LEU:HD13	1:A:756:ILE:HG12	6	0.19	0.08	0.16
(2,1364)	1:A:760:LEU:HD13	1:A:756:ILE:HG13	6	0.19	0.08	0.16
(2,1032)	1:A:785:LEU:HD21	1:A:782:VAL:HA	6	0.19	0.04	0.18
(2,1032)	1:A:785:LEU:HD22	1:A:782:VAL:HA	6	0.19	0.04	0.18
(2,1032)	1:A:785:LEU:HD23	1:A:782:VAL:HA	6	0.19	0.04	0.18
(2,1457)	1:A:785:LEU:HD21	1:A:782:VAL:HA	6	0.19	0.04	0.18
(2,1457)	1:A:785:LEU:HD22	1:A:782:VAL:HA	6	0.19	0.04	0.18
(2,1457)	1:A:785:LEU:HD23	1:A:782:VAL:HA	6	0.19	0.04	0.18
(2,141)	1:B:771:LEU:H	1:A:806:GLU:HB2	6	0.19	0.06	0.17
(2,141)	1:B:771:LEU:H	1:A:806:GLU:HB3	6	0.19	0.06	0.17
(2,219)	1:B:663:LEU:H	1:B:664:ASP:H	6	0.18	0.05	0.18
(2,225)	1:B:664:ASP:H	1:B:663:LEU:H	6	0.18	0.05	0.18
(2,653)	1:A:665:LYS:H	1:A:662:GLU:HA	6	0.18	0.06	0.16
(2,1078)	1:A:665:LYS:H	1:A:662:GLU:HA	6	0.18	0.06	0.16
(2,601)	1:B:785:LEU:H	1:B:782:VAL:HA	6	0.18	0.05	0.18
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD21	6	0.18	0.03	0.18
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD22	6	0.18	0.03	0.18
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD23	6	0.18	0.03	0.18
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD21	6	0.18	0.03	0.18
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD22	6	0.18	0.03	0.18
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD23	6	0.18	0.03	0.18
(2,701)	1:A:676:THR:HG21	1:A:666:TRP:HZ3	6	0.17	0.05	0.16
(2,701)	1:A:676:THR:HG22	1:A:666:TRP:HZ3	6	0.17	0.05	0.16
(2,701)	1:A:676:THR:HG23	1:A:666:TRP:HZ3	6	0.17	0.05	0.16
(2,1126)	1:A:676:THR:HG21	1:A:666:TRP:HZ3	6	0.17	0.05	0.16
(2,1126)	1:A:676:THR:HG22	1:A:666:TRP:HZ3	6	0.17	0.05	0.16
(2,1126)	1:A:676:THR:HG23	1:A:666:TRP:HZ3	6	0.17	0.05	0.16
(2,13)	1:B:666:TRP:HE1	1:A:666:TRP:HD1	6	0.16	0.03	0.16
(1,5)	1:B:792:ALA:O	1:B:796:TRP:H	6	0.16	0.07	0.13
(1,91)	1:B:792:ALA:O	1:B:796:TRP:H	6	0.16	0.07	0.13
(1,177)	1:B:792:ALA:O	1:B:796:TRP:H	6	0.16	0.07	0.13
(2,259)	1:B:670:TRP:H	1:B:667:ALA:HA	6	0.15	0.02	0.15
(2,904)	1:A:748:LEU:H	1:A:745:SER:HA	6	0.15	0.04	0.14
(2,1329)	1:A:748:LEU:H	1:A:745:SER:HA	6	0.15	0.04	0.14
(2,821)	1:A:705:VAL:H	1:A:702:LEU:HA	6	0.14	0.04	0.12
(2,1246)	1:A:705:VAL:H	1:A:702:LEU:HA	6	0.14	0.04	0.12
(1,47)	1:B:813:SER:O	1:B:817:ALA:H	6	0.14	0.03	0.13
(1,133)	1:B:813:SER:O	1:B:817:ALA:H	6	0.14	0.03	0.13
(1,219)	1:B:813:SER:O	1:B:817:ALA:H	6	0.14	0.03	0.13
(1,61)	1:B:830:ILE:O	1:B:834:GLN:H	6	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,147)	1:B:830:ILE:O	1:B:834:GLN:H	6	0.13	0.02	0.13
(1,233)	1:B:830:ILE:O	1:B:834:GLN:H	6	0.13	0.02	0.13
(2,576)	1:B:781:ILE:H	1:B:780:ARG:HA	6	0.12	0.01	0.11
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD11	5	0.32	0.08	0.34
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD12	5	0.32	0.08	0.34
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD13	5	0.32	0.08	0.34
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD21	5	0.32	0.08	0.34
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD22	5	0.32	0.08	0.34
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD23	5	0.32	0.08	0.34
(2,943)	1:A:763:LEU:HD11	1:A:759:ASP:HA	5	0.32	0.08	0.32
(2,943)	1:A:763:LEU:HD12	1:A:759:ASP:HA	5	0.32	0.08	0.32
(2,943)	1:A:763:LEU:HD13	1:A:759:ASP:HA	5	0.32	0.08	0.32
(2,1368)	1:A:763:LEU:HD11	1:A:759:ASP:HA	5	0.32	0.08	0.32
(2,1368)	1:A:763:LEU:HD12	1:A:759:ASP:HA	5	0.32	0.08	0.32
(2,1368)	1:A:763:LEU:HD13	1:A:759:ASP:HA	5	0.32	0.08	0.32
(2,203)	1:A:827:ASP:H	1:A:820:ILE:HG12	5	0.32	0.13	0.37
(2,203)	1:A:827:ASP:H	1:A:820:ILE:HG13	5	0.32	0.13	0.37
(2,204)	1:A:827:ASP:H	1:A:820:ILE:HG12	5	0.32	0.13	0.37
(2,204)	1:A:827:ASP:H	1:A:820:ILE:HG13	5	0.32	0.13	0.37
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD11	5	0.31	0.22	0.2
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD12	5	0.31	0.22	0.2
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD13	5	0.31	0.22	0.2
(2,854)	1:A:708:VAL:HG21	1:A:707:ARG:HD2	5	0.31	0.12	0.34
(2,854)	1:A:708:VAL:HG21	1:A:707:ARG:HD3	5	0.31	0.12	0.34
(2,854)	1:A:708:VAL:HG22	1:A:707:ARG:HD2	5	0.31	0.12	0.34
(2,854)	1:A:708:VAL:HG22	1:A:707:ARG:HD3	5	0.31	0.12	0.34
(2,854)	1:A:708:VAL:HG23	1:A:707:ARG:HD2	5	0.31	0.12	0.34
(2,854)	1:A:708:VAL:HG23	1:A:707:ARG:HD3	5	0.31	0.12	0.34
(2,1279)	1:A:708:VAL:HG21	1:A:707:ARG:HD2	5	0.31	0.12	0.34
(2,1279)	1:A:708:VAL:HG21	1:A:707:ARG:HD3	5	0.31	0.12	0.34
(2,1279)	1:A:708:VAL:HG22	1:A:707:ARG:HD2	5	0.31	0.12	0.34
(2,1279)	1:A:708:VAL:HG22	1:A:707:ARG:HD3	5	0.31	0.12	0.34
(2,1279)	1:A:708:VAL:HG23	1:A:707:ARG:HD2	5	0.31	0.12	0.34
(2,1279)	1:A:708:VAL:HG23	1:A:707:ARG:HD3	5	0.31	0.12	0.34
(2,531)	1:B:773:ASP:H	1:B:770:ARG:HD2	5	0.3	0.25	0.2
(2,531)	1:B:773:ASP:H	1:B:770:ARG:HD3	5	0.3	0.25	0.2
(2,228)	1:B:665:LYS:H	1:B:662:GLU:HA	5	0.3	0.15	0.35
(2,234)	1:B:666:TRP:H	1:B:663:LEU:HA	5	0.27	0.09	0.27
(2,752)	1:A:689:VAL:HG21	1:A:685:PHE:HE1	5	0.26	0.1	0.32
(2,752)	1:A:689:VAL:HG21	1:A:685:PHE:HE2	5	0.26	0.1	0.32
(2,752)	1:A:689:VAL:HG22	1:A:685:PHE:HE1	5	0.26	0.1	0.32
(2,752)	1:A:689:VAL:HG22	1:A:685:PHE:HE2	5	0.26	0.1	0.32

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,752)	1:A:689:VAL:HG23	1:A:685:PHE:HE1	5	0.26	0.1	0.32
(2,752)	1:A:689:VAL:HG23	1:A:685:PHE:HE2	5	0.26	0.1	0.32
(2,1177)	1:A:689:VAL:HG21	1:A:685:PHE:HE1	5	0.26	0.1	0.32
(2,1177)	1:A:689:VAL:HG21	1:A:685:PHE:HE2	5	0.26	0.1	0.32
(2,1177)	1:A:689:VAL:HG22	1:A:685:PHE:HE1	5	0.26	0.1	0.32
(2,1177)	1:A:689:VAL:HG22	1:A:685:PHE:HE2	5	0.26	0.1	0.32
(2,1177)	1:A:689:VAL:HG23	1:A:685:PHE:HE1	5	0.26	0.1	0.32
(2,1177)	1:A:689:VAL:HG23	1:A:685:PHE:HE2	5	0.26	0.1	0.32
(2,5)	1:A:663:LEU:H	1:A:661:LEU:HB2	5	0.24	0.13	0.15
(2,5)	1:A:663:LEU:H	1:A:661:LEU:HB3	5	0.24	0.13	0.15
(2,940)	1:A:760:LEU:HD11	1:A:757:TRP:HA	5	0.23	0.04	0.25
(2,940)	1:A:760:LEU:HD12	1:A:757:TRP:HA	5	0.23	0.04	0.25
(2,940)	1:A:760:LEU:HD13	1:A:757:TRP:HA	5	0.23	0.04	0.25
(2,1365)	1:A:760:LEU:HD11	1:A:757:TRP:HA	5	0.23	0.04	0.25
(2,1365)	1:A:760:LEU:HD12	1:A:757:TRP:HA	5	0.23	0.04	0.25
(2,1365)	1:A:760:LEU:HD13	1:A:757:TRP:HA	5	0.23	0.04	0.25
(2,1026)	1:A:785:LEU:H	1:A:782:VAL:HA	5	0.21	0.07	0.18
(2,1451)	1:A:785:LEU:H	1:A:782:VAL:HA	5	0.21	0.07	0.18
(2,916)	1:A:753:LEU:HD11	1:A:757:TRP:HB2	5	0.21	0.05	0.21
(2,916)	1:A:753:LEU:HD11	1:A:757:TRP:HB3	5	0.21	0.05	0.21
(2,916)	1:A:753:LEU:HD12	1:A:757:TRP:HB2	5	0.21	0.05	0.21
(2,916)	1:A:753:LEU:HD12	1:A:757:TRP:HB3	5	0.21	0.05	0.21
(2,916)	1:A:753:LEU:HD13	1:A:757:TRP:HB2	5	0.21	0.05	0.21
(2,916)	1:A:753:LEU:HD13	1:A:757:TRP:HB3	5	0.21	0.05	0.21
(2,1341)	1:A:753:LEU:HD11	1:A:757:TRP:HB2	5	0.21	0.05	0.21
(2,1341)	1:A:753:LEU:HD11	1:A:757:TRP:HB3	5	0.21	0.05	0.21
(2,1341)	1:A:753:LEU:HD12	1:A:757:TRP:HB2	5	0.21	0.05	0.21
(2,1341)	1:A:753:LEU:HD12	1:A:757:TRP:HB3	5	0.21	0.05	0.21
(2,1341)	1:A:753:LEU:HD13	1:A:757:TRP:HB2	5	0.21	0.05	0.21
(2,1341)	1:A:753:LEU:HD13	1:A:757:TRP:HB3	5	0.21	0.05	0.21
(2,711)	1:A:678:TRP:HE1	1:A:682:ILE:H	5	0.2	0.09	0.19
(2,1136)	1:A:678:TRP:HE1	1:A:682:ILE:H	5	0.2	0.09	0.19
(2,989)	1:A:778:VAL:HG21	1:A:775:LEU:HA	5	0.2	0.04	0.2
(2,989)	1:A:778:VAL:HG22	1:A:775:LEU:HA	5	0.2	0.04	0.2
(2,989)	1:A:778:VAL:HG23	1:A:775:LEU:HA	5	0.2	0.04	0.2
(2,1414)	1:A:778:VAL:HG21	1:A:775:LEU:HA	5	0.2	0.04	0.2
(2,1414)	1:A:778:VAL:HG22	1:A:775:LEU:HA	5	0.2	0.04	0.2
(2,1414)	1:A:778:VAL:HG23	1:A:775:LEU:HA	5	0.2	0.04	0.2
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD11	5	0.19	0.08	0.17
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD12	5	0.19	0.08	0.17
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD13	5	0.19	0.08	0.17
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG11	5	0.19	0.08	0.17

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG12	5	0.19	0.08	0.17
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG13	5	0.19	0.08	0.17
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG21	5	0.19	0.08	0.17
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG22	5	0.19	0.08	0.17
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG23	5	0.19	0.08	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG11	5	0.19	0.08	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG12	5	0.19	0.08	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG13	5	0.19	0.08	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG21	5	0.19	0.08	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG22	5	0.19	0.08	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG23	5	0.19	0.08	0.17
(2,718)	1:A:682:ILE:HG21	1:A:679:LEU:H	5	0.19	0.07	0.16
(2,718)	1:A:682:ILE:HG22	1:A:679:LEU:H	5	0.19	0.07	0.16
(2,718)	1:A:682:ILE:HG23	1:A:679:LEU:H	5	0.19	0.07	0.16
(2,1143)	1:A:682:ILE:HG21	1:A:679:LEU:H	5	0.19	0.07	0.16
(2,1143)	1:A:682:ILE:HG22	1:A:679:LEU:H	5	0.19	0.07	0.16
(2,1143)	1:A:682:ILE:HG23	1:A:679:LEU:H	5	0.19	0.07	0.16
(2,126)	1:A:785:LEU:HD21	1:B:749:VAL:HB	5	0.18	0.05	0.2
(2,126)	1:A:785:LEU:HD22	1:B:749:VAL:HB	5	0.18	0.05	0.2
(2,126)	1:A:785:LEU:HD23	1:B:749:VAL:HB	5	0.18	0.05	0.2
(2,780)	1:A:698:VAL:HG11	1:A:695:LEU:HA	5	0.18	0.08	0.13
(2,780)	1:A:698:VAL:HG12	1:A:695:LEU:HA	5	0.18	0.08	0.13
(2,780)	1:A:698:VAL:HG13	1:A:695:LEU:HA	5	0.18	0.08	0.13
(2,1205)	1:A:698:VAL:HG11	1:A:695:LEU:HA	5	0.18	0.08	0.13
(2,1205)	1:A:698:VAL:HG12	1:A:695:LEU:HA	5	0.18	0.08	0.13
(2,1205)	1:A:698:VAL:HG13	1:A:695:LEU:HA	5	0.18	0.08	0.13
(2,479)	1:B:748:LEU:H	1:B:745:SER:HA	5	0.18	0.06	0.16
(2,272)	1:B:674:ASP:H	1:B:677:ASN:H	5	0.18	0.04	0.18
(2,502)	1:B:755:LEU:H	1:B:752:SER:HA	5	0.18	0.02	0.19
(2,639)	1:A:661:LEU:HD11	1:A:662:GLU:HG2	5	0.17	0.03	0.18
(2,639)	1:A:661:LEU:HD11	1:A:662:GLU:HG3	5	0.17	0.03	0.18
(2,639)	1:A:661:LEU:HD12	1:A:662:GLU:HG2	5	0.17	0.03	0.18
(2,639)	1:A:661:LEU:HD12	1:A:662:GLU:HG3	5	0.17	0.03	0.18
(2,639)	1:A:661:LEU:HD13	1:A:662:GLU:HG2	5	0.17	0.03	0.18
(2,639)	1:A:661:LEU:HD13	1:A:662:GLU:HG3	5	0.17	0.03	0.18
(2,639)	1:A:661:LEU:HD21	1:A:662:GLU:HG2	5	0.17	0.03	0.18
(2,639)	1:A:661:LEU:HD21	1:A:662:GLU:HG3	5	0.17	0.03	0.18
(2,639)	1:A:661:LEU:HD22	1:A:662:GLU:HG2	5	0.17	0.03	0.18
(2,639)	1:A:661:LEU:HD22	1:A:662:GLU:HG3	5	0.17	0.03	0.18
(2,639)	1:A:661:LEU:HD23	1:A:662:GLU:HG2	5	0.17	0.03	0.18
(2,639)	1:A:661:LEU:HD23	1:A:662:GLU:HG3	5	0.17	0.03	0.18
(2,1064)	1:A:661:LEU:HD11	1:A:662:GLU:HG2	5	0.17	0.03	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1064)	1:A:661:LEU:HD11	1:A:662:GLU:HG3	5	0.17	0.03	0.18
(2,1064)	1:A:661:LEU:HD12	1:A:662:GLU:HG2	5	0.17	0.03	0.18
(2,1064)	1:A:661:LEU:HD12	1:A:662:GLU:HG3	5	0.17	0.03	0.18
(2,1064)	1:A:661:LEU:HD13	1:A:662:GLU:HG2	5	0.17	0.03	0.18
(2,1064)	1:A:661:LEU:HD13	1:A:662:GLU:HG3	5	0.17	0.03	0.18
(2,1064)	1:A:661:LEU:HD21	1:A:662:GLU:HG2	5	0.17	0.03	0.18
(2,1064)	1:A:661:LEU:HD21	1:A:662:GLU:HG3	5	0.17	0.03	0.18
(2,1064)	1:A:661:LEU:HD22	1:A:662:GLU:HG2	5	0.17	0.03	0.18
(2,1064)	1:A:661:LEU:HD22	1:A:662:GLU:HG3	5	0.17	0.03	0.18
(2,1064)	1:A:661:LEU:HD23	1:A:662:GLU:HG2	5	0.17	0.03	0.18
(2,1064)	1:A:661:LEU:HD23	1:A:662:GLU:HG3	5	0.17	0.03	0.18
(2,515)	1:B:760:LEU:HD11	1:B:757:TRP:HA	5	0.17	0.03	0.16
(2,515)	1:B:760:LEU:HD12	1:B:757:TRP:HA	5	0.17	0.03	0.16
(2,515)	1:B:760:LEU:HD13	1:B:757:TRP:HA	5	0.17	0.03	0.16
(2,519)	1:B:763:LEU:HD11	1:B:764:SER:HG	5	0.16	0.04	0.14
(2,519)	1:B:763:LEU:HD12	1:B:764:SER:HG	5	0.16	0.04	0.14
(2,519)	1:B:763:LEU:HD13	1:B:764:SER:HG	5	0.16	0.04	0.14
(2,722)	1:A:682:ILE:HD11	1:A:685:PHE:HB2	5	0.16	0.06	0.16
(2,722)	1:A:682:ILE:HD11	1:A:685:PHE:HB3	5	0.16	0.06	0.16
(2,722)	1:A:682:ILE:HD12	1:A:685:PHE:HB2	5	0.16	0.06	0.16
(2,722)	1:A:682:ILE:HD12	1:A:685:PHE:HB3	5	0.16	0.06	0.16
(2,722)	1:A:682:ILE:HD13	1:A:685:PHE:HB2	5	0.16	0.06	0.16
(2,722)	1:A:682:ILE:HD13	1:A:685:PHE:HB3	5	0.16	0.06	0.16
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB1	5	0.16	0.03	0.15
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB2	5	0.16	0.03	0.15
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB3	5	0.16	0.03	0.15
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB1	5	0.16	0.03	0.15
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB2	5	0.16	0.03	0.15
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB3	5	0.16	0.03	0.15
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB1	5	0.16	0.03	0.15
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB2	5	0.16	0.03	0.15
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB3	5	0.16	0.03	0.15
(2,1147)	1:A:682:ILE:HD11	1:A:685:PHE:HB2	5	0.16	0.06	0.16
(2,1147)	1:A:682:ILE:HD11	1:A:685:PHE:HB3	5	0.16	0.06	0.16
(2,1147)	1:A:682:ILE:HD12	1:A:685:PHE:HB2	5	0.16	0.06	0.16
(2,1147)	1:A:682:ILE:HD12	1:A:685:PHE:HB3	5	0.16	0.06	0.16
(2,1147)	1:A:682:ILE:HD13	1:A:685:PHE:HB2	5	0.16	0.06	0.16
(2,1147)	1:A:682:ILE:HD13	1:A:685:PHE:HB3	5	0.16	0.06	0.16
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB1	5	0.16	0.03	0.15
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB2	5	0.16	0.03	0.15
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB3	5	0.16	0.03	0.15
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB1	5	0.16	0.03	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB2	5	0.16	0.03	0.15
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB3	5	0.16	0.03	0.15
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB1	5	0.16	0.03	0.15
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB2	5	0.16	0.03	0.15
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB3	5	0.16	0.03	0.15
(2,253)	1:B:669:LEU:H	1:B:666:TRP:HA	5	0.16	0.02	0.16
(2,305)	1:B:684:ILE:HG21	1:B:685:PHE:HD1	5	0.15	0.04	0.13
(2,305)	1:B:684:ILE:HG21	1:B:685:PHE:HD2	5	0.15	0.04	0.13
(2,305)	1:B:684:ILE:HG22	1:B:685:PHE:HD1	5	0.15	0.04	0.13
(2,305)	1:B:684:ILE:HG22	1:B:685:PHE:HD2	5	0.15	0.04	0.13
(2,305)	1:B:684:ILE:HG23	1:B:685:PHE:HD1	5	0.15	0.04	0.13
(2,305)	1:B:684:ILE:HG23	1:B:685:PHE:HD2	5	0.15	0.04	0.13
(1,3)	1:B:791:GLU:O	1:B:795:TYR:H	5	0.15	0.01	0.16
(1,89)	1:B:791:GLU:O	1:B:795:TYR:H	5	0.15	0.01	0.16
(1,175)	1:B:791:GLU:O	1:B:795:TYR:H	5	0.15	0.01	0.16
(2,615)	1:B:796:TRP:HE1	1:B:796:TRP:H	5	0.14	0.02	0.13
(2,925)	1:A:754:ALA:HB1	1:A:758:ASP:H	5	0.14	0.02	0.13
(2,925)	1:A:754:ALA:HB2	1:A:758:ASP:H	5	0.14	0.02	0.13
(2,925)	1:A:754:ALA:HB3	1:A:758:ASP:H	5	0.14	0.02	0.13
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB1	5	0.14	0.02	0.13
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB2	5	0.14	0.02	0.13
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB3	5	0.14	0.02	0.13
(2,1350)	1:A:754:ALA:HB1	1:A:758:ASP:H	5	0.14	0.02	0.13
(2,1350)	1:A:754:ALA:HB2	1:A:758:ASP:H	5	0.14	0.02	0.13
(2,1350)	1:A:754:ALA:HB3	1:A:758:ASP:H	5	0.14	0.02	0.13
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB1	5	0.14	0.02	0.13
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB2	5	0.14	0.02	0.13
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB3	5	0.14	0.02	0.13
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG21	5	0.13	0.01	0.13
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG22	5	0.13	0.01	0.13
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG23	5	0.13	0.01	0.13
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG21	5	0.13	0.01	0.13
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG22	5	0.13	0.01	0.13
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG23	5	0.13	0.01	0.13
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG21	5	0.13	0.01	0.13
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG22	5	0.13	0.01	0.13
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG23	5	0.13	0.01	0.13
(2,956)	1:A:773:ASP:H	1:A:770:ARG:HD2	4	0.46	0.31	0.35
(2,956)	1:A:773:ASP:H	1:A:770:ARG:HD3	4	0.46	0.31	0.35
(2,1381)	1:A:773:ASP:H	1:A:770:ARG:HD2	4	0.46	0.31	0.35
(2,1381)	1:A:773:ASP:H	1:A:770:ARG:HD3	4	0.46	0.31	0.35
(2,99)	1:A:758:ASP:H	1:B:715:LEU:HD21	4	0.41	0.21	0.44

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,99)	1:A:758:ASP:H	1:B:715:LEU:HD22	4	0.41	0.21	0.44
(2,99)	1:A:758:ASP:H	1:B:715:LEU:HD23	4	0.41	0.21	0.44
(2,492)	1:B:753:LEU:HD21	1:B:750:ASN:HB2	4	0.4	0.15	0.42
(2,492)	1:B:753:LEU:HD21	1:B:750:ASN:HB3	4	0.4	0.15	0.42
(2,492)	1:B:753:LEU:HD22	1:B:750:ASN:HB2	4	0.4	0.15	0.42
(2,492)	1:B:753:LEU:HD22	1:B:750:ASN:HB3	4	0.4	0.15	0.42
(2,492)	1:B:753:LEU:HD23	1:B:750:ASN:HB2	4	0.4	0.15	0.42
(2,492)	1:B:753:LEU:HD23	1:B:750:ASN:HB3	4	0.4	0.15	0.42
(2,169)	1:B:797:TRP:HE1	1:B:848:ARG:HB2	4	0.4	0.18	0.42
(2,169)	1:B:797:TRP:HE1	1:B:848:ARG:HB3	4	0.4	0.18	0.42
(2,114)	1:A:781:ILE:HD11	1:B:743:ASP:HA	4	0.37	0.18	0.38
(2,114)	1:A:781:ILE:HD12	1:B:743:ASP:HA	4	0.37	0.18	0.38
(2,114)	1:A:781:ILE:HD13	1:B:743:ASP:HA	4	0.37	0.18	0.38
(2,1052)	1:A:819:ALA:H	1:A:820:ILE:HD11	4	0.36	0.16	0.33
(2,1052)	1:A:819:ALA:H	1:A:820:ILE:HD12	4	0.36	0.16	0.33
(2,1052)	1:A:819:ALA:H	1:A:820:ILE:HD13	4	0.36	0.16	0.33
(2,1477)	1:A:819:ALA:H	1:A:820:ILE:HD11	4	0.36	0.16	0.33
(2,1477)	1:A:819:ALA:H	1:A:820:ILE:HD12	4	0.36	0.16	0.33
(2,1477)	1:A:819:ALA:H	1:A:820:ILE:HD13	4	0.36	0.16	0.33
(2,765)	1:A:693:ILE:HG21	1:A:696:ARG:HG2	4	0.34	0.13	0.34
(2,765)	1:A:693:ILE:HG21	1:A:696:ARG:HG3	4	0.34	0.13	0.34
(2,765)	1:A:693:ILE:HG22	1:A:696:ARG:HG2	4	0.34	0.13	0.34
(2,765)	1:A:693:ILE:HG22	1:A:696:ARG:HG3	4	0.34	0.13	0.34
(2,765)	1:A:693:ILE:HG23	1:A:696:ARG:HG2	4	0.34	0.13	0.34
(2,765)	1:A:693:ILE:HG23	1:A:696:ARG:HG3	4	0.34	0.13	0.34
(2,1190)	1:A:693:ILE:HG21	1:A:696:ARG:HG2	4	0.34	0.13	0.34
(2,1190)	1:A:693:ILE:HG21	1:A:696:ARG:HG3	4	0.34	0.13	0.34
(2,1190)	1:A:693:ILE:HG22	1:A:696:ARG:HG2	4	0.34	0.13	0.34
(2,1190)	1:A:693:ILE:HG22	1:A:696:ARG:HG3	4	0.34	0.13	0.34
(2,1190)	1:A:693:ILE:HG23	1:A:696:ARG:HG2	4	0.34	0.13	0.34
(2,1190)	1:A:693:ILE:HG23	1:A:696:ARG:HG3	4	0.34	0.13	0.34
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD11	4	0.31	0.11	0.33
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD12	4	0.31	0.11	0.33
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD13	4	0.31	0.11	0.33
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD21	4	0.31	0.11	0.33
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD22	4	0.31	0.11	0.33
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD23	4	0.31	0.11	0.33
(2,241)	1:B:666:TRP:HE1	1:B:662:GLU:H	4	0.27	0.05	0.26
(2,896)	1:A:746:ILE:HD11	1:A:743:ASP:HB2	4	0.25	0.1	0.26
(2,896)	1:A:746:ILE:HD11	1:A:743:ASP:HB3	4	0.25	0.1	0.26
(2,896)	1:A:746:ILE:HD12	1:A:743:ASP:HB2	4	0.25	0.1	0.26
(2,896)	1:A:746:ILE:HD12	1:A:743:ASP:HB3	4	0.25	0.1	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,896)	1:A:746:ILE:HD13	1:A:743:ASP:HB2	4	0.25	0.1	0.26
(2,896)	1:A:746:ILE:HD13	1:A:743:ASP:HB3	4	0.25	0.1	0.26
(2,952)	1:A:771:LEU:HD21	1:A:772:ARG:HH21	4	0.25	0.06	0.26
(2,952)	1:A:771:LEU:HD21	1:A:772:ARG:HH22	4	0.25	0.06	0.26
(2,952)	1:A:771:LEU:HD22	1:A:772:ARG:HH21	4	0.25	0.06	0.26
(2,952)	1:A:771:LEU:HD22	1:A:772:ARG:HH22	4	0.25	0.06	0.26
(2,952)	1:A:771:LEU:HD23	1:A:772:ARG:HH21	4	0.25	0.06	0.26
(2,952)	1:A:771:LEU:HD23	1:A:772:ARG:HH22	4	0.25	0.06	0.26
(2,1321)	1:A:746:ILE:HD11	1:A:743:ASP:HB2	4	0.25	0.1	0.26
(2,1321)	1:A:746:ILE:HD11	1:A:743:ASP:HB3	4	0.25	0.1	0.26
(2,1321)	1:A:746:ILE:HD12	1:A:743:ASP:HB2	4	0.25	0.1	0.26
(2,1321)	1:A:746:ILE:HD12	1:A:743:ASP:HB3	4	0.25	0.1	0.26
(2,1321)	1:A:746:ILE:HD13	1:A:743:ASP:HB2	4	0.25	0.1	0.26
(2,1321)	1:A:746:ILE:HD13	1:A:743:ASP:HB3	4	0.25	0.1	0.26
(2,1377)	1:A:771:LEU:HD21	1:A:772:ARG:HH21	4	0.25	0.06	0.26
(2,1377)	1:A:771:LEU:HD21	1:A:772:ARG:HH22	4	0.25	0.06	0.26
(2,1377)	1:A:771:LEU:HD22	1:A:772:ARG:HH21	4	0.25	0.06	0.26
(2,1377)	1:A:771:LEU:HD22	1:A:772:ARG:HH22	4	0.25	0.06	0.26
(2,1377)	1:A:771:LEU:HD23	1:A:772:ARG:HH21	4	0.25	0.06	0.26
(2,1377)	1:A:771:LEU:HD23	1:A:772:ARG:HH22	4	0.25	0.06	0.26
(2,798)	1:A:701:VAL:HG21	1:A:698:VAL:HA	4	0.24	0.1	0.23
(2,798)	1:A:701:VAL:HG22	1:A:698:VAL:HA	4	0.24	0.1	0.23
(2,798)	1:A:701:VAL:HG23	1:A:698:VAL:HA	4	0.24	0.1	0.23
(2,1223)	1:A:701:VAL:HG21	1:A:698:VAL:HA	4	0.24	0.1	0.23
(2,1223)	1:A:701:VAL:HG22	1:A:698:VAL:HA	4	0.24	0.1	0.23
(2,1223)	1:A:701:VAL:HG23	1:A:698:VAL:HA	4	0.24	0.1	0.23
(2,518)	1:B:763:LEU:HD11	1:B:759:ASP:HA	4	0.23	0.09	0.23
(2,518)	1:B:763:LEU:HD12	1:B:759:ASP:HA	4	0.23	0.09	0.23
(2,518)	1:B:763:LEU:HD13	1:B:759:ASP:HA	4	0.23	0.09	0.23
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD11	4	0.23	0.08	0.2
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD12	4	0.23	0.08	0.2
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD13	4	0.23	0.08	0.2
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD21	4	0.23	0.08	0.2
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD22	4	0.23	0.08	0.2
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD23	4	0.23	0.08	0.2
(2,414)	1:B:707:ARG:H	1:B:704:LEU:HA	4	0.22	0.05	0.22
(2,697)	1:A:674:ASP:H	1:A:677:ASN:H	4	0.21	0.05	0.2
(2,1122)	1:A:674:ASP:H	1:A:677:ASN:H	4	0.21	0.05	0.2
(2,586)	1:B:782:VAL:HG21	1:B:779:THR:HA	4	0.2	0.09	0.2
(2,586)	1:B:782:VAL:HG22	1:B:779:THR:HA	4	0.2	0.09	0.2
(2,586)	1:B:782:VAL:HG23	1:B:779:THR:HA	4	0.2	0.09	0.2
(2,804)	1:A:702:LEU:HD21	1:A:706:ASN:HB2	4	0.2	0.08	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,804)	1:A:702:LEU:HD21	1:A:706:ASN:HB3	4	0.2	0.08	0.16
(2,804)	1:A:702:LEU:HD22	1:A:706:ASN:HB2	4	0.2	0.08	0.16
(2,804)	1:A:702:LEU:HD22	1:A:706:ASN:HB3	4	0.2	0.08	0.16
(2,804)	1:A:702:LEU:HD23	1:A:706:ASN:HB2	4	0.2	0.08	0.16
(2,804)	1:A:702:LEU:HD23	1:A:706:ASN:HB3	4	0.2	0.08	0.16
(2,1229)	1:A:702:LEU:HD21	1:A:706:ASN:HB2	4	0.2	0.08	0.16
(2,1229)	1:A:702:LEU:HD21	1:A:706:ASN:HB3	4	0.2	0.08	0.16
(2,1229)	1:A:702:LEU:HD22	1:A:706:ASN:HB2	4	0.2	0.08	0.16
(2,1229)	1:A:702:LEU:HD22	1:A:706:ASN:HB3	4	0.2	0.08	0.16
(2,1229)	1:A:702:LEU:HD23	1:A:706:ASN:HB2	4	0.2	0.08	0.16
(2,1229)	1:A:702:LEU:HD23	1:A:706:ASN:HB3	4	0.2	0.08	0.16
(2,898)	1:A:746:ILE:HG21	1:A:750:ASN:HD22	4	0.19	0.04	0.18
(2,898)	1:A:746:ILE:HG22	1:A:750:ASN:HD22	4	0.19	0.04	0.18
(2,898)	1:A:746:ILE:HG23	1:A:750:ASN:HD22	4	0.19	0.04	0.18
(2,1323)	1:A:746:ILE:HG21	1:A:750:ASN:HD22	4	0.19	0.04	0.18
(2,1323)	1:A:746:ILE:HG22	1:A:750:ASN:HD22	4	0.19	0.04	0.18
(2,1323)	1:A:746:ILE:HG23	1:A:750:ASN:HD22	4	0.19	0.04	0.18
(2,352)	1:B:697:ILE:HG21	1:B:694:GLY:HA2	4	0.18	0.08	0.16
(2,352)	1:B:697:ILE:HG21	1:B:694:GLY:HA3	4	0.18	0.08	0.16
(2,352)	1:B:697:ILE:HG22	1:B:694:GLY:HA2	4	0.18	0.08	0.16
(2,352)	1:B:697:ILE:HG22	1:B:694:GLY:HA3	4	0.18	0.08	0.16
(2,352)	1:B:697:ILE:HG23	1:B:694:GLY:HA2	4	0.18	0.08	0.16
(2,352)	1:B:697:ILE:HG23	1:B:694:GLY:HA3	4	0.18	0.08	0.16
(2,845)	1:A:707:ARG:H	1:A:707:ARG:HG2	4	0.18	0.07	0.15
(2,845)	1:A:707:ARG:H	1:A:707:ARG:HG3	4	0.18	0.07	0.15
(2,1270)	1:A:707:ARG:H	1:A:707:ARG:HG2	4	0.18	0.07	0.15
(2,1270)	1:A:707:ARG:H	1:A:707:ARG:HG3	4	0.18	0.07	0.15
(2,546)	1:B:776:LEU:H	1:B:773:ASP:HA	4	0.18	0.03	0.16
(2,268)	1:B:672:TRP:H	1:B:673:PHE:H	4	0.18	0.11	0.12
(2,357)	1:B:698:VAL:HG11	1:B:699:PHE:HD1	4	0.17	0.04	0.16
(2,357)	1:B:698:VAL:HG11	1:B:699:PHE:HD2	4	0.17	0.04	0.16
(2,357)	1:B:698:VAL:HG12	1:B:699:PHE:HD1	4	0.17	0.04	0.16
(2,357)	1:B:698:VAL:HG12	1:B:699:PHE:HD2	4	0.17	0.04	0.16
(2,357)	1:B:698:VAL:HG13	1:B:699:PHE:HD1	4	0.17	0.04	0.16
(2,357)	1:B:698:VAL:HG13	1:B:699:PHE:HD2	4	0.17	0.04	0.16
(2,608)	1:B:786:GLY:H	1:B:782:VAL:HA	4	0.17	0.06	0.15
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD11	4	0.17	0.04	0.16
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD12	4	0.17	0.04	0.16
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD13	4	0.17	0.04	0.16
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD21	4	0.17	0.04	0.16
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD22	4	0.17	0.04	0.16
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD23	4	0.17	0.04	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD11	4	0.17	0.04	0.16
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD12	4	0.17	0.04	0.16
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD13	4	0.17	0.04	0.16
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD21	4	0.17	0.04	0.16
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD22	4	0.17	0.04	0.16
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD23	4	0.17	0.04	0.16
(2,693)	1:A:672:TRP:H	1:A:673:PHE:H	4	0.16	0.03	0.17
(2,951)	1:A:771:LEU:HD11	1:A:768:TYR:HE1	4	0.16	0.05	0.14
(2,951)	1:A:771:LEU:HD11	1:A:768:TYR:HE2	4	0.16	0.05	0.14
(2,951)	1:A:771:LEU:HD12	1:A:768:TYR:HE1	4	0.16	0.05	0.14
(2,951)	1:A:771:LEU:HD12	1:A:768:TYR:HE2	4	0.16	0.05	0.14
(2,951)	1:A:771:LEU:HD13	1:A:768:TYR:HE1	4	0.16	0.05	0.14
(2,951)	1:A:771:LEU:HD13	1:A:768:TYR:HE2	4	0.16	0.05	0.14
(2,1118)	1:A:672:TRP:H	1:A:673:PHE:H	4	0.16	0.03	0.17
(2,1376)	1:A:771:LEU:HD11	1:A:768:TYR:HE1	4	0.16	0.05	0.14
(2,1376)	1:A:771:LEU:HD11	1:A:768:TYR:HE2	4	0.16	0.05	0.14
(2,1376)	1:A:771:LEU:HD12	1:A:768:TYR:HE1	4	0.16	0.05	0.14
(2,1376)	1:A:771:LEU:HD12	1:A:768:TYR:HE2	4	0.16	0.05	0.14
(2,1376)	1:A:771:LEU:HD13	1:A:768:TYR:HE1	4	0.16	0.05	0.14
(2,1376)	1:A:771:LEU:HD13	1:A:768:TYR:HE2	4	0.16	0.05	0.14
(2,395)	1:B:704:LEU:HD11	1:B:708:VAL:HG21	4	0.16	0.01	0.16
(2,395)	1:B:704:LEU:HD11	1:B:708:VAL:HG22	4	0.16	0.01	0.16
(2,395)	1:B:704:LEU:HD11	1:B:708:VAL:HG23	4	0.16	0.01	0.16
(2,395)	1:B:704:LEU:HD12	1:B:708:VAL:HG21	4	0.16	0.01	0.16
(2,395)	1:B:704:LEU:HD12	1:B:708:VAL:HG22	4	0.16	0.01	0.16
(2,395)	1:B:704:LEU:HD12	1:B:708:VAL:HG23	4	0.16	0.01	0.16
(2,395)	1:B:704:LEU:HD13	1:B:708:VAL:HG21	4	0.16	0.01	0.16
(2,395)	1:B:704:LEU:HD13	1:B:708:VAL:HG22	4	0.16	0.01	0.16
(2,395)	1:B:704:LEU:HD13	1:B:708:VAL:HG23	4	0.16	0.01	0.16
(2,367)	1:B:700:ALA:HB1	1:B:697:ILE:HA	4	0.16	0.04	0.15
(2,367)	1:B:700:ALA:HB2	1:B:697:ILE:HA	4	0.16	0.04	0.15
(2,367)	1:B:700:ALA:HB3	1:B:697:ILE:HA	4	0.16	0.04	0.15
(2,280)	1:B:676:THR:HG21	1:B:681:TYR:HH	4	0.15	0.03	0.15
(2,280)	1:B:676:THR:HG22	1:B:681:TYR:HH	4	0.15	0.03	0.15
(2,280)	1:B:676:THR:HG23	1:B:681:TYR:HH	4	0.15	0.03	0.15
(2,340)	1:B:693:ILE:HG21	1:B:696:ARG:HG2	4	0.15	0.03	0.16
(2,340)	1:B:693:ILE:HG21	1:B:696:ARG:HG3	4	0.15	0.03	0.16
(2,340)	1:B:693:ILE:HG22	1:B:696:ARG:HG2	4	0.15	0.03	0.16
(2,340)	1:B:693:ILE:HG22	1:B:696:ARG:HG3	4	0.15	0.03	0.16
(2,340)	1:B:693:ILE:HG23	1:B:696:ARG:HG2	4	0.15	0.03	0.16
(2,340)	1:B:693:ILE:HG23	1:B:696:ARG:HG3	4	0.15	0.03	0.16
(2,593)	1:B:784:LEU:H	1:B:781:ILE:HA	4	0.14	0.03	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,770)	1:A:695:LEU:HD21	1:A:698:VAL:HB	4	0.14	0.03	0.14
(2,770)	1:A:695:LEU:HD22	1:A:698:VAL:HB	4	0.14	0.03	0.14
(2,770)	1:A:695:LEU:HD23	1:A:698:VAL:HB	4	0.14	0.03	0.14
(2,803)	1:A:702:LEU:HD11	1:A:699:PHE:HE1	4	0.14	0.01	0.14
(2,803)	1:A:702:LEU:HD11	1:A:699:PHE:HE2	4	0.14	0.01	0.14
(2,803)	1:A:702:LEU:HD12	1:A:699:PHE:HE1	4	0.14	0.01	0.14
(2,803)	1:A:702:LEU:HD12	1:A:699:PHE:HE2	4	0.14	0.01	0.14
(2,803)	1:A:702:LEU:HD13	1:A:699:PHE:HE1	4	0.14	0.01	0.14
(2,803)	1:A:702:LEU:HD13	1:A:699:PHE:HE2	4	0.14	0.01	0.14
(2,1011)	1:A:782:VAL:HG21	1:A:779:THR:HA	4	0.14	0.02	0.15
(2,1011)	1:A:782:VAL:HG22	1:A:779:THR:HA	4	0.14	0.02	0.15
(2,1011)	1:A:782:VAL:HG23	1:A:779:THR:HA	4	0.14	0.02	0.15
(2,1195)	1:A:695:LEU:HD21	1:A:698:VAL:HB	4	0.14	0.03	0.14
(2,1195)	1:A:695:LEU:HD22	1:A:698:VAL:HB	4	0.14	0.03	0.14
(2,1195)	1:A:695:LEU:HD23	1:A:698:VAL:HB	4	0.14	0.03	0.14
(2,1228)	1:A:702:LEU:HD11	1:A:699:PHE:HE1	4	0.14	0.01	0.14
(2,1228)	1:A:702:LEU:HD11	1:A:699:PHE:HE2	4	0.14	0.01	0.14
(2,1228)	1:A:702:LEU:HD12	1:A:699:PHE:HE1	4	0.14	0.01	0.14
(2,1228)	1:A:702:LEU:HD12	1:A:699:PHE:HE2	4	0.14	0.01	0.14
(2,1228)	1:A:702:LEU:HD13	1:A:699:PHE:HE1	4	0.14	0.01	0.14
(2,1228)	1:A:702:LEU:HD13	1:A:699:PHE:HE2	4	0.14	0.01	0.14
(2,1436)	1:A:782:VAL:HG21	1:A:779:THR:HA	4	0.14	0.02	0.15
(2,1436)	1:A:782:VAL:HG22	1:A:779:THR:HA	4	0.14	0.02	0.15
(2,1436)	1:A:782:VAL:HG23	1:A:779:THR:HA	4	0.14	0.02	0.15
(2,286)	1:B:678:TRP:HE1	1:B:682:ILE:H	4	0.14	0.03	0.12
(1,73)	1:B:836:ALA:O	1:B:840:ILE:H	4	0.14	0.02	0.14
(1,159)	1:B:836:ALA:O	1:B:840:ILE:H	4	0.14	0.02	0.14
(1,245)	1:B:836:ALA:O	1:B:840:ILE:H	4	0.14	0.02	0.14
(2,465)	1:B:746:ILE:H	1:B:743:ASP:HB2	4	0.13	0.02	0.12
(2,465)	1:B:746:ILE:H	1:B:743:ASP:HB3	4	0.13	0.02	0.12
(2,60)	1:A:700:ALA:HB1	1:B:699:PHE:HD1	4	0.13	0.01	0.12
(2,60)	1:A:700:ALA:HB1	1:B:699:PHE:HD2	4	0.13	0.01	0.12
(2,60)	1:A:700:ALA:HB2	1:B:699:PHE:HD1	4	0.13	0.01	0.12
(2,60)	1:A:700:ALA:HB2	1:B:699:PHE:HD2	4	0.13	0.01	0.12
(2,60)	1:A:700:ALA:HB3	1:B:699:PHE:HD1	4	0.13	0.01	0.12
(2,60)	1:A:700:ALA:HB3	1:B:699:PHE:HD2	4	0.13	0.01	0.12
(2,666)	1:A:666:TRP:HE1	1:A:662:GLU:H	4	0.13	0.01	0.14
(2,1091)	1:A:666:TRP:HE1	1:A:662:GLU:H	4	0.13	0.01	0.14
(1,85)	1:B:850:GLY:O	1:B:854:ILE:H	4	0.13	0.01	0.12
(1,171)	1:B:850:GLY:O	1:B:854:ILE:H	4	0.13	0.01	0.12
(1,257)	1:B:850:GLY:O	1:B:854:ILE:H	4	0.13	0.01	0.12
(2,96)	1:A:755:LEU:HD11	1:B:710:GLN:HE21	4	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,96)	1:A:755:LEU:HD11	1:B:710:GLN:HE22	4	0.13	0.02	0.12
(2,96)	1:A:755:LEU:HD12	1:B:710:GLN:HE21	4	0.13	0.02	0.12
(2,96)	1:A:755:LEU:HD12	1:B:710:GLN:HE22	4	0.13	0.02	0.12
(2,96)	1:A:755:LEU:HD13	1:B:710:GLN:HE21	4	0.13	0.02	0.12
(2,96)	1:A:755:LEU:HD13	1:B:710:GLN:HE22	4	0.13	0.02	0.12
(2,276)	1:B:676:THR:HG21	1:B:666:TRP:HZ3	4	0.12	0.01	0.12
(2,276)	1:B:676:THR:HG22	1:B:666:TRP:HZ3	4	0.12	0.01	0.12
(2,276)	1:B:676:THR:HG23	1:B:666:TRP:HZ3	4	0.12	0.01	0.12
(2,672)	1:A:667:ALA:HB1	1:A:664:ASP:HA	4	0.12	0.0	0.12
(2,672)	1:A:667:ALA:HB2	1:A:664:ASP:HA	4	0.12	0.0	0.12
(2,672)	1:A:667:ALA:HB3	1:A:664:ASP:HA	4	0.12	0.0	0.12
(2,1097)	1:A:667:ALA:HB1	1:A:664:ASP:HA	4	0.12	0.0	0.12
(2,1097)	1:A:667:ALA:HB2	1:A:664:ASP:HA	4	0.12	0.0	0.12
(2,1097)	1:A:667:ALA:HB3	1:A:664:ASP:HA	4	0.12	0.0	0.12
(2,41)	1:A:693:ILE:H	1:A:693:ILE:HG12	3	1.04	0.17	1.03
(2,41)	1:A:693:ILE:H	1:A:693:ILE:HG13	3	1.04	0.17	1.03
(2,783)	1:A:698:VAL:HG11	1:A:702:LEU:HB2	3	0.65	0.07	0.66
(2,783)	1:A:698:VAL:HG11	1:A:702:LEU:HB3	3	0.65	0.07	0.66
(2,783)	1:A:698:VAL:HG12	1:A:702:LEU:HB2	3	0.65	0.07	0.66
(2,783)	1:A:698:VAL:HG12	1:A:702:LEU:HB3	3	0.65	0.07	0.66
(2,783)	1:A:698:VAL:HG13	1:A:702:LEU:HB2	3	0.65	0.07	0.66
(2,783)	1:A:698:VAL:HG13	1:A:702:LEU:HB3	3	0.65	0.07	0.66
(2,1208)	1:A:698:VAL:HG11	1:A:702:LEU:HB2	3	0.65	0.07	0.66
(2,1208)	1:A:698:VAL:HG11	1:A:702:LEU:HB3	3	0.65	0.07	0.66
(2,1208)	1:A:698:VAL:HG12	1:A:702:LEU:HB2	3	0.65	0.07	0.66
(2,1208)	1:A:698:VAL:HG12	1:A:702:LEU:HB3	3	0.65	0.07	0.66
(2,1208)	1:A:698:VAL:HG13	1:A:702:LEU:HB2	3	0.65	0.07	0.66
(2,1208)	1:A:698:VAL:HG13	1:A:702:LEU:HB3	3	0.65	0.07	0.66
(2,165)	1:A:796:TRP:HE1	1:B:755:LEU:HD21	3	0.4	0.04	0.42
(2,165)	1:A:796:TRP:HE1	1:B:755:LEU:HD22	3	0.4	0.04	0.42
(2,165)	1:A:796:TRP:HE1	1:B:755:LEU:HD23	3	0.4	0.04	0.42
(2,12)	1:A:666:TRP:HE1	1:B:666:TRP:HZ2	3	0.35	0.14	0.37
(2,470)	1:B:746:ILE:HD11	1:B:743:ASP:HA	3	0.32	0.17	0.25
(2,470)	1:B:746:ILE:HD12	1:B:743:ASP:HA	3	0.32	0.17	0.25
(2,470)	1:B:746:ILE:HD13	1:B:743:ASP:HA	3	0.32	0.17	0.25
(2,420)	1:B:707:ARG:H	1:B:707:ARG:HG2	3	0.31	0.09	0.35
(2,420)	1:B:707:ARG:H	1:B:707:ARG:HG3	3	0.31	0.09	0.35
(2,222)	1:B:663:LEU:HD21	1:B:667:ALA:HB1	3	0.3	0.08	0.32
(2,222)	1:B:663:LEU:HD21	1:B:667:ALA:HB2	3	0.3	0.08	0.32
(2,222)	1:B:663:LEU:HD21	1:B:667:ALA:HB3	3	0.3	0.08	0.32
(2,222)	1:B:663:LEU:HD22	1:B:667:ALA:HB1	3	0.3	0.08	0.32
(2,222)	1:B:663:LEU:HD22	1:B:667:ALA:HB2	3	0.3	0.08	0.32

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,222)	1:B:663:LEU:HD22	1:B:667:ALA:HB3	3	0.3	0.08	0.32
(2,222)	1:B:663:LEU:HD23	1:B:667:ALA:HB1	3	0.3	0.08	0.32
(2,222)	1:B:663:LEU:HD23	1:B:667:ALA:HB2	3	0.3	0.08	0.32
(2,222)	1:B:663:LEU:HD23	1:B:667:ALA:HB3	3	0.3	0.08	0.32
(2,863)	1:A:709:ARG:HE	1:A:709:ARG:H	3	0.3	0.16	0.23
(2,1288)	1:A:709:ARG:HE	1:A:709:ARG:H	3	0.3	0.16	0.23
(2,1057)	1:A:852:GLU:H	1:A:848:ARG:HG2	3	0.3	0.13	0.39
(2,1057)	1:A:852:GLU:H	1:A:848:ARG:HG3	3	0.3	0.13	0.39
(2,1482)	1:A:852:GLU:H	1:A:848:ARG:HG2	3	0.3	0.13	0.39
(2,1482)	1:A:852:GLU:H	1:A:848:ARG:HG3	3	0.3	0.13	0.39
(2,90)	1:B:713:SER:H	1:A:708:VAL:HG21	3	0.3	0.0	0.3
(2,90)	1:B:713:SER:H	1:A:708:VAL:HG22	3	0.3	0.0	0.3
(2,90)	1:B:713:SER:H	1:A:708:VAL:HG23	3	0.3	0.0	0.3
(2,403)	1:B:705:VAL:HG11	1:B:709:ARG:HD2	3	0.27	0.19	0.14
(2,403)	1:B:705:VAL:HG11	1:B:709:ARG:HD3	3	0.27	0.19	0.14
(2,403)	1:B:705:VAL:HG12	1:B:709:ARG:HD2	3	0.27	0.19	0.14
(2,403)	1:B:705:VAL:HG12	1:B:709:ARG:HD3	3	0.27	0.19	0.14
(2,403)	1:B:705:VAL:HG13	1:B:709:ARG:HD2	3	0.27	0.19	0.14
(2,403)	1:B:705:VAL:HG13	1:B:709:ARG:HD3	3	0.27	0.19	0.14
(2,976)	1:A:776:LEU:HD11	1:A:773:ASP:HB2	3	0.26	0.17	0.17
(2,976)	1:A:776:LEU:HD11	1:A:773:ASP:HB3	3	0.26	0.17	0.17
(2,976)	1:A:776:LEU:HD12	1:A:773:ASP:HB2	3	0.26	0.17	0.17
(2,976)	1:A:776:LEU:HD12	1:A:773:ASP:HB3	3	0.26	0.17	0.17
(2,976)	1:A:776:LEU:HD13	1:A:773:ASP:HB2	3	0.26	0.17	0.17
(2,976)	1:A:776:LEU:HD13	1:A:773:ASP:HB3	3	0.26	0.17	0.17
(2,1401)	1:A:776:LEU:HD11	1:A:773:ASP:HB2	3	0.26	0.17	0.17
(2,1401)	1:A:776:LEU:HD11	1:A:773:ASP:HB3	3	0.26	0.17	0.17
(2,1401)	1:A:776:LEU:HD12	1:A:773:ASP:HB2	3	0.26	0.17	0.17
(2,1401)	1:A:776:LEU:HD12	1:A:773:ASP:HB3	3	0.26	0.17	0.17
(2,1401)	1:A:776:LEU:HD13	1:A:773:ASP:HB2	3	0.26	0.17	0.17
(2,1401)	1:A:776:LEU:HD13	1:A:773:ASP:HB3	3	0.26	0.17	0.17
(2,758)	1:A:692:LEU:HD11	1:A:696:ARG:HH11	3	0.26	0.11	0.3
(2,758)	1:A:692:LEU:HD11	1:A:696:ARG:HH12	3	0.26	0.11	0.3
(2,758)	1:A:692:LEU:HD11	1:A:696:ARG:HH21	3	0.26	0.11	0.3
(2,758)	1:A:692:LEU:HD11	1:A:696:ARG:HH22	3	0.26	0.11	0.3
(2,758)	1:A:692:LEU:HD12	1:A:696:ARG:HH11	3	0.26	0.11	0.3
(2,758)	1:A:692:LEU:HD12	1:A:696:ARG:HH12	3	0.26	0.11	0.3
(2,758)	1:A:692:LEU:HD12	1:A:696:ARG:HH21	3	0.26	0.11	0.3
(2,758)	1:A:692:LEU:HD12	1:A:696:ARG:HH22	3	0.26	0.11	0.3
(2,758)	1:A:692:LEU:HD13	1:A:696:ARG:HH11	3	0.26	0.11	0.3
(2,758)	1:A:692:LEU:HD13	1:A:696:ARG:HH12	3	0.26	0.11	0.3
(2,758)	1:A:692:LEU:HD13	1:A:696:ARG:HH21	3	0.26	0.11	0.3

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,758)	1:A:692:LEU:HD13	1:A:696:ARG:HH22	3	0.26	0.11	0.3
(2,820)	1:A:704:LEU:HD11	1:A:708:VAL:HG21	3	0.26	0.14	0.18
(2,820)	1:A:704:LEU:HD11	1:A:708:VAL:HG22	3	0.26	0.14	0.18
(2,820)	1:A:704:LEU:HD11	1:A:708:VAL:HG23	3	0.26	0.14	0.18
(2,820)	1:A:704:LEU:HD12	1:A:708:VAL:HG21	3	0.26	0.14	0.18
(2,820)	1:A:704:LEU:HD12	1:A:708:VAL:HG22	3	0.26	0.14	0.18
(2,820)	1:A:704:LEU:HD12	1:A:708:VAL:HG23	3	0.26	0.14	0.18
(2,820)	1:A:704:LEU:HD13	1:A:708:VAL:HG21	3	0.26	0.14	0.18
(2,820)	1:A:704:LEU:HD13	1:A:708:VAL:HG22	3	0.26	0.14	0.18
(2,820)	1:A:704:LEU:HD13	1:A:708:VAL:HG23	3	0.26	0.14	0.18
(2,1183)	1:A:692:LEU:HD11	1:A:696:ARG:HH11	3	0.26	0.11	0.3
(2,1183)	1:A:692:LEU:HD11	1:A:696:ARG:HH12	3	0.26	0.11	0.3
(2,1183)	1:A:692:LEU:HD11	1:A:696:ARG:HH21	3	0.26	0.11	0.3
(2,1183)	1:A:692:LEU:HD11	1:A:696:ARG:HH22	3	0.26	0.11	0.3
(2,1183)	1:A:692:LEU:HD12	1:A:696:ARG:HH11	3	0.26	0.11	0.3
(2,1183)	1:A:692:LEU:HD12	1:A:696:ARG:HH12	3	0.26	0.11	0.3
(2,1183)	1:A:692:LEU:HD12	1:A:696:ARG:HH21	3	0.26	0.11	0.3
(2,1183)	1:A:692:LEU:HD12	1:A:696:ARG:HH22	3	0.26	0.11	0.3
(2,1183)	1:A:692:LEU:HD13	1:A:696:ARG:HH11	3	0.26	0.11	0.3
(2,1183)	1:A:692:LEU:HD13	1:A:696:ARG:HH12	3	0.26	0.11	0.3
(2,1183)	1:A:692:LEU:HD13	1:A:696:ARG:HH21	3	0.26	0.11	0.3
(2,1183)	1:A:692:LEU:HD13	1:A:696:ARG:HH22	3	0.26	0.11	0.3
(2,1245)	1:A:704:LEU:HD11	1:A:708:VAL:HG21	3	0.26	0.14	0.18
(2,1245)	1:A:704:LEU:HD11	1:A:708:VAL:HG22	3	0.26	0.14	0.18
(2,1245)	1:A:704:LEU:HD11	1:A:708:VAL:HG23	3	0.26	0.14	0.18
(2,1245)	1:A:704:LEU:HD12	1:A:708:VAL:HG21	3	0.26	0.14	0.18
(2,1245)	1:A:704:LEU:HD12	1:A:708:VAL:HG22	3	0.26	0.14	0.18
(2,1245)	1:A:704:LEU:HD12	1:A:708:VAL:HG23	3	0.26	0.14	0.18
(2,1245)	1:A:704:LEU:HD13	1:A:708:VAL:HG21	3	0.26	0.14	0.18
(2,1245)	1:A:704:LEU:HD13	1:A:708:VAL:HG22	3	0.26	0.14	0.18
(2,1245)	1:A:704:LEU:HD13	1:A:708:VAL:HG23	3	0.26	0.14	0.18
(2,719)	1:A:682:ILE:HG21	1:A:685:PHE:HB2	3	0.25	0.04	0.26
(2,719)	1:A:682:ILE:HG21	1:A:685:PHE:HB3	3	0.25	0.04	0.26
(2,719)	1:A:682:ILE:HG22	1:A:685:PHE:HB2	3	0.25	0.04	0.26
(2,719)	1:A:682:ILE:HG22	1:A:685:PHE:HB3	3	0.25	0.04	0.26
(2,719)	1:A:682:ILE:HG23	1:A:685:PHE:HB2	3	0.25	0.04	0.26
(2,719)	1:A:682:ILE:HG23	1:A:685:PHE:HB3	3	0.25	0.04	0.26
(2,757)	1:A:692:LEU:HD11	1:A:691:SER:HB2	3	0.25	0.1	0.3
(2,757)	1:A:692:LEU:HD11	1:A:691:SER:HB3	3	0.25	0.1	0.3
(2,757)	1:A:692:LEU:HD12	1:A:691:SER:HB2	3	0.25	0.1	0.3
(2,757)	1:A:692:LEU:HD12	1:A:691:SER:HB3	3	0.25	0.1	0.3
(2,757)	1:A:692:LEU:HD13	1:A:691:SER:HB2	3	0.25	0.1	0.3

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,757)	1:A:692:LEU:HD13	1:A:691:SER:HB3	3	0.25	0.1	0.3
(2,1144)	1:A:682:ILE:HG21	1:A:685:PHE:HB2	3	0.25	0.04	0.26
(2,1144)	1:A:682:ILE:HG21	1:A:685:PHE:HB3	3	0.25	0.04	0.26
(2,1144)	1:A:682:ILE:HG22	1:A:685:PHE:HB2	3	0.25	0.04	0.26
(2,1144)	1:A:682:ILE:HG22	1:A:685:PHE:HB3	3	0.25	0.04	0.26
(2,1144)	1:A:682:ILE:HG23	1:A:685:PHE:HB2	3	0.25	0.04	0.26
(2,1144)	1:A:682:ILE:HG23	1:A:685:PHE:HB3	3	0.25	0.04	0.26
(2,1182)	1:A:692:LEU:HD11	1:A:691:SER:HB2	3	0.25	0.1	0.3
(2,1182)	1:A:692:LEU:HD11	1:A:691:SER:HB3	3	0.25	0.1	0.3
(2,1182)	1:A:692:LEU:HD12	1:A:691:SER:HB2	3	0.25	0.1	0.3
(2,1182)	1:A:692:LEU:HD12	1:A:691:SER:HB3	3	0.25	0.1	0.3
(2,1182)	1:A:692:LEU:HD13	1:A:691:SER:HB2	3	0.25	0.1	0.3
(2,1182)	1:A:692:LEU:HD13	1:A:691:SER:HB3	3	0.25	0.1	0.3
(2,187)	1:B:816:ASN:H	1:B:830:ILE:HD11	3	0.25	0.08	0.22
(2,187)	1:B:816:ASN:H	1:B:830:ILE:HD12	3	0.25	0.08	0.22
(2,187)	1:B:816:ASN:H	1:B:830:ILE:HD13	3	0.25	0.08	0.22
(2,751)	1:A:689:VAL:HG21	1:A:685:PHE:HD1	3	0.24	0.04	0.26
(2,751)	1:A:689:VAL:HG21	1:A:685:PHE:HD2	3	0.24	0.04	0.26
(2,751)	1:A:689:VAL:HG22	1:A:685:PHE:HD1	3	0.24	0.04	0.26
(2,751)	1:A:689:VAL:HG22	1:A:685:PHE:HD2	3	0.24	0.04	0.26
(2,751)	1:A:689:VAL:HG23	1:A:685:PHE:HD1	3	0.24	0.04	0.26
(2,751)	1:A:689:VAL:HG23	1:A:685:PHE:HD2	3	0.24	0.04	0.26
(2,1176)	1:A:689:VAL:HG21	1:A:685:PHE:HD1	3	0.24	0.04	0.26
(2,1176)	1:A:689:VAL:HG21	1:A:685:PHE:HD2	3	0.24	0.04	0.26
(2,1176)	1:A:689:VAL:HG22	1:A:685:PHE:HD1	3	0.24	0.04	0.26
(2,1176)	1:A:689:VAL:HG22	1:A:685:PHE:HD2	3	0.24	0.04	0.26
(2,1176)	1:A:689:VAL:HG23	1:A:685:PHE:HD1	3	0.24	0.04	0.26
(2,1176)	1:A:689:VAL:HG23	1:A:685:PHE:HD2	3	0.24	0.04	0.26
(2,797)	1:A:701:VAL:HG11	1:A:698:VAL:HA	3	0.23	0.07	0.27
(2,797)	1:A:701:VAL:HG12	1:A:698:VAL:HA	3	0.23	0.07	0.27
(2,797)	1:A:701:VAL:HG13	1:A:698:VAL:HA	3	0.23	0.07	0.27
(2,1222)	1:A:701:VAL:HG11	1:A:698:VAL:HA	3	0.23	0.07	0.27
(2,1222)	1:A:701:VAL:HG12	1:A:698:VAL:HA	3	0.23	0.07	0.27
(2,1222)	1:A:701:VAL:HG13	1:A:698:VAL:HA	3	0.23	0.07	0.27
(2,982)	1:A:777:ILE:HD11	1:A:774:LEU:HA	3	0.22	0.01	0.22
(2,982)	1:A:777:ILE:HD12	1:A:774:LEU:HA	3	0.22	0.01	0.22
(2,982)	1:A:777:ILE:HD13	1:A:774:LEU:HA	3	0.22	0.01	0.22
(2,1407)	1:A:777:ILE:HD11	1:A:774:LEU:HA	3	0.22	0.01	0.22
(2,1407)	1:A:777:ILE:HD12	1:A:774:LEU:HA	3	0.22	0.01	0.22
(2,1407)	1:A:777:ILE:HD13	1:A:774:LEU:HA	3	0.22	0.01	0.22
(2,618)	1:B:797:TRP:H	1:B:796:TRP:HD1	3	0.2	0.05	0.21
(2,970)	1:A:775:LEU:HD11	1:A:772:ARG:HA	3	0.2	0.08	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,970)	1:A:775:LEU:HD12	1:A:772:ARG:HA	3	0.2	0.08	0.14
(2,970)	1:A:775:LEU:HD13	1:A:772:ARG:HA	3	0.2	0.08	0.14
(2,1395)	1:A:775:LEU:HD11	1:A:772:ARG:HA	3	0.2	0.08	0.14
(2,1395)	1:A:775:LEU:HD12	1:A:772:ARG:HA	3	0.2	0.08	0.14
(2,1395)	1:A:775:LEU:HD13	1:A:772:ARG:HA	3	0.2	0.08	0.14
(2,214)	1:B:661:LEU:HD11	1:B:662:GLU:HG2	3	0.19	0.06	0.17
(2,214)	1:B:661:LEU:HD11	1:B:662:GLU:HG3	3	0.19	0.06	0.17
(2,214)	1:B:661:LEU:HD12	1:B:662:GLU:HG2	3	0.19	0.06	0.17
(2,214)	1:B:661:LEU:HD12	1:B:662:GLU:HG3	3	0.19	0.06	0.17
(2,214)	1:B:661:LEU:HD13	1:B:662:GLU:HG2	3	0.19	0.06	0.17
(2,214)	1:B:661:LEU:HD13	1:B:662:GLU:HG3	3	0.19	0.06	0.17
(2,214)	1:B:661:LEU:HD21	1:B:662:GLU:HG2	3	0.19	0.06	0.17
(2,214)	1:B:661:LEU:HD21	1:B:662:GLU:HG3	3	0.19	0.06	0.17
(2,214)	1:B:661:LEU:HD22	1:B:662:GLU:HG2	3	0.19	0.06	0.17
(2,214)	1:B:661:LEU:HD22	1:B:662:GLU:HG3	3	0.19	0.06	0.17
(2,214)	1:B:661:LEU:HD23	1:B:662:GLU:HG2	3	0.19	0.06	0.17
(2,214)	1:B:661:LEU:HD23	1:B:662:GLU:HG3	3	0.19	0.06	0.17
(2,188)	1:A:816:ASN:H	1:A:830:ILE:HD11	3	0.19	0.02	0.2
(2,188)	1:A:816:ASN:H	1:A:830:ILE:HD12	3	0.19	0.02	0.2
(2,188)	1:A:816:ASN:H	1:A:830:ILE:HD13	3	0.19	0.02	0.2
(2,189)	1:A:816:ASN:H	1:A:830:ILE:HD11	3	0.19	0.02	0.2
(2,189)	1:A:816:ASN:H	1:A:830:ILE:HD12	3	0.19	0.02	0.2
(2,189)	1:A:816:ASN:H	1:A:830:ILE:HD13	3	0.19	0.02	0.2
(2,437)	1:B:709:ARG:HE	1:B:705:VAL:HG11	3	0.18	0.04	0.15
(2,437)	1:B:709:ARG:HE	1:B:705:VAL:HG12	3	0.18	0.04	0.15
(2,437)	1:B:709:ARG:HE	1:B:705:VAL:HG13	3	0.18	0.04	0.15
(2,580)	1:B:781:ILE:HG21	1:B:778:VAL:HA	3	0.17	0.07	0.14
(2,580)	1:B:781:ILE:HG22	1:B:778:VAL:HA	3	0.17	0.07	0.14
(2,580)	1:B:781:ILE:HG23	1:B:778:VAL:HA	3	0.17	0.07	0.14
(2,977)	1:A:777:ILE:H	1:A:774:LEU:HA	3	0.17	0.03	0.17
(2,1402)	1:A:777:ILE:H	1:A:774:LEU:HA	3	0.17	0.03	0.17
(2,55)	1:B:696:ARG:HE	1:A:694:GLY:HA2	3	0.16	0.01	0.16
(2,55)	1:B:696:ARG:HE	1:A:694:GLY:HA3	3	0.16	0.01	0.16
(2,777)	1:A:697:ILE:HG21	1:A:694:GLY:HA2	3	0.16	0.04	0.18
(2,777)	1:A:697:ILE:HG21	1:A:694:GLY:HA3	3	0.16	0.04	0.18
(2,777)	1:A:697:ILE:HG22	1:A:694:GLY:HA2	3	0.16	0.04	0.18
(2,777)	1:A:697:ILE:HG22	1:A:694:GLY:HA3	3	0.16	0.04	0.18
(2,777)	1:A:697:ILE:HG23	1:A:694:GLY:HA2	3	0.16	0.04	0.18
(2,777)	1:A:697:ILE:HG23	1:A:694:GLY:HA3	3	0.16	0.04	0.18
(2,1202)	1:A:697:ILE:HG21	1:A:694:GLY:HA2	3	0.16	0.04	0.18
(2,1202)	1:A:697:ILE:HG21	1:A:694:GLY:HA3	3	0.16	0.04	0.18
(2,1202)	1:A:697:ILE:HG22	1:A:694:GLY:HA2	3	0.16	0.04	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1202)	1:A:697:ILE:HG22	1:A:694:GLY:HA3	3	0.16	0.04	0.18
(2,1202)	1:A:697:ILE:HG23	1:A:694:GLY:HA2	3	0.16	0.04	0.18
(2,1202)	1:A:697:ILE:HG23	1:A:694:GLY:HA3	3	0.16	0.04	0.18
(2,705)	1:A:676:THR:HG21	1:A:681:TYR:HH	3	0.16	0.04	0.14
(2,705)	1:A:676:THR:HG22	1:A:681:TYR:HH	3	0.16	0.04	0.14
(2,705)	1:A:676:THR:HG23	1:A:681:TYR:HH	3	0.16	0.04	0.14
(2,1130)	1:A:676:THR:HG21	1:A:681:TYR:HH	3	0.16	0.04	0.14
(2,1130)	1:A:676:THR:HG22	1:A:681:TYR:HH	3	0.16	0.04	0.14
(2,1130)	1:A:676:THR:HG23	1:A:681:TYR:HH	3	0.16	0.04	0.14
(2,715)	1:A:680:TRP:HE1	1:A:684:ILE:HD11	3	0.16	0.03	0.17
(2,715)	1:A:680:TRP:HE1	1:A:684:ILE:HD12	3	0.16	0.03	0.17
(2,715)	1:A:680:TRP:HE1	1:A:684:ILE:HD13	3	0.16	0.03	0.17
(2,1140)	1:A:680:TRP:HE1	1:A:684:ILE:HD11	3	0.16	0.03	0.17
(2,1140)	1:A:680:TRP:HE1	1:A:684:ILE:HD12	3	0.16	0.03	0.17
(2,1140)	1:A:680:TRP:HE1	1:A:684:ILE:HD13	3	0.16	0.03	0.17
(2,153)	1:A:792:ALA:H	1:B:752:SER:HB2	3	0.15	0.02	0.15
(2,153)	1:A:792:ALA:H	1:B:752:SER:HB3	3	0.15	0.02	0.15
(2,587)	1:B:783:GLU:H	1:B:780:ARG:HA	3	0.15	0.04	0.12
(2,667)	1:A:667:ALA:H	1:A:664:ASP:HA	3	0.15	0.04	0.14
(2,1092)	1:A:667:ALA:H	1:A:664:ASP:HA	3	0.15	0.04	0.14
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD11	3	0.15	0.02	0.13
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD12	3	0.15	0.02	0.13
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD13	3	0.15	0.02	0.13
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD21	3	0.15	0.02	0.13
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD22	3	0.15	0.02	0.13
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD23	3	0.15	0.02	0.13
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD11	3	0.15	0.02	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD12	3	0.15	0.02	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD13	3	0.15	0.02	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD21	3	0.15	0.02	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD22	3	0.15	0.02	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD23	3	0.15	0.02	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD11	3	0.15	0.02	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD12	3	0.15	0.02	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD13	3	0.15	0.02	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD21	3	0.15	0.02	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD22	3	0.15	0.02	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD23	3	0.15	0.02	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD11	3	0.15	0.02	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD12	3	0.15	0.02	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD13	3	0.15	0.02	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD21	3	0.15	0.02	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD22	3	0.15	0.02	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD23	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD11	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD12	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD13	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD21	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD22	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD23	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD11	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD12	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD13	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD21	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD22	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD23	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD11	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD12	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD13	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD21	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD22	3	0.15	0.02	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD23	3	0.15	0.02	0.16
(2,292)	1:B:681:TYR:H	1:B:682:ILE:H	3	0.14	0.03	0.14
(2,599)	1:B:784:LEU:HD11	1:B:787:ARG:HD2	3	0.14	0.02	0.14
(2,599)	1:B:784:LEU:HD11	1:B:787:ARG:HD3	3	0.14	0.02	0.14
(2,599)	1:B:784:LEU:HD12	1:B:787:ARG:HD2	3	0.14	0.02	0.14
(2,599)	1:B:784:LEU:HD12	1:B:787:ARG:HD3	3	0.14	0.02	0.14
(2,599)	1:B:784:LEU:HD13	1:B:787:ARG:HD2	3	0.14	0.02	0.14
(2,599)	1:B:784:LEU:HD13	1:B:787:ARG:HD3	3	0.14	0.02	0.14
(2,684)	1:A:670:TRP:H	1:A:667:ALA:HA	3	0.14	0.01	0.14
(2,1109)	1:A:670:TRP:H	1:A:667:ALA:HA	3	0.14	0.01	0.14
(2,330)	1:B:692:LEU:HD11	1:B:689:VAL:HA	3	0.14	0.04	0.12
(2,330)	1:B:692:LEU:HD12	1:B:689:VAL:HA	3	0.14	0.04	0.12
(2,330)	1:B:692:LEU:HD13	1:B:689:VAL:HA	3	0.14	0.04	0.12
(1,4)	1:B:791:GLU:O	1:B:795:TYR:N	3	0.13	0.02	0.14
(1,17)	1:B:798:ASN:O	1:B:802:TYR:H	3	0.13	0.01	0.14
(1,90)	1:B:791:GLU:O	1:B:795:TYR:N	3	0.13	0.02	0.14
(1,103)	1:B:798:ASN:O	1:B:802:TYR:H	3	0.13	0.01	0.14
(1,176)	1:B:791:GLU:O	1:B:795:TYR:N	3	0.13	0.02	0.14
(1,189)	1:B:798:ASN:O	1:B:802:TYR:H	3	0.13	0.01	0.14
(2,336)	1:B:693:ILE:HD11	1:B:697:ILE:H	3	0.13	0.03	0.12
(2,336)	1:B:693:ILE:HD12	1:B:697:ILE:H	3	0.13	0.03	0.12
(2,336)	1:B:693:ILE:HD13	1:B:697:ILE:H	3	0.13	0.03	0.12
(2,799)	1:A:702:LEU:H	1:A:699:PHE:HA	3	0.13	0.02	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1224)	1:A:702:LEU:H	1:A:699:PHE:HA	3	0.13	0.02	0.14
(1,27)	1:B:803:TRP:O	1:B:807:LEU:H	3	0.13	0.02	0.13
(1,113)	1:B:803:TRP:O	1:B:807:LEU:H	3	0.13	0.02	0.13
(1,199)	1:B:803:TRP:O	1:B:807:LEU:H	3	0.13	0.02	0.13
(2,768)	1:A:695:LEU:HD11	1:A:691:SER:HB2	3	0.13	0.01	0.13
(2,768)	1:A:695:LEU:HD11	1:A:691:SER:HB3	3	0.13	0.01	0.13
(2,768)	1:A:695:LEU:HD12	1:A:691:SER:HB2	3	0.13	0.01	0.13
(2,768)	1:A:695:LEU:HD12	1:A:691:SER:HB3	3	0.13	0.01	0.13
(2,768)	1:A:695:LEU:HD13	1:A:691:SER:HB2	3	0.13	0.01	0.13
(2,768)	1:A:695:LEU:HD13	1:A:691:SER:HB3	3	0.13	0.01	0.13
(2,927)	1:A:755:LEU:H	1:A:752:SER:HA	3	0.13	0.01	0.13
(2,1193)	1:A:695:LEU:HD11	1:A:691:SER:HB2	3	0.13	0.01	0.13
(2,1193)	1:A:695:LEU:HD11	1:A:691:SER:HB3	3	0.13	0.01	0.13
(2,1193)	1:A:695:LEU:HD12	1:A:691:SER:HB2	3	0.13	0.01	0.13
(2,1193)	1:A:695:LEU:HD12	1:A:691:SER:HB3	3	0.13	0.01	0.13
(2,1193)	1:A:695:LEU:HD13	1:A:691:SER:HB2	3	0.13	0.01	0.13
(2,1193)	1:A:695:LEU:HD13	1:A:691:SER:HB3	3	0.13	0.01	0.13
(2,1352)	1:A:755:LEU:H	1:A:752:SER:HA	3	0.13	0.01	0.13
(2,1001)	1:A:781:ILE:H	1:A:780:ARG:HA	3	0.13	0.0	0.13
(2,1426)	1:A:781:ILE:H	1:A:780:ARG:HA	3	0.13	0.0	0.13
(1,12)	1:B:795:TYR:O	1:B:799:LEU:N	3	0.12	0.01	0.12
(1,98)	1:B:795:TYR:O	1:B:799:LEU:N	3	0.12	0.01	0.12
(1,184)	1:B:795:TYR:O	1:B:799:LEU:N	3	0.12	0.01	0.12
(2,43)	1:B:693:ILE:H	1:A:693:ILE:HD11	3	0.12	0.01	0.11
(2,43)	1:B:693:ILE:H	1:A:693:ILE:HD12	3	0.12	0.01	0.11
(2,43)	1:B:693:ILE:H	1:A:693:ILE:HD13	3	0.12	0.01	0.11
(2,445)	1:B:710:GLN:H	1:B:710:GLN:HB2	2	0.64	0.01	0.64
(2,339)	1:B:693:ILE:HG21	1:B:694:GLY:H	2	0.52	0.01	0.52
(2,339)	1:B:693:ILE:HG22	1:B:694:GLY:H	2	0.52	0.01	0.52
(2,339)	1:B:693:ILE:HG23	1:B:694:GLY:H	2	0.52	0.01	0.52
(2,491)	1:B:753:LEU:HD11	1:B:757:TRP:HB2	2	0.44	0.11	0.44
(2,491)	1:B:753:LEU:HD11	1:B:757:TRP:HB3	2	0.44	0.11	0.44
(2,491)	1:B:753:LEU:HD12	1:B:757:TRP:HB2	2	0.44	0.11	0.44
(2,491)	1:B:753:LEU:HD12	1:B:757:TRP:HB3	2	0.44	0.11	0.44
(2,491)	1:B:753:LEU:HD13	1:B:757:TRP:HB2	2	0.44	0.11	0.44
(2,491)	1:B:753:LEU:HD13	1:B:757:TRP:HB3	2	0.44	0.11	0.44
(2,882)	1:A:740:ARG:H	1:A:739:GLU:HA	2	0.38	0.1	0.38
(2,1307)	1:A:740:ARG:H	1:A:739:GLU:HA	2	0.38	0.1	0.38
(2,212)	1:A:839:ALA:H	1:A:808:LYS:HZ1	2	0.31	0.08	0.31
(2,212)	1:A:839:ALA:H	1:A:808:LYS:HZ2	2	0.31	0.08	0.31
(2,212)	1:A:839:ALA:H	1:A:808:LYS:HZ3	2	0.31	0.08	0.31
(2,213)	1:A:839:ALA:H	1:A:808:LYS:HZ1	2	0.31	0.08	0.31

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,213)	1:A:839:ALA:H	1:A:808:LYS:HZ2	2	0.31	0.08	0.31
(2,213)	1:A:839:ALA:H	1:A:808:LYS:HZ3	2	0.31	0.08	0.31
(2,373)	1:B:701:VAL:HG21	1:B:698:VAL:HA	2	0.31	0.04	0.31
(2,373)	1:B:701:VAL:HG22	1:B:698:VAL:HA	2	0.31	0.04	0.31
(2,373)	1:B:701:VAL:HG23	1:B:698:VAL:HA	2	0.31	0.04	0.31
(2,1051)	1:A:817:ALA:H	1:A:816:ASN:HB2	2	0.3	0.02	0.3
(2,1051)	1:A:817:ALA:H	1:A:816:ASN:HB3	2	0.3	0.02	0.3
(2,1476)	1:A:817:ALA:H	1:A:816:ASN:HB2	2	0.3	0.02	0.3
(2,1476)	1:A:817:ALA:H	1:A:816:ASN:HB3	2	0.3	0.02	0.3
(2,626)	1:B:817:ALA:H	1:B:816:ASN:HB2	2	0.3	0.08	0.3
(2,626)	1:B:817:ALA:H	1:B:816:ASN:HB3	2	0.3	0.08	0.3
(2,947)	1:A:764:SER:H	1:A:761:ARG:HA	2	0.29	0.04	0.29
(2,1372)	1:A:764:SER:H	1:A:761:ARG:HA	2	0.29	0.04	0.29
(2,499)	1:B:754:ALA:HB1	1:B:753:LEU:HD21	2	0.29	0.16	0.29
(2,499)	1:B:754:ALA:HB1	1:B:753:LEU:HD22	2	0.29	0.16	0.29
(2,499)	1:B:754:ALA:HB1	1:B:753:LEU:HD23	2	0.29	0.16	0.29
(2,499)	1:B:754:ALA:HB2	1:B:753:LEU:HD21	2	0.29	0.16	0.29
(2,499)	1:B:754:ALA:HB2	1:B:753:LEU:HD22	2	0.29	0.16	0.29
(2,499)	1:B:754:ALA:HB2	1:B:753:LEU:HD23	2	0.29	0.16	0.29
(2,499)	1:B:754:ALA:HB3	1:B:753:LEU:HD21	2	0.29	0.16	0.29
(2,499)	1:B:754:ALA:HB3	1:B:753:LEU:HD22	2	0.29	0.16	0.29
(2,499)	1:B:754:ALA:HB3	1:B:753:LEU:HD23	2	0.29	0.16	0.29
(2,760)	1:A:693:ILE:HD11	1:A:694:GLY:HA2	2	0.28	0.12	0.28
(2,760)	1:A:693:ILE:HD11	1:A:694:GLY:HA3	2	0.28	0.12	0.28
(2,760)	1:A:693:ILE:HD12	1:A:694:GLY:HA2	2	0.28	0.12	0.28
(2,760)	1:A:693:ILE:HD12	1:A:694:GLY:HA3	2	0.28	0.12	0.28
(2,760)	1:A:693:ILE:HD13	1:A:694:GLY:HA2	2	0.28	0.12	0.28
(2,760)	1:A:693:ILE:HD13	1:A:694:GLY:HA3	2	0.28	0.12	0.28
(2,1185)	1:A:693:ILE:HD11	1:A:694:GLY:HA2	2	0.28	0.12	0.28
(2,1185)	1:A:693:ILE:HD11	1:A:694:GLY:HA3	2	0.28	0.12	0.28
(2,1185)	1:A:693:ILE:HD12	1:A:694:GLY:HA2	2	0.28	0.12	0.28
(2,1185)	1:A:693:ILE:HD12	1:A:694:GLY:HA3	2	0.28	0.12	0.28
(2,1185)	1:A:693:ILE:HD13	1:A:694:GLY:HA2	2	0.28	0.12	0.28
(2,1185)	1:A:693:ILE:HD13	1:A:694:GLY:HA3	2	0.28	0.12	0.28
(2,438)	1:B:709:ARG:HE	1:B:709:ARG:H	2	0.28	0.02	0.28
(2,117)	1:A:781:ILE:HD11	1:B:746:ILE:HG12	2	0.27	0.05	0.27
(2,117)	1:A:781:ILE:HD11	1:B:746:ILE:HG13	2	0.27	0.05	0.27
(2,117)	1:A:781:ILE:HD12	1:B:746:ILE:HG12	2	0.27	0.05	0.27
(2,117)	1:A:781:ILE:HD12	1:B:746:ILE:HG13	2	0.27	0.05	0.27
(2,117)	1:A:781:ILE:HD13	1:B:746:ILE:HG12	2	0.27	0.05	0.27
(2,117)	1:A:781:ILE:HD13	1:B:746:ILE:HG13	2	0.27	0.05	0.27
(2,629)	1:B:835:GLY:H	1:B:834:GLN:HG2	2	0.24	0.04	0.24

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,629)	1:B:835:GLY:H	1:B:834:GLN:HG3	2	0.24	0.04	0.24
(2,102)	1:A:759:ASP:H	1:B:709:ARG:HD2	2	0.24	0.11	0.24
(2,102)	1:A:759:ASP:H	1:B:709:ARG:HD3	2	0.24	0.11	0.24
(2,744)	1:A:686:ILE:HD11	1:A:685:PHE:HD1	2	0.24	0.05	0.24
(2,744)	1:A:686:ILE:HD11	1:A:685:PHE:HD2	2	0.24	0.05	0.24
(2,744)	1:A:686:ILE:HD12	1:A:685:PHE:HD1	2	0.24	0.05	0.24
(2,744)	1:A:686:ILE:HD12	1:A:685:PHE:HD2	2	0.24	0.05	0.24
(2,744)	1:A:686:ILE:HD13	1:A:685:PHE:HD1	2	0.24	0.05	0.24
(2,744)	1:A:686:ILE:HD13	1:A:685:PHE:HD2	2	0.24	0.05	0.24
(2,1169)	1:A:686:ILE:HD11	1:A:685:PHE:HD1	2	0.24	0.05	0.24
(2,1169)	1:A:686:ILE:HD11	1:A:685:PHE:HD2	2	0.24	0.05	0.24
(2,1169)	1:A:686:ILE:HD12	1:A:685:PHE:HD1	2	0.24	0.05	0.24
(2,1169)	1:A:686:ILE:HD12	1:A:685:PHE:HD2	2	0.24	0.05	0.24
(2,1169)	1:A:686:ILE:HD13	1:A:685:PHE:HD1	2	0.24	0.05	0.24
(2,1169)	1:A:686:ILE:HD13	1:A:685:PHE:HD2	2	0.24	0.05	0.24
(2,828)	1:A:705:VAL:HG11	1:A:709:ARG:HD2	2	0.22	0.1	0.22
(2,828)	1:A:705:VAL:HG11	1:A:709:ARG:HD3	2	0.22	0.1	0.22
(2,828)	1:A:705:VAL:HG12	1:A:709:ARG:HD2	2	0.22	0.1	0.22
(2,828)	1:A:705:VAL:HG12	1:A:709:ARG:HD3	2	0.22	0.1	0.22
(2,828)	1:A:705:VAL:HG13	1:A:709:ARG:HD2	2	0.22	0.1	0.22
(2,828)	1:A:705:VAL:HG13	1:A:709:ARG:HD3	2	0.22	0.1	0.22
(2,1253)	1:A:705:VAL:HG11	1:A:709:ARG:HD2	2	0.22	0.1	0.22
(2,1253)	1:A:705:VAL:HG11	1:A:709:ARG:HD3	2	0.22	0.1	0.22
(2,1253)	1:A:705:VAL:HG12	1:A:709:ARG:HD2	2	0.22	0.1	0.22
(2,1253)	1:A:705:VAL:HG12	1:A:709:ARG:HD3	2	0.22	0.1	0.22
(2,1253)	1:A:705:VAL:HG13	1:A:709:ARG:HD2	2	0.22	0.1	0.22
(2,1253)	1:A:705:VAL:HG13	1:A:709:ARG:HD3	2	0.22	0.1	0.22
(2,327)	1:B:689:VAL:HG21	1:B:685:PHE:HE1	2	0.22	0.1	0.22
(2,327)	1:B:689:VAL:HG21	1:B:685:PHE:HE2	2	0.22	0.1	0.22
(2,327)	1:B:689:VAL:HG22	1:B:685:PHE:HE1	2	0.22	0.1	0.22
(2,327)	1:B:689:VAL:HG22	1:B:685:PHE:HE2	2	0.22	0.1	0.22
(2,327)	1:B:689:VAL:HG23	1:B:685:PHE:HE1	2	0.22	0.1	0.22
(2,327)	1:B:689:VAL:HG23	1:B:685:PHE:HE2	2	0.22	0.1	0.22
(2,748)	1:A:688:ILE:HD11	1:A:684:ILE:HD11	2	0.22	0.1	0.22
(2,748)	1:A:688:ILE:HD11	1:A:684:ILE:HD12	2	0.22	0.1	0.22
(2,748)	1:A:688:ILE:HD11	1:A:684:ILE:HD13	2	0.22	0.1	0.22
(2,748)	1:A:688:ILE:HD12	1:A:684:ILE:HD11	2	0.22	0.1	0.22
(2,748)	1:A:688:ILE:HD12	1:A:684:ILE:HD12	2	0.22	0.1	0.22
(2,748)	1:A:688:ILE:HD12	1:A:684:ILE:HD13	2	0.22	0.1	0.22
(2,748)	1:A:688:ILE:HD13	1:A:684:ILE:HD11	2	0.22	0.1	0.22
(2,748)	1:A:688:ILE:HD13	1:A:684:ILE:HD12	2	0.22	0.1	0.22
(2,748)	1:A:688:ILE:HD13	1:A:684:ILE:HD13	2	0.22	0.1	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1173)	1:A:688:ILE:HD11	1:A:684:ILE:HD11	2	0.22	0.1	0.22
(2,1173)	1:A:688:ILE:HD11	1:A:684:ILE:HD12	2	0.22	0.1	0.22
(2,1173)	1:A:688:ILE:HD11	1:A:684:ILE:HD13	2	0.22	0.1	0.22
(2,1173)	1:A:688:ILE:HD12	1:A:684:ILE:HD11	2	0.22	0.1	0.22
(2,1173)	1:A:688:ILE:HD12	1:A:684:ILE:HD12	2	0.22	0.1	0.22
(2,1173)	1:A:688:ILE:HD12	1:A:684:ILE:HD13	2	0.22	0.1	0.22
(2,1173)	1:A:688:ILE:HD13	1:A:684:ILE:HD11	2	0.22	0.1	0.22
(2,1173)	1:A:688:ILE:HD13	1:A:684:ILE:HD12	2	0.22	0.1	0.22
(2,1173)	1:A:688:ILE:HD13	1:A:684:ILE:HD13	2	0.22	0.1	0.22
(2,52)	1:B:696:ARG:H	1:A:693:ILE:HD11	2	0.21	0.03	0.21
(2,52)	1:B:696:ARG:H	1:A:693:ILE:HD12	2	0.21	0.03	0.21
(2,52)	1:B:696:ARG:H	1:A:693:ILE:HD13	2	0.21	0.03	0.21
(2,755)	1:A:692:LEU:HD11	1:A:689:VAL:HA	2	0.21	0.1	0.21
(2,755)	1:A:692:LEU:HD12	1:A:689:VAL:HA	2	0.21	0.1	0.21
(2,755)	1:A:692:LEU:HD13	1:A:689:VAL:HA	2	0.21	0.1	0.21
(2,1180)	1:A:692:LEU:HD11	1:A:689:VAL:HA	2	0.21	0.1	0.21
(2,1180)	1:A:692:LEU:HD12	1:A:689:VAL:HA	2	0.21	0.1	0.21
(2,1180)	1:A:692:LEU:HD13	1:A:689:VAL:HA	2	0.21	0.1	0.21
(2,630)	1:B:835:GLY:H	1:B:834:GLN:HE21	2	0.2	0.08	0.2
(2,630)	1:B:835:GLY:H	1:B:834:GLN:HE22	2	0.2	0.08	0.2
(2,644)	1:A:663:LEU:H	1:A:664:ASP:H	2	0.2	0.02	0.2
(2,650)	1:A:664:ASP:H	1:A:663:LEU:H	2	0.2	0.02	0.2
(2,1069)	1:A:663:LEU:H	1:A:664:ASP:H	2	0.2	0.02	0.2
(2,1075)	1:A:664:ASP:H	1:A:663:LEU:H	2	0.2	0.02	0.2
(2,354)	1:B:697:ILE:HG21	1:B:700:ALA:HB1	2	0.19	0.02	0.19
(2,354)	1:B:697:ILE:HG21	1:B:700:ALA:HB2	2	0.19	0.02	0.19
(2,354)	1:B:697:ILE:HG21	1:B:700:ALA:HB3	2	0.19	0.02	0.19
(2,354)	1:B:697:ILE:HG22	1:B:700:ALA:HB1	2	0.19	0.02	0.19
(2,354)	1:B:697:ILE:HG22	1:B:700:ALA:HB2	2	0.19	0.02	0.19
(2,354)	1:B:697:ILE:HG22	1:B:700:ALA:HB3	2	0.19	0.02	0.19
(2,354)	1:B:697:ILE:HG23	1:B:700:ALA:HB1	2	0.19	0.02	0.19
(2,354)	1:B:697:ILE:HG23	1:B:700:ALA:HB2	2	0.19	0.02	0.19
(2,354)	1:B:697:ILE:HG23	1:B:700:ALA:HB3	2	0.19	0.02	0.19
(2,191)	1:A:816:ASN:H	1:A:831:GLU:HG2	2	0.18	0.08	0.18
(2,191)	1:A:816:ASN:H	1:A:831:GLU:HG3	2	0.18	0.08	0.18
(2,192)	1:A:816:ASN:H	1:A:831:GLU:HG2	2	0.18	0.08	0.18
(2,192)	1:A:816:ASN:H	1:A:831:GLU:HG3	2	0.18	0.08	0.18
(1,55)	1:B:827:ASP:O	1:B:831:GLU:H	2	0.18	0.07	0.18
(1,141)	1:B:827:ASP:O	1:B:831:GLU:H	2	0.18	0.07	0.18
(1,227)	1:B:827:ASP:O	1:B:831:GLU:H	2	0.18	0.07	0.18
(2,557)	1:B:777:ILE:HD11	1:B:774:LEU:HA	2	0.18	0.03	0.18
(2,557)	1:B:777:ILE:HD12	1:B:774:LEU:HA	2	0.18	0.03	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,557)	1:B:777:ILE:HD13	1:B:774:LEU:HA	2	0.18	0.03	0.18
(2,123)	1:A:785:LEU:HD21	1:B:747:ARG:HD2	2	0.18	0.03	0.18
(2,123)	1:A:785:LEU:HD21	1:B:747:ARG:HD3	2	0.18	0.03	0.18
(2,123)	1:A:785:LEU:HD22	1:B:747:ARG:HD2	2	0.18	0.03	0.18
(2,123)	1:A:785:LEU:HD22	1:B:747:ARG:HD3	2	0.18	0.03	0.18
(2,123)	1:A:785:LEU:HD23	1:B:747:ARG:HD2	2	0.18	0.03	0.18
(2,123)	1:A:785:LEU:HD23	1:B:747:ARG:HD3	2	0.18	0.03	0.18
(2,564)	1:B:778:VAL:HG21	1:B:775:LEU:HA	2	0.16	0.06	0.16
(2,564)	1:B:778:VAL:HG22	1:B:775:LEU:HA	2	0.16	0.06	0.16
(2,564)	1:B:778:VAL:HG23	1:B:775:LEU:HA	2	0.16	0.06	0.16
(2,506)	1:B:755:LEU:H	1:B:756:ILE:H	2	0.16	0.05	0.16
(2,688)	1:A:670:TRP:HE1	1:A:667:ALA:HB1	2	0.16	0.05	0.16
(2,688)	1:A:670:TRP:HE1	1:A:667:ALA:HB2	2	0.16	0.05	0.16
(2,688)	1:A:670:TRP:HE1	1:A:667:ALA:HB3	2	0.16	0.05	0.16
(2,773)	1:A:695:LEU:HD21	1:A:696:ARG:HH11	2	0.16	0.01	0.16
(2,773)	1:A:695:LEU:HD21	1:A:696:ARG:HH12	2	0.16	0.01	0.16
(2,773)	1:A:695:LEU:HD22	1:A:696:ARG:HH11	2	0.16	0.01	0.16
(2,773)	1:A:695:LEU:HD22	1:A:696:ARG:HH12	2	0.16	0.01	0.16
(2,773)	1:A:695:LEU:HD23	1:A:696:ARG:HH11	2	0.16	0.01	0.16
(2,773)	1:A:695:LEU:HD23	1:A:696:ARG:HH12	2	0.16	0.01	0.16
(2,1113)	1:A:670:TRP:HE1	1:A:667:ALA:HB1	2	0.16	0.05	0.16
(2,1113)	1:A:670:TRP:HE1	1:A:667:ALA:HB2	2	0.16	0.05	0.16
(2,1113)	1:A:670:TRP:HE1	1:A:667:ALA:HB3	2	0.16	0.05	0.16
(2,1198)	1:A:695:LEU:HD21	1:A:696:ARG:HH11	2	0.16	0.01	0.16
(2,1198)	1:A:695:LEU:HD21	1:A:696:ARG:HH12	2	0.16	0.01	0.16
(2,1198)	1:A:695:LEU:HD22	1:A:696:ARG:HH11	2	0.16	0.01	0.16
(2,1198)	1:A:695:LEU:HD22	1:A:696:ARG:HH12	2	0.16	0.01	0.16
(2,1198)	1:A:695:LEU:HD23	1:A:696:ARG:HH11	2	0.16	0.01	0.16
(2,1198)	1:A:695:LEU:HD23	1:A:696:ARG:HH12	2	0.16	0.01	0.16
(2,500)	1:B:754:ALA:HB1	1:B:758:ASP:H	2	0.16	0.02	0.16
(2,500)	1:B:754:ALA:HB2	1:B:758:ASP:H	2	0.16	0.02	0.16
(2,500)	1:B:754:ALA:HB3	1:B:758:ASP:H	2	0.16	0.02	0.16
(2,509)	1:B:758:ASP:H	1:B:754:ALA:HB1	2	0.16	0.02	0.16
(2,509)	1:B:758:ASP:H	1:B:754:ALA:HB2	2	0.16	0.02	0.16
(2,509)	1:B:758:ASP:H	1:B:754:ALA:HB3	2	0.16	0.02	0.16
(2,326)	1:B:689:VAL:HG21	1:B:685:PHE:HD1	2	0.16	0.01	0.16
(2,326)	1:B:689:VAL:HG21	1:B:685:PHE:HD2	2	0.16	0.01	0.16
(2,326)	1:B:689:VAL:HG22	1:B:685:PHE:HD1	2	0.16	0.01	0.16
(2,326)	1:B:689:VAL:HG22	1:B:685:PHE:HD2	2	0.16	0.01	0.16
(2,326)	1:B:689:VAL:HG23	1:B:685:PHE:HD1	2	0.16	0.01	0.16
(2,326)	1:B:689:VAL:HG23	1:B:685:PHE:HD2	2	0.16	0.01	0.16
(2,372)	1:B:701:VAL:HG11	1:B:698:VAL:HA	2	0.16	0.01	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,372)	1:B:701:VAL:HG12	1:B:698:VAL:HA	2	0.16	0.01	0.16
(2,372)	1:B:701:VAL:HG13	1:B:698:VAL:HA	2	0.16	0.01	0.16
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD11	2	0.16	0.02	0.16
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD12	2	0.16	0.02	0.16
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD13	2	0.16	0.02	0.16
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD21	2	0.16	0.02	0.16
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD22	2	0.16	0.02	0.16
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD23	2	0.16	0.02	0.16
(2,802)	1:A:702:LEU:HD11	1:A:699:PHE:HD1	2	0.16	0.01	0.16
(2,802)	1:A:702:LEU:HD11	1:A:699:PHE:HD2	2	0.16	0.01	0.16
(2,802)	1:A:702:LEU:HD12	1:A:699:PHE:HD1	2	0.16	0.01	0.16
(2,802)	1:A:702:LEU:HD12	1:A:699:PHE:HD2	2	0.16	0.01	0.16
(2,802)	1:A:702:LEU:HD13	1:A:699:PHE:HD1	2	0.16	0.01	0.16
(2,802)	1:A:702:LEU:HD13	1:A:699:PHE:HD2	2	0.16	0.01	0.16
(2,890)	1:A:746:ILE:H	1:A:743:ASP:HB2	2	0.16	0.04	0.16
(2,890)	1:A:746:ILE:H	1:A:743:ASP:HB3	2	0.16	0.04	0.16
(2,1033)	1:A:786:GLY:H	1:A:782:VAL:HA	2	0.16	0.01	0.16
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD11	2	0.16	0.02	0.16
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD12	2	0.16	0.02	0.16
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD13	2	0.16	0.02	0.16
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD21	2	0.16	0.02	0.16
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD22	2	0.16	0.02	0.16
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD23	2	0.16	0.02	0.16
(2,1227)	1:A:702:LEU:HD11	1:A:699:PHE:HD1	2	0.16	0.01	0.16
(2,1227)	1:A:702:LEU:HD11	1:A:699:PHE:HD2	2	0.16	0.01	0.16
(2,1227)	1:A:702:LEU:HD12	1:A:699:PHE:HD1	2	0.16	0.01	0.16
(2,1227)	1:A:702:LEU:HD12	1:A:699:PHE:HD2	2	0.16	0.01	0.16
(2,1227)	1:A:702:LEU:HD13	1:A:699:PHE:HD1	2	0.16	0.01	0.16
(2,1227)	1:A:702:LEU:HD13	1:A:699:PHE:HD2	2	0.16	0.01	0.16
(2,1315)	1:A:746:ILE:H	1:A:743:ASP:HB2	2	0.16	0.04	0.16
(2,1315)	1:A:746:ILE:H	1:A:743:ASP:HB3	2	0.16	0.04	0.16
(2,1458)	1:A:786:GLY:H	1:A:782:VAL:HA	2	0.16	0.01	0.16
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD11	2	0.15	0.02	0.15
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD12	2	0.15	0.02	0.15
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD13	2	0.15	0.02	0.15
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD21	2	0.15	0.02	0.15
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD22	2	0.15	0.02	0.15
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD23	2	0.15	0.02	0.15
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD11	2	0.15	0.02	0.15
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD12	2	0.15	0.02	0.15
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD13	2	0.15	0.02	0.15
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD21	2	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD22	2	0.15	0.02	0.15
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD23	2	0.15	0.02	0.15
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD11	2	0.15	0.02	0.15
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD12	2	0.15	0.02	0.15
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD13	2	0.15	0.02	0.15
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD21	2	0.15	0.02	0.15
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD22	2	0.15	0.02	0.15
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD23	2	0.15	0.02	0.15
(2,277)	1:B:676:THR:HG21	1:B:669:LEU:HA	2	0.15	0.02	0.15
(2,277)	1:B:676:THR:HG22	1:B:669:LEU:HA	2	0.15	0.02	0.15
(2,277)	1:B:676:THR:HG23	1:B:669:LEU:HA	2	0.15	0.02	0.15
(2,288)	1:B:679:LEU:HD11	1:B:678:TRP:HH2	2	0.15	0.02	0.15
(2,288)	1:B:679:LEU:HD12	1:B:678:TRP:HH2	2	0.15	0.02	0.15
(2,288)	1:B:679:LEU:HD13	1:B:678:TRP:HH2	2	0.15	0.02	0.15
(2,288)	1:B:679:LEU:HD21	1:B:678:TRP:HH2	2	0.15	0.02	0.15
(2,288)	1:B:679:LEU:HD22	1:B:678:TRP:HH2	2	0.15	0.02	0.15
(2,288)	1:B:679:LEU:HD23	1:B:678:TRP:HH2	2	0.15	0.02	0.15
(2,338)	1:B:693:ILE:HG21	1:B:693:ILE:H	2	0.15	0.02	0.15
(2,338)	1:B:693:ILE:HG22	1:B:693:ILE:H	2	0.15	0.02	0.15
(2,338)	1:B:693:ILE:HG23	1:B:693:ILE:H	2	0.15	0.02	0.15
(2,792)	1:A:700:ALA:HB1	1:A:697:ILE:HA	2	0.15	0.01	0.15
(2,792)	1:A:700:ALA:HB2	1:A:697:ILE:HA	2	0.15	0.01	0.15
(2,792)	1:A:700:ALA:HB3	1:A:697:ILE:HA	2	0.15	0.01	0.15
(2,1217)	1:A:700:ALA:HB1	1:A:697:ILE:HA	2	0.15	0.01	0.15
(2,1217)	1:A:700:ALA:HB2	1:A:697:ILE:HA	2	0.15	0.01	0.15
(2,1217)	1:A:700:ALA:HB3	1:A:697:ILE:HA	2	0.15	0.01	0.15
(2,763)	1:A:693:ILE:HG21	1:A:693:ILE:H	2	0.14	0.03	0.14
(2,763)	1:A:693:ILE:HG22	1:A:693:ILE:H	2	0.14	0.03	0.14
(2,763)	1:A:693:ILE:HG23	1:A:693:ILE:H	2	0.14	0.03	0.14
(2,1188)	1:A:693:ILE:HG21	1:A:693:ILE:H	2	0.14	0.03	0.14
(2,1188)	1:A:693:ILE:HG22	1:A:693:ILE:H	2	0.14	0.03	0.14
(2,1188)	1:A:693:ILE:HG23	1:A:693:ILE:H	2	0.14	0.03	0.14
(2,810)	1:A:704:LEU:H	1:A:701:VAL:HA	2	0.14	0.01	0.14
(2,1012)	1:A:783:GLU:H	1:A:780:ARG:HA	2	0.14	0.02	0.14
(2,1235)	1:A:704:LEU:H	1:A:701:VAL:HA	2	0.14	0.01	0.14
(2,1437)	1:A:783:GLU:H	1:A:780:ARG:HA	2	0.14	0.02	0.14
(1,53)	1:B:826:THR:O	1:B:830:ILE:H	2	0.14	0.02	0.14
(1,71)	1:B:835:GLY:O	1:B:839:ALA:H	2	0.14	0.02	0.14
(1,139)	1:B:826:THR:O	1:B:830:ILE:H	2	0.14	0.02	0.14
(1,157)	1:B:835:GLY:O	1:B:839:ALA:H	2	0.14	0.02	0.14
(1,225)	1:B:826:THR:O	1:B:830:ILE:H	2	0.14	0.02	0.14
(1,243)	1:B:835:GLY:O	1:B:839:ALA:H	2	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,19)	1:B:678:TRP:HE1	1:A:683:ARG:HE	2	0.14	0.02	0.14
(2,743)	1:A:686:ILE:HD11	1:A:685:PHE:H	2	0.14	0.02	0.14
(2,743)	1:A:686:ILE:HD12	1:A:685:PHE:H	2	0.14	0.02	0.14
(2,743)	1:A:686:ILE:HD13	1:A:685:PHE:H	2	0.14	0.02	0.14
(2,1168)	1:A:686:ILE:HD11	1:A:685:PHE:H	2	0.14	0.02	0.14
(2,1168)	1:A:686:ILE:HD12	1:A:685:PHE:H	2	0.14	0.02	0.14
(2,1168)	1:A:686:ILE:HD13	1:A:685:PHE:H	2	0.14	0.02	0.14
(1,41)	1:B:810:SER:O	1:B:814:LEU:H	2	0.13	0.01	0.13
(1,127)	1:B:810:SER:O	1:B:814:LEU:H	2	0.13	0.01	0.13
(1,213)	1:B:810:SER:O	1:B:814:LEU:H	2	0.13	0.01	0.13
(2,407)	1:B:706:ASN:H	1:B:703:SER:HA	2	0.13	0.01	0.13
(2,429)	1:B:708:VAL:HG21	1:B:707:ARG:HD2	2	0.13	0.02	0.13
(2,429)	1:B:708:VAL:HG21	1:B:707:ARG:HD3	2	0.13	0.02	0.13
(2,429)	1:B:708:VAL:HG22	1:B:707:ARG:HD2	2	0.13	0.02	0.13
(2,429)	1:B:708:VAL:HG22	1:B:707:ARG:HD3	2	0.13	0.02	0.13
(2,429)	1:B:708:VAL:HG23	1:B:707:ARG:HD2	2	0.13	0.02	0.13
(2,429)	1:B:708:VAL:HG23	1:B:707:ARG:HD3	2	0.13	0.02	0.13
(2,713)	1:A:679:LEU:HD11	1:A:678:TRP:HH2	2	0.13	0.02	0.13
(2,713)	1:A:679:LEU:HD12	1:A:678:TRP:HH2	2	0.13	0.02	0.13
(2,713)	1:A:679:LEU:HD13	1:A:678:TRP:HH2	2	0.13	0.02	0.13
(2,713)	1:A:679:LEU:HD21	1:A:678:TRP:HH2	2	0.13	0.02	0.13
(2,713)	1:A:679:LEU:HD22	1:A:678:TRP:HH2	2	0.13	0.02	0.13
(2,713)	1:A:679:LEU:HD23	1:A:678:TRP:HH2	2	0.13	0.02	0.13
(2,1138)	1:A:679:LEU:HD11	1:A:678:TRP:HH2	2	0.13	0.02	0.13
(2,1138)	1:A:679:LEU:HD12	1:A:678:TRP:HH2	2	0.13	0.02	0.13
(2,1138)	1:A:679:LEU:HD13	1:A:678:TRP:HH2	2	0.13	0.02	0.13
(2,1138)	1:A:679:LEU:HD21	1:A:678:TRP:HH2	2	0.13	0.02	0.13
(2,1138)	1:A:679:LEU:HD22	1:A:678:TRP:HH2	2	0.13	0.02	0.13
(2,1138)	1:A:679:LEU:HD23	1:A:678:TRP:HH2	2	0.13	0.02	0.13
(1,69)	1:B:834:GLN:O	1:B:838:ARG:H	2	0.12	0.02	0.12
(1,155)	1:B:834:GLN:O	1:B:838:ARG:H	2	0.12	0.02	0.12
(1,241)	1:B:834:GLN:O	1:B:838:ARG:H	2	0.12	0.02	0.12
(2,301)	1:B:684:ILE:HD11	1:B:681:TYR:HA	2	0.12	0.02	0.12
(2,301)	1:B:684:ILE:HD12	1:B:681:TYR:HA	2	0.12	0.02	0.12
(2,301)	1:B:684:ILE:HD13	1:B:681:TYR:HA	2	0.12	0.02	0.12
(2,358)	1:B:698:VAL:HG11	1:B:702:LEU:HB2	2	0.12	0.01	0.12
(2,358)	1:B:698:VAL:HG11	1:B:702:LEU:HB3	2	0.12	0.01	0.12
(2,358)	1:B:698:VAL:HG12	1:B:702:LEU:HB2	2	0.12	0.01	0.12
(2,358)	1:B:698:VAL:HG12	1:B:702:LEU:HB3	2	0.12	0.01	0.12
(2,358)	1:B:698:VAL:HG13	1:B:702:LEU:HB2	2	0.12	0.01	0.12
(2,358)	1:B:698:VAL:HG13	1:B:702:LEU:HB3	2	0.12	0.01	0.12
(2,541)	1:B:775:LEU:H	1:B:774:LEU:HA	2	0.12	0.01	0.12

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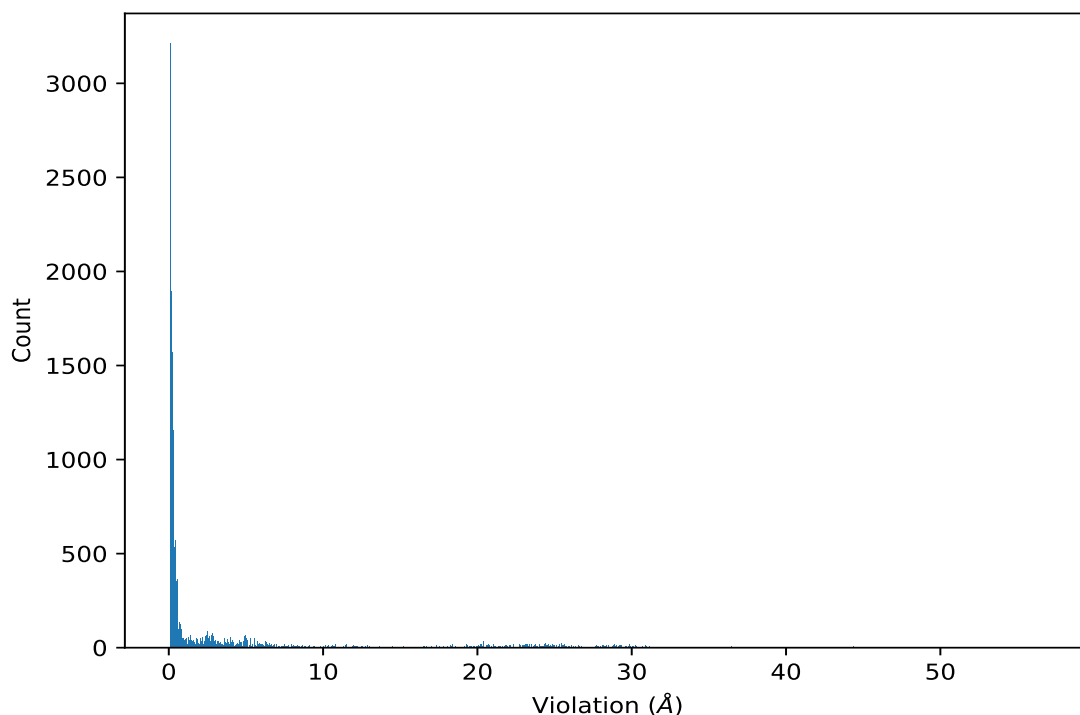
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,15)	1:B:797:TRP:O	1:B:801:GLN:H	2	0.12	0.0	0.12
(1,101)	1:B:797:TRP:O	1:B:801:GLN:H	2	0.12	0.0	0.12
(1,187)	1:B:797:TRP:O	1:B:801:GLN:H	2	0.12	0.0	0.12
(2,304)	1:B:684:ILE:HG21	1:B:685:PHE:HB2	2	0.12	0.01	0.12
(2,304)	1:B:684:ILE:HG21	1:B:685:PHE:HB3	2	0.12	0.01	0.12
(2,304)	1:B:684:ILE:HG22	1:B:685:PHE:HB2	2	0.12	0.01	0.12
(2,304)	1:B:684:ILE:HG22	1:B:685:PHE:HB3	2	0.12	0.01	0.12
(2,304)	1:B:684:ILE:HG23	1:B:685:PHE:HB2	2	0.12	0.01	0.12
(2,304)	1:B:684:ILE:HG23	1:B:685:PHE:HB3	2	0.12	0.01	0.12
(1,67)	1:B:833:VAL:O	1:B:837:SER:H	2	0.12	0.0	0.12
(1,153)	1:B:833:VAL:O	1:B:837:SER:H	2	0.12	0.0	0.12
(1,239)	1:B:833:VAL:O	1:B:837:SER:H	2	0.12	0.0	0.12
(2,324)	1:B:688:ILE:HG21	1:B:692:LEU:HG	2	0.12	0.0	0.12
(2,324)	1:B:688:ILE:HG22	1:B:692:LEU:HG	2	0.12	0.0	0.12
(2,324)	1:B:688:ILE:HG23	1:B:692:LEU:HG	2	0.12	0.0	0.12
(2,717)	1:A:681:TYR:H	1:A:682:ILE:H	2	0.11	0.0	0.11
(2,1142)	1:A:681:TYR:H	1:A:682:ILE:H	2	0.11	0.0	0.11

<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 9.5 All violated distance restraints [i](#)

### 9.5.1 Histogram : Distribution of distance violations [i](#)

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



### 9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,181)	1:B:806:GLU:H	1:A:772:ARG:HE	1	56.95
(2,181)	1:B:806:GLU:H	1:A:772:ARG:HE	4	56.86
(2,181)	1:B:806:GLU:H	1:A:772:ARG:HE	8	56.35
(2,181)	1:B:806:GLU:H	1:A:772:ARG:HE	15	56.0
(2,181)	1:B:806:GLU:H	1:A:772:ARG:HE	5	55.88
(2,181)	1:B:806:GLU:H	1:A:772:ARG:HE	10	55.73
(2,181)	1:B:806:GLU:H	1:A:772:ARG:HE	6	55.56
(2,181)	1:B:806:GLU:H	1:A:772:ARG:HE	12	55.54
(2,181)	1:B:806:GLU:H	1:A:772:ARG:HE	3	55.51
(2,181)	1:B:806:GLU:H	1:A:772:ARG:HE	13	55.28
(2,181)	1:B:806:GLU:H	1:A:772:ARG:HE	14	54.55
(2,181)	1:B:806:GLU:H	1:A:772:ARG:HE	7	54.51
(2,181)	1:B:806:GLU:H	1:A:772:ARG:HE	11	54.48
(2,181)	1:B:806:GLU:H	1:A:772:ARG:HE	2	54.31
(2,181)	1:B:806:GLU:H	1:A:772:ARG:HE	9	53.78
(2,178)	1:B:806:GLU:H	1:A:771:LEU:HG	3	52.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,182)	1:A:806:GLU:H	1:A:772:ARG:HE	1	52.01
(2,178)	1:B:806:GLU:H	1:A:771:LEU:HG	12	51.93
(2,182)	1:A:806:GLU:H	1:A:772:ARG:HE	5	51.89
(2,178)	1:B:806:GLU:H	1:A:771:LEU:HG	1	51.85
(2,178)	1:B:806:GLU:H	1:A:771:LEU:HG	13	51.72
(2,178)	1:B:806:GLU:H	1:A:771:LEU:HG	4	51.44
(2,178)	1:B:806:GLU:H	1:A:771:LEU:HG	8	51.4
(2,182)	1:A:806:GLU:H	1:A:772:ARG:HE	4	51.37
(2,178)	1:B:806:GLU:H	1:A:771:LEU:HG	2	51.28
(2,182)	1:A:806:GLU:H	1:A:772:ARG:HE	12	51.23
(2,182)	1:A:806:GLU:H	1:A:772:ARG:HE	3	51.01
(2,182)	1:A:806:GLU:H	1:A:772:ARG:HE	6	50.82
(2,182)	1:A:806:GLU:H	1:A:772:ARG:HE	15	50.73
(2,182)	1:A:806:GLU:H	1:A:772:ARG:HE	14	50.68
(2,178)	1:B:806:GLU:H	1:A:771:LEU:HG	14	50.41
(2,178)	1:B:806:GLU:H	1:A:771:LEU:HG	9	50.4
(2,178)	1:B:806:GLU:H	1:A:771:LEU:HG	15	50.36
(2,182)	1:A:806:GLU:H	1:A:772:ARG:HE	11	50.32
(2,178)	1:B:806:GLU:H	1:A:771:LEU:HG	6	50.29
(2,182)	1:A:806:GLU:H	1:A:772:ARG:HE	8	50.16
(2,178)	1:B:806:GLU:H	1:A:771:LEU:HG	5	50.07
(2,178)	1:B:806:GLU:H	1:A:771:LEU:HG	7	50.04
(2,178)	1:B:806:GLU:H	1:A:771:LEU:HG	10	50.0
(2,182)	1:A:806:GLU:H	1:A:772:ARG:HE	13	49.87
(2,182)	1:A:806:GLU:H	1:A:772:ARG:HE	10	49.81
(2,182)	1:A:806:GLU:H	1:A:772:ARG:HE	7	49.73
(2,182)	1:A:806:GLU:H	1:A:772:ARG:HE	2	49.41
(2,178)	1:B:806:GLU:H	1:A:771:LEU:HG	11	49.28
(2,179)	1:A:806:GLU:H	1:A:771:LEU:HG	1	49.11
(2,182)	1:A:806:GLU:H	1:A:772:ARG:HE	9	48.77
(2,179)	1:A:806:GLU:H	1:A:771:LEU:HG	4	48.35
(2,179)	1:A:806:GLU:H	1:A:771:LEU:HG	2	48.27
(2,179)	1:A:806:GLU:H	1:A:771:LEU:HG	14	48.24
(2,179)	1:A:806:GLU:H	1:A:771:LEU:HG	5	48.2
(2,179)	1:A:806:GLU:H	1:A:771:LEU:HG	3	47.82
(2,179)	1:A:806:GLU:H	1:A:771:LEU:HG	9	47.61
(2,179)	1:A:806:GLU:H	1:A:771:LEU:HG	12	47.6
(2,179)	1:A:806:GLU:H	1:A:771:LEU:HG	6	47.56
(2,179)	1:A:806:GLU:H	1:A:771:LEU:HG	15	47.47
(2,179)	1:A:806:GLU:H	1:A:771:LEU:HG	11	47.36
(2,179)	1:A:806:GLU:H	1:A:771:LEU:HG	10	47.35
(2,179)	1:A:806:GLU:H	1:A:771:LEU:HG	8	47.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,179)	1:A:806:GLU:H	1:A:771:LEU:HG	7	47.22
(2,179)	1:A:806:GLU:H	1:A:771:LEU:HG	13	46.85
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB2	8	45.51
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB3	8	45.51
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB2	3	44.99
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB3	3	44.99
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB2	14	44.82
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB3	14	44.82
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB2	1	44.78
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB3	1	44.78
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB2	2	44.52
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB3	2	44.52
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB2	12	44.48
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB3	12	44.48
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB2	4	44.39
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB3	4	44.39
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB2	13	44.38
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB3	13	44.38
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB2	6	44.35
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB3	6	44.35
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB2	7	44.14
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB3	7	44.14
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB2	9	44.05
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB3	9	44.05
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB2	15	44.02
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB3	15	44.02
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB2	10	43.72
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB3	10	43.72
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB2	5	43.52
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB3	5	43.52
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB2	11	42.99
(2,140)	1:A:771:LEU:H	1:B:806:GLU:HB3	11	42.99
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB2	14	42.7
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB3	14	42.7
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB2	1	42.29
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB3	1	42.29
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB2	12	42.15
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB3	12	42.15
(2,175)	1:B:803:TRP:HE1	1:A:764:SER:HG	2	41.98
(2,175)	1:B:803:TRP:HE1	1:A:764:SER:HG	13	41.97
(2,175)	1:B:803:TRP:HE1	1:A:764:SER:HG	8	41.96
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB2	8	41.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB3	8	41.95
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB2	2	41.89
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB3	2	41.89
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB2	4	41.83
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB3	4	41.83
(2,175)	1:B:803:TRP:HE1	1:A:764:SER:HG	12	41.64
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB2	5	41.58
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB3	5	41.58
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB2	3	41.55
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB3	3	41.55
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB2	9	41.53
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB3	9	41.53
(2,175)	1:B:803:TRP:HE1	1:A:764:SER:HG	3	41.38
(2,175)	1:B:803:TRP:HE1	1:A:764:SER:HG	9	41.25
(2,175)	1:B:803:TRP:HE1	1:A:764:SER:HG	14	41.15
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB2	10	41.15
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB3	10	41.15
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB2	6	41.1
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB3	6	41.1
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB2	7	41.09
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB3	7	41.09
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB2	13	40.91
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB3	13	40.91
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB2	15	40.84
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB3	15	40.84
(2,175)	1:B:803:TRP:HE1	1:A:764:SER:HG	4	40.8
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB2	11	40.79
(2,139)	1:A:771:LEU:H	1:A:806:GLU:HB3	11	40.79
(2,175)	1:B:803:TRP:HE1	1:A:764:SER:HG	6	40.59
(2,175)	1:B:803:TRP:HE1	1:A:764:SER:HG	7	40.51
(2,175)	1:B:803:TRP:HE1	1:A:764:SER:HG	1	40.5
(2,175)	1:B:803:TRP:HE1	1:A:764:SER:HG	10	40.41
(2,175)	1:B:803:TRP:HE1	1:A:764:SER:HG	5	40.34
(2,175)	1:B:803:TRP:HE1	1:A:764:SER:HG	15	39.42
(2,176)	1:A:803:TRP:HE1	1:A:764:SER:HG	7	39.33
(2,176)	1:A:803:TRP:HE1	1:A:764:SER:HG	14	39.0
(2,176)	1:A:803:TRP:HE1	1:A:764:SER:HG	9	38.98
(2,176)	1:A:803:TRP:HE1	1:A:764:SER:HG	8	38.36
(2,176)	1:A:803:TRP:HE1	1:A:764:SER:HG	1	38.01
(2,175)	1:B:803:TRP:HE1	1:A:764:SER:HG	11	37.96
(2,176)	1:A:803:TRP:HE1	1:A:764:SER:HG	3	37.93
(2,176)	1:A:803:TRP:HE1	1:A:764:SER:HG	12	37.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,176)	1:A:803:TRP:HE1	1:A:764:SER:HG	2	37.76
(2,176)	1:A:803:TRP:HE1	1:A:764:SER:HG	5	37.65
(2,176)	1:A:803:TRP:HE1	1:A:764:SER:HG	6	37.34
(2,176)	1:A:803:TRP:HE1	1:A:764:SER:HG	4	37.24
(2,176)	1:A:803:TRP:HE1	1:A:764:SER:HG	13	37.2
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB2	4	37.09
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB3	4	37.09
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB2	8	36.59
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB3	8	36.59
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB2	7	36.56
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB3	7	36.56
(2,176)	1:A:803:TRP:HE1	1:A:764:SER:HG	11	36.47
(2,176)	1:A:803:TRP:HE1	1:A:764:SER:HG	10	36.45
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB2	12	36.45
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB3	12	36.45
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB2	13	36.45
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB3	13	36.45
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB2	9	36.23
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB3	9	36.23
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB2	14	36.12
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB3	14	36.12
(2,176)	1:A:803:TRP:HE1	1:A:764:SER:HG	15	36.06
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB2	3	35.98
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB3	3	35.98
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB2	2	35.87
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB3	2	35.87
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB2	6	35.6
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB3	6	35.6
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB2	15	35.35
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB3	15	35.35
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB2	1	35.34
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB3	1	35.34
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB2	10	35.18
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB3	10	35.18
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB2	5	35.12
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB3	5	35.12
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB2	11	34.76
(2,172)	1:B:803:TRP:HE1	1:A:764:SER:HB3	11	34.76
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB2	7	34.36
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB3	7	34.36
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB2	14	33.55
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB3	14	33.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB2	9	33.51
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB3	9	33.51
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB2	1	33.09
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB3	1	33.09
(2,133)	1:A:756:ILE:H	1:A:796:TRP:HE1	14	32.85
(2,133)	1:A:756:ILE:H	1:A:796:TRP:HE1	11	32.72
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB2	4	32.64
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB3	4	32.64
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB2	8	32.58
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB3	8	32.58
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB2	3	32.46
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB3	3	32.46
(2,133)	1:A:756:ILE:H	1:A:796:TRP:HE1	12	32.46
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB2	6	32.43
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB3	6	32.43
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB2	12	32.35
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB3	12	32.35
(2,133)	1:A:756:ILE:H	1:A:796:TRP:HE1	6	32.31
(2,133)	1:A:756:ILE:H	1:A:796:TRP:HE1	2	32.2
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB2	5	32.13
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB3	5	32.13
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB2	2	32.08
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB3	2	32.08
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB2	11	32.08
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB3	11	32.08
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB2	13	31.83
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB3	13	31.83
(2,133)	1:A:756:ILE:H	1:A:796:TRP:HE1	1	31.82
(2,134)	1:A:756:ILE:H	1:B:796:TRP:HE1	9	31.8
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB2	10	31.69
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB3	10	31.69
(2,134)	1:A:756:ILE:H	1:B:796:TRP:HE1	4	31.67
(2,133)	1:A:756:ILE:H	1:A:796:TRP:HE1	9	31.64
(2,134)	1:A:756:ILE:H	1:B:796:TRP:HE1	5	31.61
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB2	8	31.53
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB3	8	31.53
(2,133)	1:A:756:ILE:H	1:A:796:TRP:HE1	4	31.53
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB2	10	31.48
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB3	10	31.48
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG12	10	31.45
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG13	10	31.45
(2,134)	1:A:756:ILE:H	1:B:796:TRP:HE1	3	31.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,134)	1:A:756:ILE:H	1:B:796:TRP:HE1	13	31.41
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG12	10	31.37
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG13	10	31.37
(2,134)	1:A:756:ILE:H	1:B:796:TRP:HE1	2	31.36
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG12	13	31.28
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG13	13	31.28
(2,133)	1:A:756:ILE:H	1:A:796:TRP:HE1	10	31.26
(2,133)	1:A:756:ILE:H	1:A:796:TRP:HE1	8	31.24
(2,133)	1:A:756:ILE:H	1:A:796:TRP:HE1	7	31.23
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG12	3	31.22
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG13	3	31.22
(2,133)	1:A:756:ILE:H	1:A:796:TRP:HE1	3	31.22
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB2	15	31.2
(2,173)	1:A:803:TRP:HE1	1:A:764:SER:HB3	15	31.2
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG12	11	31.19
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG13	11	31.19
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG12	11	31.19
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG13	11	31.19
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD2	5	31.17
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD3	5	31.17
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB2	11	31.14
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB3	11	31.14
(2,134)	1:A:756:ILE:H	1:B:796:TRP:HE1	12	31.14
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG12	13	31.05
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG13	13	31.05
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG12	8	31.01
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG13	8	31.01
(2,134)	1:A:756:ILE:H	1:B:796:TRP:HE1	7	31.01
(2,133)	1:A:756:ILE:H	1:A:796:TRP:HE1	15	30.99
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG12	8	30.98
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG13	8	30.98
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD2	14	30.97
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD3	14	30.97
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB2	5	30.95
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB3	5	30.95
(2,133)	1:A:756:ILE:H	1:A:796:TRP:HE1	5	30.92
(2,133)	1:A:756:ILE:H	1:A:796:TRP:HE1	13	30.92
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG12	1	30.91
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG13	1	30.91
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD2	9	30.91
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD3	9	30.91
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG12	1	30.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG13	1	30.89
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB2	9	30.88
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB3	9	30.88
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG12	3	30.86
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG13	3	30.86
(2,134)	1:A:756:ILE:H	1:B:796:TRP:HE1	10	30.86
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB2	2	30.85
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB3	2	30.85
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB2	14	30.85
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB3	14	30.85
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG12	2	30.82
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG13	2	30.82
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD2	2	30.82
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD3	2	30.82
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD2	15	30.79
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD3	15	30.79
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG12	14	30.75
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG13	14	30.75
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB2	9	30.71
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB3	9	30.71
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB2	4	30.7
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB3	4	30.7
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB2	12	30.66
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB3	12	30.66
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG12	14	30.66
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG13	14	30.66
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB2	6	30.6
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB3	6	30.6
(2,134)	1:A:756:ILE:H	1:B:796:TRP:HE1	14	30.55
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB2	12	30.54
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB3	12	30.54
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD2	3	30.54
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD3	3	30.54
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG12	2	30.46
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG13	2	30.46
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG12	15	30.45
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG13	15	30.45
(2,134)	1:A:756:ILE:H	1:B:796:TRP:HE1	1	30.44
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD2	12	30.42
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD3	12	30.42
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG12	15	30.37
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG13	15	30.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD2	6	30.35
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD3	6	30.35
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG12	12	30.33
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG13	12	30.33
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD2	1	30.33
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD3	1	30.33
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG12	9	30.32
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG13	9	30.32
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD2	13	30.32
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD3	13	30.32
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG12	4	30.28
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG13	4	30.28
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG12	5	30.28
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG13	5	30.28
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG21	8	30.28
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG22	8	30.28
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG23	8	30.28
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG21	13	30.27
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG22	13	30.27
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG23	13	30.27
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG12	6	30.24
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG13	6	30.24
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG21	15	30.23
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG22	15	30.23
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG23	15	30.23
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG12	12	30.22
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG13	12	30.22
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG21	7	30.22
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG22	7	30.22
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG23	7	30.22
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG12	4	30.21
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG13	4	30.21
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG12	6	30.21
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG13	6	30.21
(2,134)	1:A:756:ILE:H	1:B:796:TRP:HE1	15	30.17
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB2	3	30.15
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB3	3	30.15
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG21	3	30.15
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG22	3	30.15
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG23	3	30.15
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB2	13	30.12
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB3	13	30.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB2	6	30.09
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB3	6	30.09
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG12	9	30.09
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG13	9	30.09
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG12	7	30.06
(2,146)	1:A:782:VAL:H	1:A:746:ILE:HG13	7	30.06
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB2	7	30.04
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB3	7	30.04
(2,134)	1:A:756:ILE:H	1:B:796:TRP:HE1	6	30.04
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG21	6	30.04
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG22	6	30.04
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG23	6	30.04
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB2	5	30.01
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB3	5	30.01
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB2	13	29.96
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB3	13	29.96
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB2	1	29.93
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB3	1	29.93
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG12	5	29.92
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG13	5	29.92
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD2	2	29.91
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD3	2	29.91
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD2	8	29.89
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD3	8	29.89
(2,134)	1:A:756:ILE:H	1:B:796:TRP:HE1	8	29.88
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD2	4	29.87
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD3	4	29.87
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG12	8	29.85
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG13	8	29.85
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG12	7	29.84
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG13	7	29.84
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG12	15	29.84
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG13	15	29.84
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD2	11	29.84
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD3	11	29.84
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG21	10	29.84
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG22	10	29.84
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG23	10	29.84
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG12	13	29.83
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG13	13	29.83
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB2	7	29.82
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB3	7	29.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB2	2	29.8
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB3	2	29.8
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB2	4	29.8
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB3	4	29.8
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG12	7	29.78
(2,143)	1:A:781:ILE:H	1:A:746:ILE:HG13	7	29.78
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD2	7	29.78
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD3	7	29.78
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB2	15	29.75
(2,152)	1:A:792:ALA:H	1:A:752:SER:HB3	15	29.75
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB2	3	29.75
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB3	3	29.75
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB2	2	29.73
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB3	2	29.73
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG12	3	29.69
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG13	3	29.69
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB2	5	29.68
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB3	5	29.68
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD2	11	29.67
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD3	11	29.67
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB2	1	29.65
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB3	1	29.65
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB2	14	29.64
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB3	14	29.64
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD2	10	29.6
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD3	10	29.6
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD2	4	29.58
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD3	4	29.58
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG21	12	29.55
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG22	12	29.55
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG23	12	29.55
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG21	5	29.49
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG22	5	29.49
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG23	5	29.49
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG12	4	29.46
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG13	4	29.46
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB2	9	29.43
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB3	9	29.43
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB2	15	29.42
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB3	15	29.42
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD2	10	29.39
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD3	10	29.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG21	2	29.35
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG22	2	29.35
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG23	2	29.35
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG12	10	29.34
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG13	10	29.34
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB2	14	29.34
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB3	14	29.34
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD2	8	29.33
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD3	8	29.33
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB2	11	29.32
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB3	11	29.32
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG12	6	29.32
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG13	6	29.32
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG21	10	29.3
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG22	10	29.3
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG23	10	29.3
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB2	12	29.28
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB3	12	29.28
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG12	11	29.26
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG13	11	29.26
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD2	7	29.26
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD3	7	29.26
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD2	7	29.26
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD3	7	29.26
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB2	10	29.25
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB3	10	29.25
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG21	1	29.25
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG22	1	29.25
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG23	1	29.25
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB2	4	29.24
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB3	4	29.24
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB2	12	29.23
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB3	12	29.23
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD2	11	29.21
(2,137)	1:A:756:ILE:H	1:B:794:LYS:HD3	11	29.21
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD2	12	29.21
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD3	12	29.21
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG21	11	29.21
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG22	11	29.21
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG23	11	29.21
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG12	5	29.2
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG13	5	29.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB2	2	29.18
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB3	2	29.18
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG21	14	29.17
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG22	14	29.17
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG23	14	29.17
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG21	8	29.08
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG22	8	29.08
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG23	8	29.08
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD2	9	29.04
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD3	9	29.04
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB2	1	29.04
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB3	1	29.04
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG21	9	29.03
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG22	9	29.03
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG23	9	29.03
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB2	15	29.02
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB3	15	29.02
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG21	13	29.0
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG22	13	29.0
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG23	13	29.0
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG21	4	29.0
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG22	4	29.0
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG23	4	29.0
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD2	14	28.98
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD3	14	28.98
(2,134)	1:A:756:ILE:H	1:B:796:TRP:HE1	11	28.98
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD1	14	28.97
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD2	14	28.97
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB2	6	28.96
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB3	6	28.96
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD2	4	28.95
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD3	4	28.95
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD2	9	28.91
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD3	9	28.91
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB2	11	28.9
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB3	11	28.9
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB2	1	28.87
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB3	1	28.87
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG21	3	28.87
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG22	3	28.87
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG23	3	28.87
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG12	9	28.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG13	9	28.85
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB2	6	28.85
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB3	6	28.85
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB2	13	28.85
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB3	13	28.85
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG21	11	28.85
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG22	11	28.85
(2,109)	1:B:781:ILE:H	1:A:746:ILE:HG23	11	28.85
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG12	2	28.84
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG13	2	28.84
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG21	1	28.83
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG22	1	28.83
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG23	1	28.83
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG12	12	28.82
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG13	12	28.82
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB2	3	28.81
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB3	3	28.81
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB2	8	28.8
(2,151)	1:B:792:ALA:H	1:A:752:SER:HB3	8	28.8
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD2	13	28.8
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD3	13	28.8
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD2	1	28.79
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD3	1	28.79
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD1	5	28.78
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD2	5	28.78
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD2	13	28.77
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD3	13	28.77
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB2	4	28.76
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB3	4	28.76
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD1	2	28.75
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD2	2	28.75
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG12	14	28.73
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG13	14	28.73
(2,113)	1:A:781:ILE:HD11	1:A:743:ASP:HA	10	28.72
(2,113)	1:A:781:ILE:HD12	1:A:743:ASP:HA	10	28.72
(2,113)	1:A:781:ILE:HD13	1:A:743:ASP:HA	10	28.72
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD2	15	28.72
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD3	15	28.72
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD2	5	28.71
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD3	5	28.71
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG21	14	28.68
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG22	14	28.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG23	14	28.68
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG12	1	28.63
(2,144)	1:B:781:ILE:H	1:A:746:ILE:HG13	1	28.63
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD1	2	28.61
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD2	2	28.61
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD2	14	28.58
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD3	14	28.58
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD2	15	28.55
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD3	15	28.55
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD2	3	28.53
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD3	3	28.53
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG21	2	28.53
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG22	2	28.53
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG23	2	28.53
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD1	1	28.51
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD2	1	28.51
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD2	1	28.47
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD3	1	28.47
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD1	3	28.47
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD2	3	28.47
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG12	7	28.46
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG13	7	28.46
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD1	15	28.46
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD2	15	28.46
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG21	12	28.46
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG22	12	28.46
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG23	12	28.46
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD2	12	28.46
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD3	12	28.46
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB2	3	28.41
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB3	3	28.41
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG21	15	28.41
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG22	15	28.41
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG23	15	28.41
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD2	2	28.4
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD3	2	28.4
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD1	9	28.39
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD2	9	28.39
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD2	8	28.36
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD3	8	28.36
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG12	3	28.35
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG13	3	28.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD1	12	28.35
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD2	12	28.35
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB2	7	28.35
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB3	7	28.35
(2,125)	1:A:785:LEU:HD21	1:A:749:VAL:HB	8	28.34
(2,125)	1:A:785:LEU:HD22	1:A:749:VAL:HB	8	28.34
(2,125)	1:A:785:LEU:HD23	1:A:749:VAL:HB	8	28.34
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD1	12	28.33
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD2	12	28.33
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG12	4	28.32
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG13	4	28.32
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG21	6	28.31
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG22	6	28.31
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG23	6	28.31
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB2	8	28.28
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB3	8	28.28
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG12	15	28.27
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG13	15	28.27
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD2	6	28.27
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD3	6	28.27
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD1	11	28.25
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD2	11	28.25
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG21	9	28.24
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG22	9	28.24
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG23	9	28.24
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD2	3	28.24
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD3	3	28.24
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD2	6	28.23
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD3	6	28.23
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG12	8	28.2
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG13	8	28.2
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB2	10	28.19
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB3	10	28.19
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD1	1	28.18
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD2	1	28.18
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD1	6	28.18
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD2	6	28.18
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG21	7	28.17
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG22	7	28.17
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG23	7	28.17
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG12	5	28.13
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG13	5	28.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB2	14	28.13
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB3	14	28.13
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD1	13	28.12
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD2	13	28.12
(2,125)	1:A:785:LEU:HD21	1:A:749:VAL:HB	14	28.11
(2,125)	1:A:785:LEU:HD22	1:A:749:VAL:HB	14	28.11
(2,125)	1:A:785:LEU:HD23	1:A:749:VAL:HB	14	28.11
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG12	6	28.1
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG13	6	28.1
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG12	13	28.0
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG13	13	28.0
(2,113)	1:A:781:ILE:HD11	1:A:743:ASP:HA	15	28.0
(2,113)	1:A:781:ILE:HD12	1:A:743:ASP:HA	15	28.0
(2,113)	1:A:781:ILE:HD13	1:A:743:ASP:HA	15	28.0
(2,113)	1:A:781:ILE:HD11	1:A:743:ASP:HA	6	27.99
(2,113)	1:A:781:ILE:HD12	1:A:743:ASP:HA	6	27.99
(2,113)	1:A:781:ILE:HD13	1:A:743:ASP:HA	6	27.99
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG21	4	27.99
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG22	4	27.99
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG23	4	27.99
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD2	10	27.93
(2,136)	1:A:756:ILE:H	1:A:794:LYS:HD3	10	27.93
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD2	5	27.87
(2,103)	1:B:763:LEU:H	1:A:742:ARG:HD3	5	27.87
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD1	14	27.84
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD2	14	27.84
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG21	5	27.83
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG22	5	27.83
(2,110)	1:A:781:ILE:H	1:A:746:ILE:HG23	5	27.83
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB2	7	27.8
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB3	7	27.8
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD1	6	27.79
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD2	6	27.79
(2,125)	1:A:785:LEU:HD21	1:A:749:VAL:HB	11	27.79
(2,125)	1:A:785:LEU:HD22	1:A:749:VAL:HB	11	27.79
(2,125)	1:A:785:LEU:HD23	1:A:749:VAL:HB	11	27.79
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG12	10	27.76
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG13	10	27.76
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB2	9	27.76
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB3	9	27.76
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD1	3	27.74
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD2	3	27.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG12	11	27.73
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG13	11	27.73
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD1	11	27.73
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD2	11	27.73
(2,113)	1:A:781:ILE:HD11	1:A:743:ASP:HA	4	27.73
(2,113)	1:A:781:ILE:HD12	1:A:743:ASP:HA	4	27.73
(2,113)	1:A:781:ILE:HD13	1:A:743:ASP:HA	4	27.73
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD1	4	27.72
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD2	4	27.72
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB2	8	27.71
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB3	8	27.71
(2,113)	1:A:781:ILE:HD11	1:A:743:ASP:HA	2	27.69
(2,113)	1:A:781:ILE:HD12	1:A:743:ASP:HA	2	27.69
(2,113)	1:A:781:ILE:HD13	1:A:743:ASP:HA	2	27.69
(2,113)	1:A:781:ILE:HD11	1:A:743:ASP:HA	8	27.69
(2,113)	1:A:781:ILE:HD12	1:A:743:ASP:HA	8	27.69
(2,113)	1:A:781:ILE:HD13	1:A:743:ASP:HA	8	27.69
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG12	9	27.65
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG13	9	27.65
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB2	5	27.62
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB3	5	27.62
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD1	4	27.61
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD2	4	27.61
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD1	8	27.6
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD2	8	27.6
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB2	11	27.59
(2,128)	1:A:756:ILE:H	1:B:795:TYR:HB3	11	27.59
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG12	2	27.55
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG13	2	27.55
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG12	1	27.53
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG13	1	27.53
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD1	7	27.51
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD2	7	27.51
(2,125)	1:A:785:LEU:HD21	1:A:749:VAL:HB	12	27.42
(2,125)	1:A:785:LEU:HD22	1:A:749:VAL:HB	12	27.42
(2,125)	1:A:785:LEU:HD23	1:A:749:VAL:HB	12	27.42
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG12	12	27.38
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG13	12	27.38
(2,125)	1:A:785:LEU:HD21	1:A:749:VAL:HB	10	27.38
(2,125)	1:A:785:LEU:HD22	1:A:749:VAL:HB	10	27.38
(2,125)	1:A:785:LEU:HD23	1:A:749:VAL:HB	10	27.38
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB2	15	27.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB3	15	27.26
(2,113)	1:A:781:ILE:HD11	1:A:743:ASP:HA	13	27.24
(2,113)	1:A:781:ILE:HD12	1:A:743:ASP:HA	13	27.24
(2,113)	1:A:781:ILE:HD13	1:A:743:ASP:HA	13	27.24
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB2	10	27.22
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB3	10	27.22
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB2	13	27.19
(2,127)	1:A:756:ILE:H	1:A:795:TYR:HB3	13	27.19
(2,125)	1:A:785:LEU:HD21	1:A:749:VAL:HB	6	27.16
(2,125)	1:A:785:LEU:HD22	1:A:749:VAL:HB	6	27.16
(2,125)	1:A:785:LEU:HD23	1:A:749:VAL:HB	6	27.16
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD1	9	27.14
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD2	9	27.14
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG12	14	27.12
(2,145)	1:B:782:VAL:H	1:A:746:ILE:HG13	14	27.12
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD1	8	27.07
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD2	8	27.07
(2,113)	1:A:781:ILE:HD11	1:A:743:ASP:HA	3	27.04
(2,113)	1:A:781:ILE:HD12	1:A:743:ASP:HA	3	27.04
(2,113)	1:A:781:ILE:HD13	1:A:743:ASP:HA	3	27.04
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD1	7	26.99
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD2	7	26.99
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD1	5	26.87
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD2	5	26.87
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD1	10	26.86
(2,131)	1:A:756:ILE:H	1:B:795:TYR:HD2	10	26.86
(2,125)	1:A:785:LEU:HD21	1:A:749:VAL:HB	9	26.78
(2,125)	1:A:785:LEU:HD22	1:A:749:VAL:HB	9	26.78
(2,125)	1:A:785:LEU:HD23	1:A:749:VAL:HB	9	26.78
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD1	10	26.74
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD2	10	26.74
(2,125)	1:A:785:LEU:HD21	1:A:749:VAL:HB	15	26.72
(2,125)	1:A:785:LEU:HD22	1:A:749:VAL:HB	15	26.72
(2,125)	1:A:785:LEU:HD23	1:A:749:VAL:HB	15	26.72
(2,124)	1:B:785:LEU:HD21	1:A:749:VAL:HB	15	26.71
(2,124)	1:B:785:LEU:HD22	1:A:749:VAL:HB	15	26.71
(2,124)	1:B:785:LEU:HD23	1:A:749:VAL:HB	15	26.71
(2,113)	1:A:781:ILE:HD11	1:A:743:ASP:HA	14	26.7
(2,113)	1:A:781:ILE:HD12	1:A:743:ASP:HA	14	26.7
(2,113)	1:A:781:ILE:HD13	1:A:743:ASP:HA	14	26.7
(2,113)	1:A:781:ILE:HD11	1:A:743:ASP:HA	9	26.65
(2,113)	1:A:781:ILE:HD12	1:A:743:ASP:HA	9	26.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,113)	1:A:781:ILE:HD13	1:A:743:ASP:HA	9	26.65
(2,113)	1:A:781:ILE:HD11	1:A:743:ASP:HA	12	26.65
(2,113)	1:A:781:ILE:HD12	1:A:743:ASP:HA	12	26.65
(2,113)	1:A:781:ILE:HD13	1:A:743:ASP:HA	12	26.65
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD1	15	26.59
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD2	15	26.59
(2,124)	1:B:785:LEU:HD21	1:A:749:VAL:HB	7	26.59
(2,124)	1:B:785:LEU:HD22	1:A:749:VAL:HB	7	26.59
(2,124)	1:B:785:LEU:HD23	1:A:749:VAL:HB	7	26.59
(2,112)	1:B:781:ILE:HD11	1:A:743:ASP:HA	7	26.58
(2,112)	1:B:781:ILE:HD12	1:A:743:ASP:HA	7	26.58
(2,112)	1:B:781:ILE:HD13	1:A:743:ASP:HA	7	26.58
(2,113)	1:A:781:ILE:HD11	1:A:743:ASP:HA	11	26.56
(2,113)	1:A:781:ILE:HD12	1:A:743:ASP:HA	11	26.56
(2,113)	1:A:781:ILE:HD13	1:A:743:ASP:HA	11	26.56
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD1	13	26.48
(2,130)	1:A:756:ILE:H	1:A:795:TYR:HD2	13	26.48
(2,112)	1:B:781:ILE:HD11	1:A:743:ASP:HA	10	26.43
(2,112)	1:B:781:ILE:HD12	1:A:743:ASP:HA	10	26.43
(2,112)	1:B:781:ILE:HD13	1:A:743:ASP:HA	10	26.43
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD11	11	26.4
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD12	11	26.4
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD13	11	26.4
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD21	11	26.4
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD22	11	26.4
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD23	11	26.4
(2,113)	1:A:781:ILE:HD11	1:A:743:ASP:HA	1	26.38
(2,113)	1:A:781:ILE:HD12	1:A:743:ASP:HA	1	26.38
(2,113)	1:A:781:ILE:HD13	1:A:743:ASP:HA	1	26.38
(2,112)	1:B:781:ILE:HD11	1:A:743:ASP:HA	2	26.33
(2,112)	1:B:781:ILE:HD12	1:A:743:ASP:HA	2	26.33
(2,112)	1:B:781:ILE:HD13	1:A:743:ASP:HA	2	26.33
(2,124)	1:B:785:LEU:HD21	1:A:749:VAL:HB	13	26.23
(2,124)	1:B:785:LEU:HD22	1:A:749:VAL:HB	13	26.23
(2,124)	1:B:785:LEU:HD23	1:A:749:VAL:HB	13	26.23
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD11	8	26.21
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD12	8	26.21
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD13	8	26.21
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD21	8	26.21
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD22	8	26.21
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD23	8	26.21
(2,124)	1:B:785:LEU:HD21	1:A:749:VAL:HB	3	26.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,124)	1:B:785:LEU:HD22	1:A:749:VAL:HB	3	26.09
(2,124)	1:B:785:LEU:HD23	1:A:749:VAL:HB	3	26.09
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD2	8	26.07
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD3	8	26.07
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD2	8	26.07
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD3	8	26.07
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD2	8	26.07
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD3	8	26.07
(2,124)	1:B:785:LEU:HD21	1:A:749:VAL:HB	14	26.06
(2,124)	1:B:785:LEU:HD22	1:A:749:VAL:HB	14	26.06
(2,124)	1:B:785:LEU:HD23	1:A:749:VAL:HB	14	26.06
(2,125)	1:A:785:LEU:HD21	1:A:749:VAL:HB	2	26.02
(2,125)	1:A:785:LEU:HD22	1:A:749:VAL:HB	2	26.02
(2,125)	1:A:785:LEU:HD23	1:A:749:VAL:HB	2	26.02
(2,113)	1:A:781:ILE:HD11	1:A:743:ASP:HA	5	25.99
(2,113)	1:A:781:ILE:HD12	1:A:743:ASP:HA	5	25.99
(2,113)	1:A:781:ILE:HD13	1:A:743:ASP:HA	5	25.99
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD11	10	25.98
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD12	10	25.98
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD13	10	25.98
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD21	10	25.98
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD22	10	25.98
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD23	10	25.98
(2,124)	1:B:785:LEU:HD21	1:A:749:VAL:HB	12	25.93
(2,124)	1:B:785:LEU:HD22	1:A:749:VAL:HB	12	25.93
(2,124)	1:B:785:LEU:HD23	1:A:749:VAL:HB	12	25.93
(2,112)	1:B:781:ILE:HD11	1:A:743:ASP:HA	5	25.93
(2,112)	1:B:781:ILE:HD12	1:A:743:ASP:HA	5	25.93
(2,112)	1:B:781:ILE:HD13	1:A:743:ASP:HA	5	25.93
(2,124)	1:B:785:LEU:HD21	1:A:749:VAL:HB	5	25.89
(2,124)	1:B:785:LEU:HD22	1:A:749:VAL:HB	5	25.89
(2,124)	1:B:785:LEU:HD23	1:A:749:VAL:HB	5	25.89
(2,125)	1:A:785:LEU:HD21	1:A:749:VAL:HB	3	25.79
(2,125)	1:A:785:LEU:HD22	1:A:749:VAL:HB	3	25.79
(2,125)	1:A:785:LEU:HD23	1:A:749:VAL:HB	3	25.79
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD2	3	25.77
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD3	3	25.77
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD2	3	25.77
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD3	3	25.77
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD2	3	25.77
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD3	3	25.77
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD2	10	25.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD3	10	25.71
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD2	10	25.71
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD3	10	25.71
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD2	10	25.71
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD3	10	25.71
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD11	13	25.7
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD12	13	25.7
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD13	13	25.7
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD21	13	25.7
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD22	13	25.7
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD23	13	25.7
(2,125)	1:A:785:LEU:HD21	1:A:749:VAL:HB	1	25.69
(2,125)	1:A:785:LEU:HD22	1:A:749:VAL:HB	1	25.69
(2,125)	1:A:785:LEU:HD23	1:A:749:VAL:HB	1	25.69
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD2	4	25.68
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD3	4	25.68
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD11	15	25.66
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD12	15	25.66
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD13	15	25.66
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD21	15	25.66
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD22	15	25.66
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD23	15	25.66
(2,125)	1:A:785:LEU:HD21	1:A:749:VAL:HB	13	25.66
(2,125)	1:A:785:LEU:HD22	1:A:749:VAL:HB	13	25.66
(2,125)	1:A:785:LEU:HD23	1:A:749:VAL:HB	13	25.66
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD2	1	25.65
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD3	1	25.65
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD2	1	25.65
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD3	1	25.65
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD2	1	25.65
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD3	1	25.65
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD2	7	25.65
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD3	7	25.65
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD2	7	25.65
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD3	7	25.65
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD2	7	25.65
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD3	7	25.65
(2,124)	1:B:785:LEU:HD21	1:A:749:VAL:HB	8	25.62
(2,124)	1:B:785:LEU:HD22	1:A:749:VAL:HB	8	25.62
(2,124)	1:B:785:LEU:HD23	1:A:749:VAL:HB	8	25.62
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD2	4	25.58
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD3	4	25.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD2	4	25.58
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD3	4	25.58
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD2	4	25.58
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD3	4	25.58
(2,124)	1:B:785:LEU:HD21	1:A:749:VAL:HB	9	25.57
(2,124)	1:B:785:LEU:HD22	1:A:749:VAL:HB	9	25.57
(2,124)	1:B:785:LEU:HD23	1:A:749:VAL:HB	9	25.57
(2,112)	1:B:781:ILE:HD11	1:A:743:ASP:HA	1	25.57
(2,112)	1:B:781:ILE:HD12	1:A:743:ASP:HA	1	25.57
(2,112)	1:B:781:ILE:HD13	1:A:743:ASP:HA	1	25.57
(2,112)	1:B:781:ILE:HD11	1:A:743:ASP:HA	15	25.55
(2,112)	1:B:781:ILE:HD12	1:A:743:ASP:HA	15	25.55
(2,112)	1:B:781:ILE:HD13	1:A:743:ASP:HA	15	25.55
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD2	11	25.53
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD3	11	25.53
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD2	11	25.53
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD3	11	25.53
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD2	11	25.53
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD3	11	25.53
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD11	9	25.52
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD12	9	25.52
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD13	9	25.52
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD21	9	25.52
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD22	9	25.52
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD23	9	25.52
(2,112)	1:B:781:ILE:HD11	1:A:743:ASP:HA	11	25.51
(2,112)	1:B:781:ILE:HD12	1:A:743:ASP:HA	11	25.51
(2,112)	1:B:781:ILE:HD13	1:A:743:ASP:HA	11	25.51
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD11	12	25.49
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD12	12	25.49
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD13	12	25.49
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD21	12	25.49
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD22	12	25.49
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD23	12	25.49
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD2	6	25.49
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD3	6	25.49
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD2	6	25.49
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD3	6	25.49
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD2	6	25.49
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD3	6	25.49
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD11	2	25.47
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD12	2	25.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD13	2	25.47
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD21	2	25.47
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD22	2	25.47
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD23	2	25.47
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD11	5	25.46
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD12	5	25.46
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD13	5	25.46
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD21	5	25.46
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD22	5	25.46
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD23	5	25.46
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD2	12	25.42
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD3	12	25.42
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD2	12	25.42
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD3	12	25.42
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD2	12	25.42
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD3	12	25.42
(2,113)	1:A:781:ILE:HD11	1:A:743:ASP:HA	7	25.38
(2,113)	1:A:781:ILE:HD12	1:A:743:ASP:HA	7	25.38
(2,113)	1:A:781:ILE:HD13	1:A:743:ASP:HA	7	25.38
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD2	13	25.34
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD3	13	25.34
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD2	13	25.34
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD3	13	25.34
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD2	13	25.34
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD3	13	25.34
(2,125)	1:A:785:LEU:HD21	1:A:749:VAL:HB	7	25.32
(2,125)	1:A:785:LEU:HD22	1:A:749:VAL:HB	7	25.32
(2,125)	1:A:785:LEU:HD23	1:A:749:VAL:HB	7	25.32
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG12	10	25.31
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG13	10	25.31
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG12	10	25.31
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG13	10	25.31
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG12	10	25.31
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG13	10	25.31
(2,125)	1:A:785:LEU:HD21	1:A:749:VAL:HB	5	25.3
(2,125)	1:A:785:LEU:HD22	1:A:749:VAL:HB	5	25.3
(2,125)	1:A:785:LEU:HD23	1:A:749:VAL:HB	5	25.3
(2,112)	1:B:781:ILE:HD11	1:A:743:ASP:HA	14	25.3
(2,112)	1:B:781:ILE:HD12	1:A:743:ASP:HA	14	25.3
(2,112)	1:B:781:ILE:HD13	1:A:743:ASP:HA	14	25.3
(2,112)	1:B:781:ILE:HD11	1:A:743:ASP:HA	8	25.29
(2,112)	1:B:781:ILE:HD12	1:A:743:ASP:HA	8	25.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,112)	1:B:781:ILE:HD13	1:A:743:ASP:HA	8	25.29
(2,125)	1:A:785:LEU:HD21	1:A:749:VAL:HB	4	25.26
(2,125)	1:A:785:LEU:HD22	1:A:749:VAL:HB	4	25.26
(2,125)	1:A:785:LEU:HD23	1:A:749:VAL:HB	4	25.26
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD11	9	25.15
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD12	9	25.15
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD13	9	25.15
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD21	9	25.15
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD22	9	25.15
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD23	9	25.15
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD11	6	25.13
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD12	6	25.13
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD13	6	25.13
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD21	6	25.13
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD22	6	25.13
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD23	6	25.13
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD21	4	25.01
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD22	4	25.01
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD23	4	25.01
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD2	9	25.01
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD3	9	25.01
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD2	9	25.01
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD3	9	25.01
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD2	9	25.01
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD3	9	25.01
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD11	7	24.99
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD12	7	24.99
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD13	7	24.99
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD21	7	24.99
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD22	7	24.99
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD23	7	24.99
(2,124)	1:B:785:LEU:HD21	1:A:749:VAL:HB	6	24.99
(2,124)	1:B:785:LEU:HD22	1:A:749:VAL:HB	6	24.99
(2,124)	1:B:785:LEU:HD23	1:A:749:VAL:HB	6	24.99
(2,124)	1:B:785:LEU:HD21	1:A:749:VAL:HB	11	24.97
(2,124)	1:B:785:LEU:HD22	1:A:749:VAL:HB	11	24.97
(2,124)	1:B:785:LEU:HD23	1:A:749:VAL:HB	11	24.97
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD11	3	24.93
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD12	3	24.93
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD13	3	24.93
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD21	3	24.93
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD22	3	24.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD23	3	24.93
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD21	9	24.92
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD22	9	24.92
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD23	9	24.92
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD11	3	24.92
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD12	3	24.92
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD13	3	24.92
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD21	3	24.92
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD22	3	24.92
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD23	3	24.92
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD11	5	24.89
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD12	5	24.89
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD13	5	24.89
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD21	5	24.89
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD22	5	24.89
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD23	5	24.89
(2,124)	1:B:785:LEU:HD21	1:A:749:VAL:HB	10	24.89
(2,124)	1:B:785:LEU:HD22	1:A:749:VAL:HB	10	24.89
(2,124)	1:B:785:LEU:HD23	1:A:749:VAL:HB	10	24.89
(2,112)	1:B:781:ILE:HD11	1:A:743:ASP:HA	9	24.89
(2,112)	1:B:781:ILE:HD12	1:A:743:ASP:HA	9	24.89
(2,112)	1:B:781:ILE:HD13	1:A:743:ASP:HA	9	24.89
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD2	8	24.89
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD3	8	24.89
(2,112)	1:B:781:ILE:HD11	1:A:743:ASP:HA	4	24.87
(2,112)	1:B:781:ILE:HD12	1:A:743:ASP:HA	4	24.87
(2,112)	1:B:781:ILE:HD13	1:A:743:ASP:HA	4	24.87
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD11	4	24.82
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD12	4	24.82
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD13	4	24.82
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD21	4	24.82
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD22	4	24.82
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD23	4	24.82
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD11	11	24.78
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD12	11	24.78
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD13	11	24.78
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD21	11	24.78
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD22	11	24.78
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD23	11	24.78
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD2	14	24.74
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD3	14	24.74
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD2	14	24.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD3	14	24.74
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD2	14	24.74
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD3	14	24.74
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD11	2	24.71
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD12	2	24.71
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD13	2	24.71
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD21	2	24.71
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD22	2	24.71
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD23	2	24.71
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD21	13	24.7
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD22	13	24.7
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD23	13	24.7
(2,124)	1:B:785:LEU:HD21	1:A:749:VAL:HB	1	24.67
(2,124)	1:B:785:LEU:HD22	1:A:749:VAL:HB	1	24.67
(2,124)	1:B:785:LEU:HD23	1:A:749:VAL:HB	1	24.67
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD11	14	24.65
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD12	14	24.65
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD13	14	24.65
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD21	14	24.65
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD22	14	24.65
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD23	14	24.65
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG12	6	24.64
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG13	6	24.64
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG12	6	24.64
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG13	6	24.64
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG12	6	24.64
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG13	6	24.64
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD2	1	24.64
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD3	1	24.64
(2,112)	1:B:781:ILE:HD11	1:A:743:ASP:HA	13	24.62
(2,112)	1:B:781:ILE:HD12	1:A:743:ASP:HA	13	24.62
(2,112)	1:B:781:ILE:HD13	1:A:743:ASP:HA	13	24.62
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD2	15	24.53
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD3	15	24.53
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD2	15	24.53
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD3	15	24.53
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD2	15	24.53
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD3	15	24.53
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD11	8	24.51
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD12	8	24.51
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD13	8	24.51
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD21	8	24.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD22	8	24.51
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD23	8	24.51
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD21	14	24.49
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD22	14	24.49
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD23	14	24.49
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD2	10	24.49
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD3	10	24.49
(2,124)	1:B:785:LEU:HD21	1:A:749:VAL:HB	2	24.46
(2,124)	1:B:785:LEU:HD22	1:A:749:VAL:HB	2	24.46
(2,124)	1:B:785:LEU:HD23	1:A:749:VAL:HB	2	24.46
(2,112)	1:B:781:ILE:HD11	1:A:743:ASP:HA	6	24.46
(2,112)	1:B:781:ILE:HD12	1:A:743:ASP:HA	6	24.46
(2,112)	1:B:781:ILE:HD13	1:A:743:ASP:HA	6	24.46
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD2	9	24.46
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD3	9	24.46
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD11	6	24.45
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD12	6	24.45
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD13	6	24.45
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD21	6	24.45
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD22	6	24.45
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD23	6	24.45
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD2	13	24.45
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD3	13	24.45
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG12	2	24.44
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG13	2	24.44
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG12	2	24.44
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG13	2	24.44
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG12	2	24.44
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG13	2	24.44
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD2	5	24.43
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD3	5	24.43
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD2	5	24.43
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD3	5	24.43
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD2	5	24.43
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD3	5	24.43
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD11	13	24.41
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD12	13	24.41
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD13	13	24.41
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD21	13	24.41
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD22	13	24.41
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD23	13	24.41
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD11	12	24.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD12	12	24.39
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD13	12	24.39
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD21	12	24.39
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD22	12	24.39
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD23	12	24.39
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD2	7	24.39
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD3	7	24.39
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD11	15	24.36
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD12	15	24.36
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD13	15	24.36
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD21	15	24.36
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD22	15	24.36
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD23	15	24.36
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD11	14	24.36
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD12	14	24.36
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD13	14	24.36
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD21	14	24.36
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD22	14	24.36
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD23	14	24.36
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD21	1	24.33
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD22	1	24.33
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD23	1	24.33
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD21	7	24.32
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD22	7	24.32
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD23	7	24.32
(2,112)	1:B:781:ILE:HD11	1:A:743:ASP:HA	3	24.32
(2,112)	1:B:781:ILE:HD12	1:A:743:ASP:HA	3	24.32
(2,112)	1:B:781:ILE:HD13	1:A:743:ASP:HA	3	24.32
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB2	11	24.31
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB3	11	24.31
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD11	1	24.26
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD12	1	24.26
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD13	1	24.26
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD21	1	24.26
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD22	1	24.26
(2,155)	1:A:792:ALA:H	1:A:753:LEU:HD23	1	24.26
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD2	12	24.23
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD3	12	24.23
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD11	7	24.21
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD12	7	24.21
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD13	7	24.21
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD21	7	24.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD22	7	24.21
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD23	7	24.21
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD2	3	24.21
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD3	3	24.21
(2,124)	1:B:785:LEU:HD21	1:A:749:VAL:HB	4	24.19
(2,124)	1:B:785:LEU:HD22	1:A:749:VAL:HB	4	24.19
(2,124)	1:B:785:LEU:HD23	1:A:749:VAL:HB	4	24.19
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD11	1	24.18
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD12	1	24.18
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD13	1	24.18
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD21	1	24.18
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD22	1	24.18
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD23	1	24.18
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD2	14	24.1
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD3	14	24.1
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG12	4	24.08
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG13	4	24.08
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG12	4	24.08
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG13	4	24.08
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG12	4	24.08
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG13	4	24.08
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD2	2	24.08
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD3	2	24.08
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD2	11	24.06
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD3	11	24.06
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD21	1	24.04
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD22	1	24.04
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD23	1	24.04
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD21	11	24.03
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD22	11	24.03
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD23	11	24.03
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD11	10	24.03
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD12	10	24.03
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD13	10	24.03
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD21	10	24.03
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD22	10	24.03
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD23	10	24.03
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD2	2	24.03
(2,107)	1:A:777:ILE:HD11	1:A:742:ARG:HD3	2	24.03
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD2	2	24.03
(2,107)	1:A:777:ILE:HD12	1:A:742:ARG:HD3	2	24.03
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD2	2	24.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,107)	1:A:777:ILE:HD13	1:A:742:ARG:HD3	2	24.03
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD21	2	23.98
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD22	2	23.98
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD23	2	23.98
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG12	15	23.89
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG13	15	23.89
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG12	15	23.89
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG13	15	23.89
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG12	15	23.89
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG13	15	23.89
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB2	5	23.86
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB3	5	23.86
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG12	11	23.81
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG13	11	23.81
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG12	11	23.81
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG13	11	23.81
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG12	11	23.81
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG13	11	23.81
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD11	4	23.78
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD12	4	23.78
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD13	4	23.78
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD21	4	23.78
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD22	4	23.78
(2,154)	1:B:792:ALA:H	1:A:753:LEU:HD23	4	23.78
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG12	7	23.76
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG13	7	23.76
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG12	7	23.76
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG13	7	23.76
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG12	7	23.76
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG13	7	23.76
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG12	10	23.75
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG13	10	23.75
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG12	10	23.75
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG13	10	23.75
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG12	10	23.75
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG13	10	23.75
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD21	6	23.74
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD22	6	23.74
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD23	6	23.74
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB2	15	23.72
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB3	15	23.72
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG12	2	23.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG13	2	23.72
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG12	2	23.72
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG13	2	23.72
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG12	2	23.72
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG13	2	23.72
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD21	2	23.66
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD22	2	23.66
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD23	2	23.66
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD2	5	23.62
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD3	5	23.62
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG12	15	23.61
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG13	15	23.61
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG12	15	23.61
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG13	15	23.61
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG12	15	23.61
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG13	15	23.61
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD21	5	23.57
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD22	5	23.57
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD23	5	23.57
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD2	15	23.57
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD3	15	23.57
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD21	4	23.51
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD22	4	23.51
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD23	4	23.51
(2,112)	1:B:781:ILE:HD11	1:A:743:ASP:HA	12	23.5
(2,112)	1:B:781:ILE:HD12	1:A:743:ASP:HA	12	23.5
(2,112)	1:B:781:ILE:HD13	1:A:743:ASP:HA	12	23.5
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD2	1	23.5
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD3	1	23.5
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD2	1	23.5
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD3	1	23.5
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD2	1	23.5
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD3	1	23.5
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD2	7	23.5
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD3	7	23.5
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD2	7	23.5
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD3	7	23.5
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD2	7	23.5
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD3	7	23.5
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG12	8	23.49
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG13	8	23.49
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG12	8	23.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG13	8	23.49
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG12	8	23.49
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG13	8	23.49
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG12	3	23.48
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG13	3	23.48
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG12	3	23.48
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG13	3	23.48
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG12	3	23.48
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG13	3	23.48
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD2	6	23.46
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD3	6	23.46
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD2	6	23.46
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD3	6	23.46
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD2	6	23.46
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD3	6	23.46
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD2	6	23.45
(2,104)	1:A:763:LEU:H	1:A:742:ARG:HD3	6	23.45
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD21	3	23.43
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD22	3	23.43
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD23	3	23.43
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD2	9	23.4
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD3	9	23.4
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD2	9	23.4
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD3	9	23.4
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD2	9	23.4
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD3	9	23.4
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD21	14	23.39
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD22	14	23.39
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD23	14	23.39
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD2	11	23.38
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD3	11	23.38
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD2	11	23.38
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD3	11	23.38
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD2	11	23.38
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD3	11	23.38
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD21	10	23.37
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD22	10	23.37
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD23	10	23.37
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD21	3	23.33
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD22	3	23.33
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD23	3	23.33
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB2	9	23.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB3	9	23.32
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB2	6	23.31
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB3	6	23.31
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG12	13	23.27
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG13	13	23.27
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG12	13	23.27
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG13	13	23.27
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG12	13	23.27
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG13	13	23.27
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG12	14	23.25
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG13	14	23.25
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG12	14	23.25
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG13	14	23.25
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG12	14	23.25
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG13	14	23.25
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD2	10	23.25
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD3	10	23.25
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD2	10	23.25
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD3	10	23.25
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD2	10	23.25
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD3	10	23.25
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD21	6	23.23
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD22	6	23.23
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD23	6	23.23
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG12	11	23.22
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG13	11	23.22
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG12	11	23.22
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG13	11	23.22
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG12	11	23.22
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG13	11	23.22
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD2	15	23.2
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD3	15	23.2
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD2	15	23.2
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD3	15	23.2
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD2	15	23.2
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD3	15	23.2
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG12	14	23.19
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG13	14	23.19
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG12	14	23.19
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG13	14	23.19
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG12	14	23.19
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG13	14	23.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG12	5	23.18
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG13	5	23.18
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG12	5	23.18
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG13	5	23.18
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG12	5	23.18
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG13	5	23.18
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG12	9	23.14
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG13	9	23.14
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG12	9	23.14
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG13	9	23.14
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG12	9	23.14
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG13	9	23.14
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB2	3	23.11
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB3	3	23.11
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG12	1	23.1
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG13	1	23.1
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG12	1	23.1
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG13	1	23.1
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG12	1	23.1
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG13	1	23.1
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD2	13	23.1
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD3	13	23.1
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD2	13	23.1
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD3	13	23.1
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD2	13	23.1
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD3	13	23.1
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD21	10	23.09
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD22	10	23.09
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD23	10	23.09
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD2	3	23.07
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD3	3	23.07
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD2	3	23.07
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD3	3	23.07
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD2	3	23.07
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD3	3	23.07
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB2	2	23.06
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB3	2	23.06
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG12	1	23.04
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG13	1	23.04
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG12	1	23.04
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG13	1	23.04
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG12	1	23.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG13	1	23.04
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD2	6	22.99
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD3	6	22.99
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD2	6	22.99
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD3	6	22.99
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD2	6	22.99
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD3	6	22.99
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD21	5	22.97
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD22	5	22.97
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD23	5	22.97
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD21	7	22.96
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD22	7	22.96
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD23	7	22.96
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB2	13	22.95
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB3	13	22.95
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD21	12	22.95
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD22	12	22.95
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD23	12	22.95
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG12	4	22.92
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG13	4	22.92
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG12	4	22.92
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG13	4	22.92
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG12	4	22.92
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG13	4	22.92
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD21	9	22.84
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD22	9	22.84
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD23	9	22.84
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB2	1	22.81
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB3	1	22.81
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG12	12	22.79
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG13	12	22.79
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG12	12	22.79
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG13	12	22.79
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG12	12	22.79
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG13	12	22.79
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB2	12	22.78
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB3	12	22.78
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG12	8	22.76
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG13	8	22.76
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG12	8	22.76
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG13	8	22.76
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG12	8	22.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG13	8	22.76
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD2	8	22.73
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD3	8	22.73
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD2	8	22.73
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD3	8	22.73
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD2	8	22.73
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD3	8	22.73
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG12	3	22.72
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG13	3	22.72
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG12	3	22.72
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG13	3	22.72
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG12	3	22.72
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG13	3	22.72
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB2	7	22.71
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB3	7	22.71
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD21	8	22.71
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD22	8	22.71
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD23	8	22.71
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD21	13	22.66
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD22	13	22.66
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD23	13	22.66
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB2	10	22.63
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB3	10	22.63
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD21	15	22.59
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD22	15	22.59
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD23	15	22.59
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB2	8	22.51
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB3	8	22.51
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG12	13	22.31
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG13	13	22.31
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG12	13	22.31
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG13	13	22.31
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG12	13	22.31
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG13	13	22.31
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD2	9	22.3
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD3	9	22.3
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD2	9	22.3
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD3	9	22.3
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD2	9	22.3
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD3	9	22.3
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG12	9	22.3
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG13	9	22.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG12	9	22.3
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG13	9	22.3
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG12	9	22.3
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG13	9	22.3
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD21	8	22.29
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD22	8	22.29
(2,164)	1:A:796:TRP:HE1	1:A:755:LEU:HD23	8	22.29
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB2	14	22.25
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB3	14	22.25
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD2	12	22.19
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD3	12	22.19
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD2	12	22.19
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD3	12	22.19
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD2	12	22.19
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD3	12	22.19
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD2	14	22.17
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD3	14	22.17
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD2	14	22.17
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD3	14	22.17
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD2	14	22.17
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD3	14	22.17
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD21	11	22.14
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD22	11	22.14
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD23	11	22.14
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD2	2	22.09
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD3	2	22.09
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD2	2	22.09
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD3	2	22.09
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD2	2	22.09
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD3	2	22.09
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD21	15	22.05
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD22	15	22.05
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD23	15	22.05
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD2	4	22.05
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD3	4	22.05
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD2	4	22.05
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD3	4	22.05
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD2	4	22.05
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD3	4	22.05
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD21	12	22.04
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD22	12	22.04
(2,163)	1:B:796:TRP:HE1	1:A:755:LEU:HD23	12	22.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB2	11	21.91
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB3	11	21.91
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB2	11	21.91
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB3	11	21.91
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB2	11	21.91
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB3	11	21.91
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG12	5	21.9
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG13	5	21.9
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG12	5	21.9
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG13	5	21.9
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG12	5	21.9
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG13	5	21.9
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG12	7	21.88
(2,116)	1:A:781:ILE:HD11	1:A:746:ILE:HG13	7	21.88
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG12	7	21.88
(2,116)	1:A:781:ILE:HD12	1:A:746:ILE:HG13	7	21.88
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG12	7	21.88
(2,116)	1:A:781:ILE:HD13	1:A:746:ILE:HG13	7	21.88
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD2	5	21.84
(2,106)	1:B:777:ILE:HD11	1:A:742:ARG:HD3	5	21.84
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD2	5	21.84
(2,106)	1:B:777:ILE:HD12	1:A:742:ARG:HD3	5	21.84
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD2	5	21.84
(2,106)	1:B:777:ILE:HD13	1:A:742:ARG:HD3	5	21.84
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG12	6	21.81
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG13	6	21.81
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG12	6	21.81
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG13	6	21.81
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG12	6	21.81
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG13	6	21.81
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB2	4	21.75
(2,92)	1:A:754:ALA:H	1:A:716:SER:HB3	4	21.75
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB2	9	21.75
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB3	9	21.75
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB2	9	21.75
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB3	9	21.75
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB2	9	21.75
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB3	9	21.75
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD2	10	21.6
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD3	10	21.6
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD2	10	21.6
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD3	10	21.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD2	10	21.6
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD3	10	21.6
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB2	15	21.53
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB3	15	21.53
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB2	15	21.53
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB3	15	21.53
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB2	15	21.53
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB3	15	21.53
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD2	11	21.45
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD3	11	21.45
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD2	11	21.45
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD3	11	21.45
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD2	11	21.45
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD3	11	21.45
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB2	9	21.39
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB3	9	21.39
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD2	2	21.35
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD3	2	21.35
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD2	2	21.35
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD3	2	21.35
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD2	2	21.35
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD3	2	21.35
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB2	5	21.17
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB3	5	21.17
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB2	5	21.17
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB3	5	21.17
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB2	5	21.17
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB3	5	21.17
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD2	13	21.16
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD3	13	21.16
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG12	12	21.11
(2,115)	1:B:781:ILE:HD11	1:A:746:ILE:HG13	12	21.11
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG12	12	21.11
(2,115)	1:B:781:ILE:HD12	1:A:746:ILE:HG13	12	21.11
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG12	12	21.11
(2,115)	1:B:781:ILE:HD13	1:A:746:ILE:HG13	12	21.11
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD2	14	21.04
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD3	14	21.04
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD2	14	21.04
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD3	14	21.04
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD2	14	21.04
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD3	14	21.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB2	3	21.04
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB3	3	21.04
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB2	3	21.04
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB3	3	21.04
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB2	3	21.04
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB3	3	21.04
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD2	7	21.01
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD3	7	21.01
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD2	7	21.01
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD3	7	21.01
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD2	7	21.01
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD3	7	21.01
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB2	3	20.96
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB3	3	20.96
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB2	1	20.95
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB3	1	20.95
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB2	11	20.92
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB3	11	20.92
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD2	3	20.91
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD3	3	20.91
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD2	3	20.91
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD3	3	20.91
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD2	3	20.91
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD3	3	20.91
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB2	2	20.81
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB3	2	20.81
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD2	15	20.79
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD3	15	20.79
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD2	15	20.79
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD3	15	20.79
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD2	15	20.79
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD3	15	20.79
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB2	6	20.75
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB3	6	20.75
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB2	6	20.75
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB3	6	20.75
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB2	6	20.75
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB3	6	20.75
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD2	1	20.74
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD3	1	20.74
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD2	1	20.74
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD3	1	20.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD2	1	20.74
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD3	1	20.74
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD2	12	20.74
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD3	12	20.74
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB2	8	20.71
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB3	8	20.71
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB2	8	20.71
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB3	8	20.71
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB2	8	20.71
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB3	8	20.71
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD2	8	20.71
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD3	8	20.71
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB2	10	20.65
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB3	10	20.65
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB2	10	20.65
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB3	10	20.65
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB2	10	20.65
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB3	10	20.65
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB2	12	20.65
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB3	12	20.65
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB2	12	20.65
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB3	12	20.65
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB2	12	20.65
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB3	12	20.65
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD2	2	20.59
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD3	2	20.59
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD2	10	20.58
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD3	10	20.58
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD2	10	20.58
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD3	10	20.58
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD2	10	20.58
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD3	10	20.58
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD2	1	20.56
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD3	1	20.56
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD2	1	20.56
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD3	1	20.56
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD2	1	20.56
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD3	1	20.56
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD2	5	20.45
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD3	5	20.45
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD2	5	20.45
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD3	5	20.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD2	5	20.45
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD3	5	20.45
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB2	8	20.44
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB3	8	20.44
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD2	3	20.44
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD3	3	20.44
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD2	3	20.44
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD3	3	20.44
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD2	3	20.44
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD3	3	20.44
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB2	4	20.44
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB3	4	20.44
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB2	4	20.44
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB3	4	20.44
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB2	4	20.44
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB3	4	20.44
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD2	7	20.44
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD3	7	20.44
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB2	1	20.42
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB3	1	20.42
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB2	1	20.42
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB3	1	20.42
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB2	1	20.42
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB3	1	20.42
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD2	12	20.41
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD3	12	20.41
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD2	12	20.41
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD3	12	20.41
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD2	12	20.41
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD3	12	20.41
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD2	15	20.34
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD3	15	20.34
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB2	10	20.3
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB3	10	20.3
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB2	15	20.3
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB3	15	20.3
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD2	13	20.29
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD3	13	20.29
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD2	13	20.29
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD3	13	20.29
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD2	13	20.29
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD3	13	20.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB2	14	20.26
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB3	14	20.26
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB2	14	20.26
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB3	14	20.26
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB2	14	20.26
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB3	14	20.26
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB2	2	20.25
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB3	2	20.25
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB2	2	20.25
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB3	2	20.25
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB2	2	20.25
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB3	2	20.25
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB2	12	20.24
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB3	12	20.24
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB2	5	20.22
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB3	5	20.22
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD2	14	20.22
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD3	14	20.22
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD2	14	20.22
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD3	14	20.22
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD2	14	20.22
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD3	14	20.22
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB2	13	20.21
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB3	13	20.21
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB2	13	20.21
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB3	13	20.21
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB2	13	20.21
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB3	13	20.21
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD2	2	20.13
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD3	2	20.13
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD2	2	20.13
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD3	2	20.13
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD2	2	20.13
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD3	2	20.13
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB2	4	20.08
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB3	4	20.08
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD2	15	20.06
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD3	15	20.06
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD2	15	20.06
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD3	15	20.06
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD2	15	20.06
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD3	15	20.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB2	8	20.06
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB3	8	20.06
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB2	8	20.06
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB3	8	20.06
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB2	8	20.06
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB3	8	20.06
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD2	12	20.01
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD3	12	20.01
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD2	12	20.01
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD3	12	20.01
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD2	12	20.01
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD3	12	20.01
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD2	11	19.98
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD3	11	19.98
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD2	11	19.98
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD3	11	19.98
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD2	11	19.98
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD3	11	19.98
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB2	6	19.94
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB3	6	19.94
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD2	11	19.92
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD3	11	19.92
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD2	6	19.91
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD3	6	19.91
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD2	6	19.91
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD3	6	19.91
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD2	6	19.91
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD3	6	19.91
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD2	8	19.84
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD3	8	19.84
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD2	8	19.84
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD3	8	19.84
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD2	8	19.84
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD3	8	19.84
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD2	1	19.82
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD3	1	19.82
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD2	3	19.82
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD3	3	19.82
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB2	14	19.76
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB3	14	19.76
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB2	14	19.76
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB3	14	19.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB2	14	19.76
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB3	14	19.76
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB2	14	19.64
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB3	14	19.64
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD2	9	19.6
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD3	9	19.6
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD2	9	19.6
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD3	9	19.6
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD2	9	19.6
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD3	9	19.6
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD2	10	19.57
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD3	10	19.57
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB2	7	19.55
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB3	7	19.55
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD2	6	19.52
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD3	6	19.52
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB2	13	19.51
(2,91)	1:B:754:ALA:H	1:A:716:SER:HB3	13	19.51
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB2	12	19.5
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB3	12	19.5
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB2	12	19.5
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB3	12	19.5
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB2	12	19.5
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB3	12	19.5
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB2	11	19.46
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB3	11	19.46
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB2	11	19.46
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB3	11	19.46
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB2	11	19.46
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB3	11	19.46
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD2	4	19.41
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD3	4	19.41
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD2	9	19.4
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD3	9	19.4
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD2	5	19.38
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD3	5	19.38
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD2	5	19.38
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD3	5	19.38
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD2	5	19.38
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD3	5	19.38
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD2	4	19.38
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD3	4	19.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD2	4	19.38
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD3	4	19.38
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD2	4	19.38
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD3	4	19.38
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD2	13	19.34
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD3	13	19.34
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD2	13	19.34
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD3	13	19.34
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD2	13	19.34
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD3	13	19.34
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB2	7	19.31
(2,120)	1:A:785:LEU:HD21	1:A:716:SER:HB3	7	19.31
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB2	7	19.31
(2,120)	1:A:785:LEU:HD22	1:A:716:SER:HB3	7	19.31
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB2	7	19.31
(2,120)	1:A:785:LEU:HD23	1:A:716:SER:HB3	7	19.31
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD2	8	19.3
(2,121)	1:B:785:LEU:HD21	1:A:747:ARG:HD3	8	19.3
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD2	8	19.3
(2,121)	1:B:785:LEU:HD22	1:A:747:ARG:HD3	8	19.3
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD2	8	19.3
(2,121)	1:B:785:LEU:HD23	1:A:747:ARG:HD3	8	19.3
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB2	6	19.29
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB3	6	19.29
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB2	6	19.29
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB3	6	19.29
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB2	6	19.29
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB3	6	19.29
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD21	4	19.23
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD22	4	19.23
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD23	4	19.23
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB2	10	19.2
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB3	10	19.2
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB2	10	19.2
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB3	10	19.2
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB2	10	19.2
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB3	10	19.2
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD21	3	19.02
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD22	3	19.02
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD23	3	19.02
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD2	14	18.97
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD3	14	18.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB2	2	18.55
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB3	2	18.55
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB2	2	18.55
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB3	2	18.55
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB2	2	18.55
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB3	2	18.55
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD21	12	18.54
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD22	12	18.54
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD23	12	18.54
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD21	13	18.49
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD22	13	18.49
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD23	13	18.49
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD21	9	18.4
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD22	9	18.4
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD23	9	18.4
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB2	4	18.4
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB3	4	18.4
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB2	4	18.4
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB3	4	18.4
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB2	4	18.4
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB3	4	18.4
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB2	15	18.37
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB3	15	18.37
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB2	15	18.37
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB3	15	18.37
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB2	15	18.37
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB3	15	18.37
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD2	5	18.37
(2,100)	1:B:759:ASP:H	1:A:709:ARG:HD3	5	18.37
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD2	4	18.31
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD3	4	18.31
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD2	4	18.31
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD3	4	18.31
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD2	4	18.31
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD3	4	18.31
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD21	7	18.21
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD22	7	18.21
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD23	7	18.21
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB2	9	18.21
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB3	9	18.21
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB2	9	18.21
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB3	9	18.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB2	9	18.21
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB3	9	18.21
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD21	8	18.2
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD22	8	18.2
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD23	8	18.2
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB2	3	18.06
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB3	3	18.06
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB2	3	18.06
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB3	3	18.06
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB2	3	18.06
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB3	3	18.06
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD21	1	18.02
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD22	1	18.02
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD23	1	18.02
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD21	14	17.96
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD22	14	17.96
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD23	14	17.96
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD2	7	17.82
(2,122)	1:A:785:LEU:HD21	1:A:747:ARG:HD3	7	17.82
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD2	7	17.82
(2,122)	1:A:785:LEU:HD22	1:A:747:ARG:HD3	7	17.82
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD2	7	17.82
(2,122)	1:A:785:LEU:HD23	1:A:747:ARG:HD3	7	17.82
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB2	1	17.58
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB3	1	17.58
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB2	1	17.58
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB3	1	17.58
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB2	1	17.58
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB3	1	17.58
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD21	2	17.5
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD22	2	17.5
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD23	2	17.5
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD21	10	17.48
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD22	10	17.48
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD23	10	17.48
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD21	5	17.42
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD22	5	17.42
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD23	5	17.42
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB2	7	17.31
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB3	7	17.31
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB2	7	17.31
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB3	7	17.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB2	7	17.31
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB3	7	17.31
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB2	5	17.3
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB3	5	17.3
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB2	5	17.3
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB3	5	17.3
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB2	5	17.3
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB3	5	17.3
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD21	11	17.26
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD22	11	17.26
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD23	11	17.26
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD21	6	17.08
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD22	6	17.08
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD23	6	17.08
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB2	13	17.04
(2,119)	1:A:785:LEU:HD21	1:B:716:SER:HB3	13	17.04
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB2	13	17.04
(2,119)	1:A:785:LEU:HD22	1:B:716:SER:HB3	13	17.04
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB2	13	17.04
(2,119)	1:A:785:LEU:HD23	1:B:716:SER:HB3	13	17.04
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD21	13	16.94
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD22	13	16.94
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD23	13	16.94
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD21	1	16.8
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD22	1	16.8
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD23	1	16.8
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD21	3	16.7
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD22	3	16.7
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD23	3	16.7
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD21	5	16.7
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD22	5	16.7
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD23	5	16.7
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD21	14	16.58
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD22	14	16.58
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD23	14	16.58
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD21	15	16.57
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD22	15	16.57
(2,98)	1:A:758:ASP:H	1:A:715:LEU:HD23	15	16.57
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD21	4	16.56
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD22	4	16.56
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD23	4	16.56
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD21	12	16.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD22	12	16.49
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD23	12	16.49
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD21	10	16.48
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD22	10	16.48
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD23	10	16.48
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD21	8	16.44
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD22	8	16.44
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD23	8	16.44
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD21	15	16.12
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD22	15	16.12
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD23	15	16.12
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD21	7	15.87
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD22	7	15.87
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD23	7	15.87
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD2	9	15.82
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD3	9	15.82
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD21	2	15.8
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD22	2	15.8
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD23	2	15.8
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD21	11	15.78
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD22	11	15.78
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD23	11	15.78
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD2	1	15.67
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD3	1	15.67
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB2	1	15.58
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB3	1	15.58
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB2	5	15.49
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB3	5	15.49
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB2	3	15.4
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB3	3	15.4
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD2	8	15.4
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD3	8	15.4
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD21	6	15.39
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD22	6	15.39
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD23	6	15.39
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB2	2	15.31
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB3	2	15.31
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD21	9	15.26
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD22	9	15.26
(2,97)	1:B:758:ASP:H	1:A:715:LEU:HD23	9	15.26
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD2	5	15.23
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD3	5	15.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB2	13	15.22
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB3	13	15.22
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD2	2	15.22
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD3	2	15.22
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB2	14	15.18
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB3	14	15.18
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB2	6	15.11
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB3	6	15.11
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD2	12	15.08
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD3	12	15.08
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB2	4	15.05
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB3	4	15.05
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD2	4	14.98
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD3	4	14.98
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB2	12	14.87
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB3	12	14.87
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB2	15	14.85
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB3	15	14.85
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD2	3	14.76
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD3	3	14.76
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB2	7	14.69
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB3	7	14.69
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB2	11	14.66
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB3	11	14.66
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB2	8	14.6
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB3	8	14.6
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB2	10	14.55
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB3	10	14.55
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB2	4	14.54
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB3	4	14.54
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD2	10	14.52
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD3	10	14.52
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB2	5	14.5
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB3	5	14.5
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB2	9	14.46
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB3	9	14.46
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD2	13	14.42
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD3	13	14.42
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD2	15	14.39
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD3	15	14.39
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB2	9	14.37
(2,86)	1:A:711:GLY:H	1:B:758:ASP:HB3	9	14.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD2	14	14.34
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD3	14	14.34
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD2	6	14.21
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD3	6	14.21
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB2	8	14.1
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB3	8	14.1
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB2	2	14.08
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB3	2	14.08
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD2	7	14.04
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD3	7	14.04
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB2	1	14.0
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB3	1	14.0
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB2	12	13.8
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB3	12	13.8
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB2	3	13.79
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB3	3	13.79
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE21	11	13.69
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE22	11	13.69
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE21	11	13.69
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE22	11	13.69
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE21	11	13.69
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE22	11	13.69
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB2	14	13.54
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB3	14	13.54
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD2	11	13.53
(2,101)	1:A:759:ASP:H	1:A:709:ARG:HD3	11	13.53
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB2	7	13.49
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB3	7	13.49
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB2	13	13.19
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB3	13	13.19
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB2	6	13.15
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB3	6	13.15
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB2	10	13.07
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB3	10	13.07
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE21	2	13.01
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE22	2	13.01
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE21	2	13.01
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE22	2	13.01
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE21	2	13.01
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE22	2	13.01
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE21	14	12.89
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE22	14	12.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE21	14	12.89
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE22	14	12.89
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE21	14	12.89
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE22	14	12.89
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE21	3	12.88
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE22	3	12.88
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE21	3	12.88
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE22	3	12.88
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE21	3	12.88
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE22	3	12.88
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE21	4	12.78
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE22	4	12.78
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE21	4	12.78
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE22	4	12.78
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE21	4	12.78
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE22	4	12.78
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB2	11	12.74
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB3	11	12.74
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB2	15	12.69
(2,85)	1:A:711:GLY:H	1:A:758:ASP:HB3	15	12.69
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE21	12	12.58
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE22	12	12.58
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE21	12	12.58
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE22	12	12.58
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE21	12	12.58
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE22	12	12.58
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE21	1	12.54
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE22	1	12.54
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE21	1	12.54
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE22	1	12.54
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE21	1	12.54
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE22	1	12.54
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE21	10	12.47
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE22	10	12.47
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE21	10	12.47
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE22	10	12.47
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE21	10	12.47
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE22	10	12.47
(2,21)	1:A:678:TRP:HE1	1:B:683:ARG:HE	7	12.42
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE21	7	12.24
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE22	7	12.24
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE21	7	12.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE22	7	12.24
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE21	7	12.24
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE22	7	12.24
(2,21)	1:A:678:TRP:HE1	1:B:683:ARG:HE	1	12.21
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE21	8	12.19
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE22	8	12.19
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE21	8	12.19
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE22	8	12.19
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE21	8	12.19
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE22	8	12.19
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD2	10	12.1
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD3	10	12.1
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD2	9	12.08
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD3	9	12.08
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE21	5	12.06
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE22	5	12.06
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE21	5	12.06
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE22	5	12.06
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE21	5	12.06
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE22	5	12.06
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE21	9	12.02
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE22	9	12.02
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE21	9	12.02
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE22	9	12.02
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE21	9	12.02
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE22	9	12.02
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE21	6	11.99
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE22	6	11.99
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE21	6	11.99
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE22	6	11.99
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE21	6	11.99
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE22	6	11.99
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE21	15	11.98
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE22	15	11.98
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE21	15	11.98
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE22	15	11.98
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE21	15	11.98
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE22	15	11.98
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE21	9	11.86
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE22	9	11.86
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE21	9	11.86
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE22	9	11.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE21	9	11.86
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE22	9	11.86
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD2	11	11.8
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD3	11	11.8
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD2	5	11.7
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD3	5	11.7
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE21	1	11.54
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE22	1	11.54
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE21	1	11.54
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE22	1	11.54
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE21	1	11.54
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE22	1	11.54
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD2	8	11.54
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD3	8	11.54
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD2	14	11.54
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD3	14	11.54
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE21	13	11.53
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE22	13	11.53
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE21	13	11.53
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE22	13	11.53
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE21	13	11.53
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE22	13	11.53
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE21	4	11.49
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE22	4	11.49
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE21	4	11.49
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE22	4	11.49
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE21	4	11.49
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE22	4	11.49
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD11	9	11.47
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD12	9	11.47
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD13	9	11.47
(2,79)	1:B:708:VAL:HG21	1:A:714:PRO:HA	11	11.46
(2,79)	1:B:708:VAL:HG22	1:A:714:PRO:HA	11	11.46
(2,79)	1:B:708:VAL:HG23	1:A:714:PRO:HA	11	11.46
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD11	10	11.45
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD12	10	11.45
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD13	10	11.45
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD2	7	11.44
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD3	7	11.44
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD2	2	11.39
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD3	2	11.39
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE21	12	11.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE22	12	11.32
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE21	12	11.32
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE22	12	11.32
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE21	12	11.32
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE22	12	11.32
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD11	3	11.28
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD12	3	11.28
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD13	3	11.28
(2,21)	1:A:678:TRP:HE1	1:B:683:ARG:HE	14	11.25
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD2	12	11.19
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD3	12	11.19
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD11	7	11.18
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD12	7	11.18
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD13	7	11.18
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD2	15	11.04
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD3	15	11.04
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD2	3	10.98
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD3	3	10.98
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD11	12	10.97
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD12	12	10.97
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD13	12	10.97
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD2	6	10.92
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD3	6	10.92
(2,21)	1:A:678:TRP:HE1	1:B:683:ARG:HE	8	10.84
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB2	11	10.82
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB3	11	10.82
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE21	14	10.79
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE22	14	10.79
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE21	14	10.79
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE22	14	10.79
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE21	14	10.79
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE22	14	10.79
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD2	4	10.79
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD3	4	10.79
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB2	13	10.78
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB3	13	10.78
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE21	2	10.76
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE22	2	10.76
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE21	2	10.76
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE22	2	10.76
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE21	2	10.76
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE22	2	10.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD2	13	10.75
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD3	13	10.75
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE21	13	10.71
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE22	13	10.71
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE21	13	10.71
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE22	13	10.71
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE21	13	10.71
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE22	13	10.71
(2,21)	1:A:678:TRP:HE1	1:B:683:ARG:HE	10	10.71
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB2	14	10.67
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB3	14	10.67
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB2	5	10.66
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB3	5	10.66
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB2	12	10.66
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB3	12	10.66
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD2	1	10.65
(2,82)	1:B:709:ARG:H	1:A:714:PRO:HD3	1	10.65
(2,79)	1:B:708:VAL:HG21	1:A:714:PRO:HA	5	10.64
(2,79)	1:B:708:VAL:HG22	1:A:714:PRO:HA	5	10.64
(2,79)	1:B:708:VAL:HG23	1:A:714:PRO:HA	5	10.64
(2,79)	1:B:708:VAL:HG21	1:A:714:PRO:HA	9	10.63
(2,79)	1:B:708:VAL:HG22	1:A:714:PRO:HA	9	10.63
(2,79)	1:B:708:VAL:HG23	1:A:714:PRO:HA	9	10.63
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB2	3	10.63
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB3	3	10.63
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE21	8	10.61
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE22	8	10.61
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE21	8	10.61
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE22	8	10.61
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE21	8	10.61
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE22	8	10.61
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE21	10	10.59
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE22	10	10.59
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE21	10	10.59
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE22	10	10.59
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE21	10	10.59
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE22	10	10.59
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB2	1	10.54
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB3	1	10.54
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB2	2	10.45
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB3	2	10.45
(2,21)	1:A:678:TRP:HE1	1:B:683:ARG:HE	12	10.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE21	15	10.39
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE22	15	10.39
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE21	15	10.39
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE22	15	10.39
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE21	15	10.39
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE22	15	10.39
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD11	5	10.39
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD12	5	10.39
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD13	5	10.39
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD11	11	10.38
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD12	11	10.38
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD13	11	10.38
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD11	13	10.34
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD12	13	10.34
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD13	13	10.34
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE21	7	10.33
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE22	7	10.33
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE21	7	10.33
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE22	7	10.33
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE21	7	10.33
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE22	7	10.33
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB2	15	10.31
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB3	15	10.31
(2,79)	1:B:708:VAL:HG21	1:A:714:PRO:HA	1	10.29
(2,79)	1:B:708:VAL:HG22	1:A:714:PRO:HA	1	10.29
(2,79)	1:B:708:VAL:HG23	1:A:714:PRO:HA	1	10.29
(2,21)	1:A:678:TRP:HE1	1:B:683:ARG:HE	11	10.29
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE21	6	10.26
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE22	6	10.26
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE21	6	10.26
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE22	6	10.26
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE21	6	10.26
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE22	6	10.26
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB2	8	10.21
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB3	8	10.21
(2,79)	1:B:708:VAL:HG21	1:A:714:PRO:HA	4	10.19
(2,79)	1:B:708:VAL:HG22	1:A:714:PRO:HA	4	10.19
(2,79)	1:B:708:VAL:HG23	1:A:714:PRO:HA	4	10.19
(2,79)	1:B:708:VAL:HG21	1:A:714:PRO:HA	6	10.19
(2,79)	1:B:708:VAL:HG22	1:A:714:PRO:HA	6	10.19
(2,79)	1:B:708:VAL:HG23	1:A:714:PRO:HA	6	10.19
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE21	5	10.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,94)	1:B:755:LEU:HD11	1:A:710:GLN:HE22	5	10.18
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE21	5	10.18
(2,94)	1:B:755:LEU:HD12	1:A:710:GLN:HE22	5	10.18
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE21	5	10.18
(2,94)	1:B:755:LEU:HD13	1:A:710:GLN:HE22	5	10.18
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB2	9	10.13
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB3	9	10.13
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB2	7	10.02
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB3	7	10.02
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE21	11	10.0
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE22	11	10.0
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE21	11	10.0
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE22	11	10.0
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE21	11	10.0
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE22	11	10.0
(2,21)	1:A:678:TRP:HE1	1:B:683:ARG:HE	6	9.98
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD11	15	9.89
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD12	15	9.89
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD13	15	9.89
(2,21)	1:A:678:TRP:HE1	1:B:683:ARG:HE	15	9.84
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE21	3	9.8
(2,95)	1:A:755:LEU:HD11	1:A:710:GLN:HE22	3	9.8
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE21	3	9.8
(2,95)	1:A:755:LEU:HD12	1:A:710:GLN:HE22	3	9.8
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE21	3	9.8
(2,95)	1:A:755:LEU:HD13	1:A:710:GLN:HE22	3	9.8
(2,21)	1:A:678:TRP:HE1	1:B:683:ARG:HE	2	9.77
(2,21)	1:A:678:TRP:HE1	1:B:683:ARG:HE	3	9.77
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG21	1	9.67
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG22	1	9.67
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG23	1	9.67
(2,79)	1:B:708:VAL:HG21	1:A:714:PRO:HA	15	9.63
(2,79)	1:B:708:VAL:HG22	1:A:714:PRO:HA	15	9.63
(2,79)	1:B:708:VAL:HG23	1:A:714:PRO:HA	15	9.63
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB2	12	9.55
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB3	12	9.55
(2,79)	1:B:708:VAL:HG21	1:A:714:PRO:HA	7	9.49
(2,79)	1:B:708:VAL:HG22	1:A:714:PRO:HA	7	9.49
(2,79)	1:B:708:VAL:HG23	1:A:714:PRO:HA	7	9.49
(2,79)	1:B:708:VAL:HG21	1:A:714:PRO:HA	14	9.47
(2,79)	1:B:708:VAL:HG22	1:A:714:PRO:HA	14	9.47
(2,79)	1:B:708:VAL:HG23	1:A:714:PRO:HA	14	9.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB2	10	9.46
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB3	10	9.46
(2,79)	1:B:708:VAL:HG21	1:A:714:PRO:HA	12	9.44
(2,79)	1:B:708:VAL:HG22	1:A:714:PRO:HA	12	9.44
(2,79)	1:B:708:VAL:HG23	1:A:714:PRO:HA	12	9.44
(2,79)	1:B:708:VAL:HG21	1:A:714:PRO:HA	10	9.42
(2,79)	1:B:708:VAL:HG22	1:A:714:PRO:HA	10	9.42
(2,79)	1:B:708:VAL:HG23	1:A:714:PRO:HA	10	9.42
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD11	14	9.37
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD12	14	9.37
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD13	14	9.37
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG21	10	9.35
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG22	10	9.35
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG23	10	9.35
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB2	11	9.33
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB3	11	9.33
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD11	11	9.24
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD12	11	9.24
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD13	11	9.24
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB2	4	9.24
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB3	4	9.24
(2,79)	1:B:708:VAL:HG21	1:A:714:PRO:HA	13	9.16
(2,79)	1:B:708:VAL:HG22	1:A:714:PRO:HA	13	9.16
(2,79)	1:B:708:VAL:HG23	1:A:714:PRO:HA	13	9.16
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG21	4	9.13
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG22	4	9.13
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG23	4	9.13
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD11	4	9.13
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD12	4	9.13
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD13	4	9.13
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD11	10	9.1
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD12	10	9.1
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD13	10	9.1
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB2	1	9.1
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB3	1	9.1
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG21	6	9.07
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG22	6	9.07
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG23	6	9.07
(2,79)	1:B:708:VAL:HG21	1:A:714:PRO:HA	3	9.07
(2,79)	1:B:708:VAL:HG22	1:A:714:PRO:HA	3	9.07
(2,79)	1:B:708:VAL:HG23	1:A:714:PRO:HA	3	9.07
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB2	2	9.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB3	2	9.06
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG21	9	8.92
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG22	9	8.92
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG23	9	8.92
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD11	9	8.87
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD12	9	8.87
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD13	9	8.87
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG21	14	8.86
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG22	14	8.86
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG23	14	8.86
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD11	2	8.75
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD12	2	8.75
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD13	2	8.75
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD11	7	8.75
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD12	7	8.75
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD13	7	8.75
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB2	13	8.7
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB3	13	8.7
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG21	12	8.69
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG22	12	8.69
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG23	12	8.69
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD11	4	8.69
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD12	4	8.69
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD13	4	8.69
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB2	6	8.68
(2,16)	1:B:670:TRP:HE1	1:A:660:LEU:HB3	6	8.68
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB2	14	8.67
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB3	14	8.67
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB2	3	8.66
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB3	3	8.66
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB2	15	8.61
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB3	15	8.61
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD11	8	8.61
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD12	8	8.61
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD13	8	8.61
(2,79)	1:B:708:VAL:HG21	1:A:714:PRO:HA	8	8.6
(2,79)	1:B:708:VAL:HG22	1:A:714:PRO:HA	8	8.6
(2,79)	1:B:708:VAL:HG23	1:A:714:PRO:HA	8	8.6
(2,79)	1:B:708:VAL:HG21	1:A:714:PRO:HA	2	8.59
(2,79)	1:B:708:VAL:HG22	1:A:714:PRO:HA	2	8.59
(2,79)	1:B:708:VAL:HG23	1:A:714:PRO:HA	2	8.59
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD11	14	8.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD12	14	8.57
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD13	14	8.57
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG21	11	8.48
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG22	11	8.48
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG23	11	8.48
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD11	8	8.47
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD12	8	8.47
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD13	8	8.47
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD11	6	8.45
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD12	6	8.45
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD13	6	8.45
(2,21)	1:A:678:TRP:HE1	1:B:683:ARG:HE	9	8.44
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB2	2	8.41
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB3	2	8.41
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB2	9	8.41
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB3	9	8.41
(2,21)	1:A:678:TRP:HE1	1:B:683:ARG:HE	4	8.38
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD11	1	8.34
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD12	1	8.34
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD13	1	8.34
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG21	5	8.33
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG22	5	8.33
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG23	5	8.33
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB2	15	8.31
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB3	15	8.31
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG21	2	8.3
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG22	2	8.3
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG23	2	8.3
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG21	3	8.28
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG22	3	8.28
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG23	3	8.28
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB2	12	8.26
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB3	12	8.26
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB2	7	8.26
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB3	7	8.26
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD2	9	8.22
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD3	9	8.22
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD2	9	8.22
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD3	9	8.22
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD2	9	8.22
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD3	9	8.22
(2,21)	1:A:678:TRP:HE1	1:B:683:ARG:HE	13	8.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG21	13	8.21
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG22	13	8.21
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG23	13	8.21
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB2	5	8.2
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB3	5	8.2
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD11	6	8.2
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD12	6	8.2
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD13	6	8.2
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD11	15	8.2
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD12	15	8.2
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD13	15	8.2
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB2	6	8.14
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB3	6	8.14
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB2	10	8.12
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB3	10	8.12
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD11	1	8.1
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD12	1	8.1
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD13	1	8.1
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD2	11	8.07
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD3	11	8.07
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD2	11	8.07
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD3	11	8.07
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD2	11	8.07
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD3	11	8.07
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD2	1	8.05
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD3	1	8.05
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD2	1	8.05
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD3	1	8.05
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD2	1	8.05
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD3	1	8.05
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG21	8	8.04
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG22	8	8.04
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG23	8	8.04
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB2	3	8.03
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB3	3	8.03
(2,21)	1:A:678:TRP:HE1	1:B:683:ARG:HE	5	8.02
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB2	5	8.01
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB3	5	8.01
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD2	10	7.98
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD3	10	7.98
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD2	10	7.98
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD3	10	7.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD2	10	7.98
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD3	10	7.98
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB2	1	7.97
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB3	1	7.97
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB2	1	7.97
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB3	1	7.97
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB2	1	7.97
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB3	1	7.97
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD2	4	7.95
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD3	4	7.95
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD2	4	7.95
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD3	4	7.95
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD2	4	7.95
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD3	4	7.95
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB2	12	7.9
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB3	12	7.9
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB2	12	7.9
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB3	12	7.9
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB2	12	7.9
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB3	12	7.9
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD11	5	7.89
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD12	5	7.89
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD13	5	7.89
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB2	8	7.84
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB3	8	7.84
(2,20)	1:A:678:TRP:HE1	1:A:683:ARG:HE	3	7.78
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG21	7	7.77
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG22	7	7.77
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG23	7	7.77
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB2	11	7.76
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB3	11	7.76
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD11	2	7.76
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD12	2	7.76
(2,24)	1:A:678:TRP:HE1	1:B:687:ILE:HD13	2	7.76
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB2	14	7.75
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB3	14	7.75
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB2	4	7.73
(2,17)	1:A:670:TRP:HE1	1:A:660:LEU:HB3	4	7.73
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD11	12	7.68
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD12	12	7.68
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD13	12	7.68
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD2	6	7.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD3	6	7.66
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD2	6	7.66
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD3	6	7.66
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD2	6	7.66
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD3	6	7.66
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD2	5	7.62
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD3	5	7.62
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD2	5	7.62
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD3	5	7.62
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD2	5	7.62
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD3	5	7.62
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB2	1	7.59
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB3	1	7.59
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB2	10	7.57
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB3	10	7.57
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB2	10	7.57
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB3	10	7.57
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB2	10	7.57
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB3	10	7.57
(2,2)	1:A:661:LEU:HD11	1:A:680:TRP:HE1	2	7.49
(2,2)	1:A:661:LEU:HD12	1:A:680:TRP:HE1	2	7.49
(2,2)	1:A:661:LEU:HD13	1:A:680:TRP:HE1	2	7.49
(2,2)	1:A:661:LEU:HD21	1:A:680:TRP:HE1	2	7.49
(2,2)	1:A:661:LEU:HD22	1:A:680:TRP:HE1	2	7.49
(2,2)	1:A:661:LEU:HD23	1:A:680:TRP:HE1	2	7.49
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB2	11	7.47
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB3	11	7.47
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB2	11	7.47
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB3	11	7.47
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB2	11	7.47
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB3	11	7.47
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB2	6	7.46
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB3	6	7.46
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB2	6	7.46
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB3	6	7.46
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB2	6	7.46
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB3	6	7.46
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD11	3	7.45
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD12	3	7.45
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD13	3	7.45
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB2	7	7.43
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB3	7	7.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB2	13	7.42
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB3	13	7.42
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB2	9	7.4
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB3	9	7.4
(2,20)	1:A:678:TRP:HE1	1:A:683:ARG:HE	15	7.4
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD2	14	7.39
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD3	14	7.39
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD2	14	7.39
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD3	14	7.39
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD2	14	7.39
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD3	14	7.39
(2,80)	1:A:708:VAL:HG21	1:A:714:PRO:HA	11	7.37
(2,80)	1:A:708:VAL:HG22	1:A:714:PRO:HA	11	7.37
(2,80)	1:A:708:VAL:HG23	1:A:714:PRO:HA	11	7.37
(2,20)	1:A:678:TRP:HE1	1:A:683:ARG:HE	10	7.36
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD2	12	7.35
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD3	12	7.35
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD2	12	7.35
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD3	12	7.35
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD2	12	7.35
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD3	12	7.35
(2,20)	1:A:678:TRP:HE1	1:A:683:ARG:HE	4	7.3
(2,20)	1:A:678:TRP:HE1	1:A:683:ARG:HE	6	7.3
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB2	4	7.28
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB3	4	7.28
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB2	4	7.28
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB3	4	7.28
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB2	4	7.28
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB3	4	7.28
(2,20)	1:A:678:TRP:HE1	1:A:683:ARG:HE	1	7.26
(2,20)	1:A:678:TRP:HE1	1:A:683:ARG:HE	14	7.17
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD2	7	7.15
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD3	7	7.15
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD2	7	7.15
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD3	7	7.15
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD2	7	7.15
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD3	7	7.15
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA2	13	7.15
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA3	13	7.15
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB2	14	7.12
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB3	14	7.12
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB2	14	7.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB3	14	7.12
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB2	14	7.12
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB3	14	7.12
(2,20)	1:A:678:TRP:HE1	1:A:683:ARG:HE	12	7.12
(2,20)	1:A:678:TRP:HE1	1:A:683:ARG:HE	8	7.06
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA2	15	7.03
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA3	15	7.03
(2,20)	1:A:678:TRP:HE1	1:A:683:ARG:HE	7	7.03
(2,20)	1:A:678:TRP:HE1	1:A:683:ARG:HE	5	6.99
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD2	8	6.98
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD3	8	6.98
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD2	8	6.98
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD3	8	6.98
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD2	8	6.98
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD3	8	6.98
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD2	13	6.96
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD3	13	6.96
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD2	13	6.96
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD3	13	6.96
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD2	13	6.96
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD3	13	6.96
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD11	13	6.95
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD12	13	6.95
(2,23)	1:A:678:TRP:HE1	1:A:687:ILE:HD13	13	6.95
(2,20)	1:A:678:TRP:HE1	1:A:683:ARG:HE	9	6.93
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB2	12	6.89
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB3	12	6.89
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB2	12	6.89
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB3	12	6.89
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB2	12	6.89
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB3	12	6.89
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB2	3	6.88
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB3	3	6.88
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB2	3	6.88
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB3	3	6.88
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB2	3	6.88
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB3	3	6.88
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB2	2	6.86
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB3	2	6.86
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB2	2	6.86
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB3	2	6.86
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB2	2	6.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB3	2	6.86
(2,20)	1:A:678:TRP:HE1	1:A:683:ARG:HE	13	6.86
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB2	11	6.83
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB3	11	6.83
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB2	11	6.83
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB3	11	6.83
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB2	11	6.83
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB3	11	6.83
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB2	4	6.83
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB3	4	6.83
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD2	2	6.82
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD3	2	6.82
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD2	2	6.82
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD3	2	6.82
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD2	2	6.82
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD3	2	6.82
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB2	9	6.82
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB3	9	6.82
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB2	9	6.82
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB3	9	6.82
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB2	9	6.82
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB3	9	6.82
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB2	5	6.79
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB3	5	6.79
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB2	5	6.79
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB3	5	6.79
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB2	5	6.79
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB3	5	6.79
(2,39)	1:A:692:LEU:HD21	1:B:694:GLY:H	6	6.78
(2,39)	1:A:692:LEU:HD22	1:B:694:GLY:H	6	6.78
(2,39)	1:A:692:LEU:HD23	1:B:694:GLY:H	6	6.78
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA2	5	6.75
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA3	5	6.75
(2,39)	1:A:692:LEU:HD21	1:B:694:GLY:H	13	6.75
(2,39)	1:A:692:LEU:HD22	1:B:694:GLY:H	13	6.75
(2,39)	1:A:692:LEU:HD23	1:B:694:GLY:H	13	6.75
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD2	3	6.72
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD3	3	6.72
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD2	3	6.72
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD3	3	6.72
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD2	3	6.72
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD3	3	6.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:A:678:TRP:HE1	1:A:683:ARG:HE	11	6.7
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD2	15	6.68
(2,76)	1:B:708:VAL:HG21	1:A:714:PRO:HD3	15	6.68
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD2	15	6.68
(2,76)	1:B:708:VAL:HG22	1:A:714:PRO:HD3	15	6.68
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD2	15	6.68
(2,76)	1:B:708:VAL:HG23	1:A:714:PRO:HD3	15	6.68
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB2	10	6.68
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB3	10	6.68
(2,2)	1:A:661:LEU:HD11	1:A:680:TRP:HE1	5	6.68
(2,2)	1:A:661:LEU:HD12	1:A:680:TRP:HE1	5	6.68
(2,2)	1:A:661:LEU:HD13	1:A:680:TRP:HE1	5	6.68
(2,2)	1:A:661:LEU:HD21	1:A:680:TRP:HE1	5	6.68
(2,2)	1:A:661:LEU:HD22	1:A:680:TRP:HE1	5	6.68
(2,2)	1:A:661:LEU:HD23	1:A:680:TRP:HE1	5	6.68
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD2	8	6.67
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD3	8	6.67
(2,39)	1:A:692:LEU:HD21	1:B:694:GLY:H	15	6.61
(2,39)	1:A:692:LEU:HD22	1:B:694:GLY:H	15	6.61
(2,39)	1:A:692:LEU:HD23	1:B:694:GLY:H	15	6.61
(2,80)	1:A:708:VAL:HG21	1:A:714:PRO:HA	15	6.59
(2,80)	1:A:708:VAL:HG22	1:A:714:PRO:HA	15	6.59
(2,80)	1:A:708:VAL:HG23	1:A:714:PRO:HA	15	6.59
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG21	15	6.57
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG22	15	6.57
(2,89)	1:A:713:SER:H	1:B:708:VAL:HG23	15	6.57
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB2	4	6.57
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB3	4	6.57
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB2	4	6.57
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB3	4	6.57
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB2	4	6.57
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB3	4	6.57
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB2	8	6.54
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB3	8	6.54
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB2	8	6.54
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB3	8	6.54
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB2	8	6.54
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB3	8	6.54
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA2	6	6.53
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA3	6	6.53
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB2	14	6.51
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB3	14	6.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB2	14	6.51
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB3	14	6.51
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB2	14	6.51
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB3	14	6.51
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB2	15	6.51
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB3	15	6.51
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB2	15	6.51
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB3	15	6.51
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB2	15	6.51
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB3	15	6.51
(2,39)	1:A:692:LEU:HD21	1:B:694:GLY:H	3	6.5
(2,39)	1:A:692:LEU:HD22	1:B:694:GLY:H	3	6.5
(2,39)	1:A:692:LEU:HD23	1:B:694:GLY:H	3	6.5
(2,80)	1:A:708:VAL:HG21	1:A:714:PRO:HA	8	6.47
(2,80)	1:A:708:VAL:HG22	1:A:714:PRO:HA	8	6.47
(2,80)	1:A:708:VAL:HG23	1:A:714:PRO:HA	8	6.47
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD1	9	6.45
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD2	9	6.45
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD1	9	6.45
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD2	9	6.45
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD1	9	6.45
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD2	9	6.45
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD1	9	6.45
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD2	9	6.45
(2,39)	1:A:692:LEU:HD21	1:B:694:GLY:H	5	6.45
(2,39)	1:A:692:LEU:HD22	1:B:694:GLY:H	5	6.45
(2,39)	1:A:692:LEU:HD23	1:B:694:GLY:H	5	6.45
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB2	13	6.44
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB3	13	6.44
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB2	13	6.44
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB3	13	6.44
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB2	13	6.44
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB3	13	6.44
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD2	11	6.43
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD3	11	6.43
(2,20)	1:A:678:TRP:HE1	1:A:683:ARG:HE	2	6.43
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA2	3	6.42
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA3	3	6.42
(2,80)	1:A:708:VAL:HG21	1:A:714:PRO:HA	5	6.41
(2,80)	1:A:708:VAL:HG22	1:A:714:PRO:HA	5	6.41
(2,80)	1:A:708:VAL:HG23	1:A:714:PRO:HA	5	6.41
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB2	8	6.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB3	8	6.4
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB2	8	6.39
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB3	8	6.39
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB2	8	6.39
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB3	8	6.39
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB2	8	6.39
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB3	8	6.39
(2,39)	1:A:692:LEU:HD21	1:B:694:GLY:H	12	6.38
(2,39)	1:A:692:LEU:HD22	1:B:694:GLY:H	12	6.38
(2,39)	1:A:692:LEU:HD23	1:B:694:GLY:H	12	6.38
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB2	1	6.36
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB3	1	6.36
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB2	1	6.36
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB3	1	6.36
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB2	1	6.36
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB3	1	6.36
(2,39)	1:A:692:LEU:HD21	1:B:694:GLY:H	10	6.36
(2,39)	1:A:692:LEU:HD22	1:B:694:GLY:H	10	6.36
(2,39)	1:A:692:LEU:HD23	1:B:694:GLY:H	10	6.36
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD2	11	6.35
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD3	11	6.35
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD2	11	6.35
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD3	11	6.35
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD2	11	6.35
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD3	11	6.35
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD2	2	6.34
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD3	2	6.34
(2,2)	1:A:661:LEU:HD11	1:A:680:TRP:HE1	1	6.34
(2,2)	1:A:661:LEU:HD12	1:A:680:TRP:HE1	1	6.34
(2,2)	1:A:661:LEU:HD13	1:A:680:TRP:HE1	1	6.34
(2,2)	1:A:661:LEU:HD21	1:A:680:TRP:HE1	1	6.34
(2,2)	1:A:661:LEU:HD22	1:A:680:TRP:HE1	1	6.34
(2,2)	1:A:661:LEU:HD23	1:A:680:TRP:HE1	1	6.34
(2,2)	1:A:661:LEU:HD11	1:A:680:TRP:HE1	3	6.34
(2,2)	1:A:661:LEU:HD12	1:A:680:TRP:HE1	3	6.34
(2,2)	1:A:661:LEU:HD13	1:A:680:TRP:HE1	3	6.34
(2,2)	1:A:661:LEU:HD21	1:A:680:TRP:HE1	3	6.34
(2,2)	1:A:661:LEU:HD22	1:A:680:TRP:HE1	3	6.34
(2,2)	1:A:661:LEU:HD23	1:A:680:TRP:HE1	3	6.34
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB2	13	6.33
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB3	13	6.33
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB2	13	6.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB3	13	6.33
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB2	13	6.33
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB3	13	6.33
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA2	2	6.32
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA3	2	6.32
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA2	4	6.31
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA3	4	6.31
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD2	7	6.3
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD3	7	6.3
(2,80)	1:A:708:VAL:HG21	1:A:714:PRO:HA	7	6.3
(2,80)	1:A:708:VAL:HG22	1:A:714:PRO:HA	7	6.3
(2,80)	1:A:708:VAL:HG23	1:A:714:PRO:HA	7	6.3
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA2	9	6.28
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA3	9	6.28
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD21	6	6.28
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD22	6	6.28
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD23	6	6.28
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	10	6.28
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	10	6.28
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	10	6.28
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	10	6.28
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	10	6.28
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	10	6.28
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	10	6.28
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	10	6.28
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	10	6.28
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	10	6.28
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	10	6.28
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	10	6.28
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	10	6.28
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	10	6.28
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	10	6.28
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	10	6.28
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD2	8	6.26
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD3	8	6.26
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD2	8	6.26
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD3	8	6.26
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD2	8	6.26
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD3	8	6.26
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD21	13	6.25
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD22	13	6.25
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD23	13	6.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB2	6	6.19
(2,7)	1:B:664:ASP:H	1:A:660:LEU:HB3	6	6.19
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD2	12	6.15
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD3	12	6.15
(2,39)	1:A:692:LEU:HD21	1:B:694:GLY:H	14	6.15
(2,39)	1:A:692:LEU:HD22	1:B:694:GLY:H	14	6.15
(2,39)	1:A:692:LEU:HD23	1:B:694:GLY:H	14	6.15
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD2	7	6.13
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD3	7	6.13
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD2	7	6.13
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD3	7	6.13
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD2	7	6.13
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD3	7	6.13
(2,39)	1:A:692:LEU:HD21	1:B:694:GLY:H	9	6.12
(2,39)	1:A:692:LEU:HD22	1:B:694:GLY:H	9	6.12
(2,39)	1:A:692:LEU:HD23	1:B:694:GLY:H	9	6.12
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD21	15	6.11
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD22	15	6.11
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD23	15	6.11
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD2	10	6.1
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD3	10	6.1
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD2	10	6.1
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD3	10	6.1
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD2	10	6.1
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD3	10	6.1
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB2	15	6.1
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB3	15	6.1
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB2	15	6.1
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB3	15	6.1
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB2	15	6.1
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB3	15	6.1
(2,39)	1:A:692:LEU:HD21	1:B:694:GLY:H	1	6.09
(2,39)	1:A:692:LEU:HD22	1:B:694:GLY:H	1	6.09
(2,39)	1:A:692:LEU:HD23	1:B:694:GLY:H	1	6.09
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA2	1	6.07
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA3	1	6.07
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA2	7	6.06
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA3	7	6.06
(2,3)	1:A:661:LEU:HD11	1:B:680:TRP:HE1	11	6.05
(2,3)	1:A:661:LEU:HD12	1:B:680:TRP:HE1	11	6.05
(2,3)	1:A:661:LEU:HD13	1:B:680:TRP:HE1	11	6.05
(2,3)	1:A:661:LEU:HD21	1:B:680:TRP:HE1	11	6.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:A:661:LEU:HD22	1:B:680:TRP:HE1	11	6.05
(2,3)	1:A:661:LEU:HD23	1:B:680:TRP:HE1	11	6.05
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD2	5	6.03
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD3	5	6.03
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD2	14	6.0
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD3	14	6.0
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB2	7	6.0
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB3	7	6.0
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB2	7	6.0
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB3	7	6.0
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB2	7	6.0
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB3	7	6.0
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD21	3	6.0
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD22	3	6.0
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD23	3	6.0
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD2	15	5.98
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD3	15	5.98
(2,80)	1:A:708:VAL:HG21	1:A:714:PRO:HA	2	5.97
(2,80)	1:A:708:VAL:HG22	1:A:714:PRO:HA	2	5.97
(2,80)	1:A:708:VAL:HG23	1:A:714:PRO:HA	2	5.97
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD1	1	5.96
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD2	1	5.96
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD1	1	5.96
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD2	1	5.96
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD1	1	5.96
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD2	1	5.96
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD1	1	5.96
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD2	1	5.96
(2,39)	1:A:692:LEU:HD21	1:B:694:GLY:H	2	5.96
(2,39)	1:A:692:LEU:HD22	1:B:694:GLY:H	2	5.96
(2,39)	1:A:692:LEU:HD23	1:B:694:GLY:H	2	5.96
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD2	1	5.95
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD3	1	5.95
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD21	5	5.95
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD22	5	5.95
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD23	5	5.95
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD2	10	5.94
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD3	10	5.94
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB1	12	5.94
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB2	12	5.94
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB3	12	5.94
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB1	12	5.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB2	12	5.94
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB3	12	5.94
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB1	12	5.94
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB2	12	5.94
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB3	12	5.94
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB2	7	5.9
(2,70)	1:B:708:VAL:HG21	1:A:712:TYR:HB3	7	5.9
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB2	7	5.9
(2,70)	1:B:708:VAL:HG22	1:A:712:TYR:HB3	7	5.9
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB2	7	5.9
(2,70)	1:B:708:VAL:HG23	1:A:712:TYR:HB3	7	5.9
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB1	15	5.88
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB2	15	5.88
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB3	15	5.88
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB1	15	5.88
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB2	15	5.88
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB3	15	5.88
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB1	15	5.88
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB2	15	5.88
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB3	15	5.88
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD21	12	5.88
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD22	12	5.88
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD23	12	5.88
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD2	15	5.86
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD3	15	5.86
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD2	15	5.86
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD3	15	5.86
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD2	15	5.86
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD3	15	5.86
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD21	10	5.86
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD22	10	5.86
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD23	10	5.86
(2,39)	1:A:692:LEU:HD21	1:B:694:GLY:H	11	5.86
(2,39)	1:A:692:LEU:HD22	1:B:694:GLY:H	11	5.86
(2,39)	1:A:692:LEU:HD23	1:B:694:GLY:H	11	5.86
(2,80)	1:A:708:VAL:HG21	1:A:714:PRO:HA	10	5.85
(2,80)	1:A:708:VAL:HG22	1:A:714:PRO:HA	10	5.85
(2,80)	1:A:708:VAL:HG23	1:A:714:PRO:HA	10	5.85
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA2	10	5.85
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA3	10	5.85
(2,39)	1:A:692:LEU:HD21	1:B:694:GLY:H	7	5.84
(2,39)	1:A:692:LEU:HD22	1:B:694:GLY:H	7	5.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,39)	1:A:692:LEU:HD23	1:B:694:GLY:H	7	5.84
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA2	12	5.83
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA3	12	5.83
(2,2)	1:A:661:LEU:HD11	1:A:680:TRP:HE1	8	5.83
(2,2)	1:A:661:LEU:HD12	1:A:680:TRP:HE1	8	5.83
(2,2)	1:A:661:LEU:HD13	1:A:680:TRP:HE1	8	5.83
(2,2)	1:A:661:LEU:HD21	1:A:680:TRP:HE1	8	5.83
(2,2)	1:A:661:LEU:HD22	1:A:680:TRP:HE1	8	5.83
(2,2)	1:A:661:LEU:HD23	1:A:680:TRP:HE1	8	5.83
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD2	4	5.82
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD3	4	5.82
(2,3)	1:A:661:LEU:HD11	1:B:680:TRP:HE1	1	5.79
(2,3)	1:A:661:LEU:HD12	1:B:680:TRP:HE1	1	5.79
(2,3)	1:A:661:LEU:HD13	1:B:680:TRP:HE1	1	5.79
(2,3)	1:A:661:LEU:HD21	1:B:680:TRP:HE1	1	5.79
(2,3)	1:A:661:LEU:HD22	1:B:680:TRP:HE1	1	5.79
(2,3)	1:A:661:LEU:HD23	1:B:680:TRP:HE1	1	5.79
(2,3)	1:A:661:LEU:HD11	1:B:680:TRP:HE1	7	5.78
(2,3)	1:A:661:LEU:HD12	1:B:680:TRP:HE1	7	5.78
(2,3)	1:A:661:LEU:HD13	1:B:680:TRP:HE1	7	5.78
(2,3)	1:A:661:LEU:HD21	1:B:680:TRP:HE1	7	5.78
(2,3)	1:A:661:LEU:HD22	1:B:680:TRP:HE1	7	5.78
(2,3)	1:A:661:LEU:HD23	1:B:680:TRP:HE1	7	5.78
(2,2)	1:A:661:LEU:HD11	1:A:680:TRP:HE1	10	5.77
(2,2)	1:A:661:LEU:HD12	1:A:680:TRP:HE1	10	5.77
(2,2)	1:A:661:LEU:HD13	1:A:680:TRP:HE1	10	5.77
(2,2)	1:A:661:LEU:HD21	1:A:680:TRP:HE1	10	5.77
(2,2)	1:A:661:LEU:HD22	1:A:680:TRP:HE1	10	5.77
(2,2)	1:A:661:LEU:HD23	1:A:680:TRP:HE1	10	5.77
(2,2)	1:A:661:LEU:HD11	1:A:680:TRP:HE1	13	5.77
(2,2)	1:A:661:LEU:HD12	1:A:680:TRP:HE1	13	5.77
(2,2)	1:A:661:LEU:HD13	1:A:680:TRP:HE1	13	5.77
(2,2)	1:A:661:LEU:HD21	1:A:680:TRP:HE1	13	5.77
(2,2)	1:A:661:LEU:HD22	1:A:680:TRP:HE1	13	5.77
(2,2)	1:A:661:LEU:HD23	1:A:680:TRP:HE1	13	5.77
(2,80)	1:A:708:VAL:HG21	1:A:714:PRO:HA	1	5.76
(2,80)	1:A:708:VAL:HG22	1:A:714:PRO:HA	1	5.76
(2,80)	1:A:708:VAL:HG23	1:A:714:PRO:HA	1	5.76
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH21	13	5.76
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH22	13	5.76
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH21	13	5.76
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH22	13	5.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH21	13	5.76
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH22	13	5.76
(2,80)	1:A:708:VAL:HG21	1:A:714:PRO:HA	14	5.75
(2,80)	1:A:708:VAL:HG22	1:A:714:PRO:HA	14	5.75
(2,80)	1:A:708:VAL:HG23	1:A:714:PRO:HA	14	5.75
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB2	2	5.74
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB3	2	5.74
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB2	2	5.74
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB3	2	5.74
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB2	2	5.74
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB3	2	5.74
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB2	10	5.74
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB3	10	5.74
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB2	10	5.74
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB3	10	5.74
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB2	10	5.74
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB3	10	5.74
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD2	9	5.73
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD3	9	5.73
(2,80)	1:A:708:VAL:HG21	1:A:714:PRO:HA	12	5.73
(2,80)	1:A:708:VAL:HG22	1:A:714:PRO:HA	12	5.73
(2,80)	1:A:708:VAL:HG23	1:A:714:PRO:HA	12	5.73
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD2	14	5.71
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD3	14	5.71
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD2	14	5.71
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD3	14	5.71
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD2	14	5.71
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD3	14	5.71
(2,80)	1:A:708:VAL:HG21	1:A:714:PRO:HA	6	5.69
(2,80)	1:A:708:VAL:HG22	1:A:714:PRO:HA	6	5.69
(2,80)	1:A:708:VAL:HG23	1:A:714:PRO:HA	6	5.69
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD21	14	5.65
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD22	14	5.65
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD23	14	5.65
(2,80)	1:A:708:VAL:HG21	1:A:714:PRO:HA	9	5.63
(2,80)	1:A:708:VAL:HG22	1:A:714:PRO:HA	9	5.63
(2,80)	1:A:708:VAL:HG23	1:A:714:PRO:HA	9	5.63
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD21	9	5.62
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD22	9	5.62
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD23	9	5.62
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD1	14	5.61
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD2	14	5.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD1	14	5.61
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD2	14	5.61
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD1	14	5.61
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD2	14	5.61
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD1	14	5.61
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD2	14	5.61
(2,2)	1:A:661:LEU:HD11	1:A:680:TRP:HE1	7	5.6
(2,2)	1:A:661:LEU:HD12	1:A:680:TRP:HE1	7	5.6
(2,2)	1:A:661:LEU:HD13	1:A:680:TRP:HE1	7	5.6
(2,2)	1:A:661:LEU:HD21	1:A:680:TRP:HE1	7	5.6
(2,2)	1:A:661:LEU:HD22	1:A:680:TRP:HE1	7	5.6
(2,2)	1:A:661:LEU:HD23	1:A:680:TRP:HE1	7	5.6
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	4	5.6
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	4	5.6
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	4	5.6
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	4	5.6
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	4	5.6
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	4	5.6
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	4	5.6
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	4	5.6
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	4	5.6
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	4	5.6
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	4	5.6
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	4	5.6
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	4	5.6
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	4	5.6
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	4	5.6
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	4	5.6
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD2	1	5.59
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD3	1	5.59
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD2	1	5.59
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD3	1	5.59
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD2	1	5.59
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD3	1	5.59
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD21	1	5.59
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD22	1	5.59
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD23	1	5.59
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD2	3	5.58
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD3	3	5.58
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD2	5	5.58
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD3	5	5.58
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD2	5	5.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD3	5	5.58
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD2	5	5.58
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD3	5	5.58
(2,80)	1:A:708:VAL:HG21	1:A:714:PRO:HA	3	5.57
(2,80)	1:A:708:VAL:HG22	1:A:714:PRO:HA	3	5.57
(2,80)	1:A:708:VAL:HG23	1:A:714:PRO:HA	3	5.57
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD2	2	5.57
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD3	2	5.57
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD2	2	5.57
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD3	2	5.57
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD2	2	5.57
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD3	2	5.57
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD2	6	5.54
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD3	6	5.54
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD2	6	5.54
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD3	6	5.54
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD2	6	5.54
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD3	6	5.54
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB1	9	5.53
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB2	9	5.53
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB3	9	5.53
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB1	9	5.53
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB2	9	5.53
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB3	9	5.53
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB1	9	5.53
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB2	9	5.53
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB3	9	5.53
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH21	1	5.52
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH22	1	5.52
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH21	1	5.52
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH22	1	5.52
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH21	1	5.52
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH22	1	5.52
(2,39)	1:A:692:LEU:HD21	1:B:694:GLY:H	4	5.52
(2,39)	1:A:692:LEU:HD22	1:B:694:GLY:H	4	5.52
(2,39)	1:A:692:LEU:HD23	1:B:694:GLY:H	4	5.52
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD2	6	5.5
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD3	6	5.5
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD2	12	5.5
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD3	12	5.5
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD2	12	5.5
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD3	12	5.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD2	12	5.5
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD3	12	5.5
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD21	2	5.46
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD22	2	5.46
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD23	2	5.46
(2,3)	1:A:661:LEU:HD11	1:B:680:TRP:HE1	12	5.42
(2,3)	1:A:661:LEU:HD12	1:B:680:TRP:HE1	12	5.42
(2,3)	1:A:661:LEU:HD13	1:B:680:TRP:HE1	12	5.42
(2,3)	1:A:661:LEU:HD21	1:B:680:TRP:HE1	12	5.42
(2,3)	1:A:661:LEU:HD22	1:B:680:TRP:HE1	12	5.42
(2,3)	1:A:661:LEU:HD23	1:B:680:TRP:HE1	12	5.42
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB1	1	5.41
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB2	1	5.41
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB3	1	5.41
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB1	1	5.41
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB2	1	5.41
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB3	1	5.41
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB1	1	5.41
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB2	1	5.41
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB3	1	5.41
(2,2)	1:A:661:LEU:HD11	1:A:680:TRP:HE1	12	5.4
(2,2)	1:A:661:LEU:HD12	1:A:680:TRP:HE1	12	5.4
(2,2)	1:A:661:LEU:HD13	1:A:680:TRP:HE1	12	5.4
(2,2)	1:A:661:LEU:HD21	1:A:680:TRP:HE1	12	5.4
(2,2)	1:A:661:LEU:HD22	1:A:680:TRP:HE1	12	5.4
(2,2)	1:A:661:LEU:HD23	1:A:680:TRP:HE1	12	5.4
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD2	13	5.38
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD3	13	5.38
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD2	13	5.38
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD3	13	5.38
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD2	13	5.38
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD3	13	5.38
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD21	11	5.36
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD22	11	5.36
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD23	11	5.36
(2,80)	1:A:708:VAL:HG21	1:A:714:PRO:HA	13	5.34
(2,80)	1:A:708:VAL:HG22	1:A:714:PRO:HA	13	5.34
(2,80)	1:A:708:VAL:HG23	1:A:714:PRO:HA	13	5.34
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD21	7	5.34
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD22	7	5.34
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD23	7	5.34
(2,80)	1:A:708:VAL:HG21	1:A:714:PRO:HA	4	5.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,80)	1:A:708:VAL:HG22	1:A:714:PRO:HA	4	5.33
(2,80)	1:A:708:VAL:HG23	1:A:714:PRO:HA	4	5.33
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH21	14	5.33
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH22	14	5.33
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH21	14	5.33
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH22	14	5.33
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH21	14	5.33
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH22	14	5.33
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD2	3	5.32
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD3	3	5.32
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD2	3	5.32
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD3	3	5.32
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD2	3	5.32
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD3	3	5.32
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD2	13	5.31
(2,83)	1:A:709:ARG:H	1:A:714:PRO:HD3	13	5.31
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	2	5.29
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	2	5.29
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	2	5.29
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	2	5.29
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	2	5.29
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	2	5.29
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	2	5.29
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	2	5.29
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	2	5.29
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	2	5.29
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	2	5.29
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	2	5.29
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	2	5.29
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	2	5.29
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	2	5.29
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	2	5.29
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB1	13	5.28
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB2	13	5.28
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB3	13	5.28
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB1	13	5.28
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB2	13	5.28
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB3	13	5.28
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB1	13	5.28
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB2	13	5.28
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB3	13	5.28
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA2	14	5.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA3	14	5.28
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB1	6	5.27
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB2	6	5.27
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB3	6	5.27
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB1	6	5.27
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB2	6	5.27
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB3	6	5.27
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB1	6	5.27
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB2	6	5.27
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB3	6	5.27
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	9	5.27
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	9	5.27
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	9	5.27
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	9	5.27
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	9	5.27
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	9	5.27
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	9	5.27
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	9	5.27
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	9	5.27
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	9	5.27
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	9	5.27
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	9	5.27
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	9	5.27
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	9	5.27
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	9	5.27
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	9	5.27
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD2	9	5.23
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD3	9	5.23
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD2	9	5.23
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD3	9	5.23
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD2	9	5.23
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD3	9	5.23
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB1	11	5.2
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB2	11	5.2
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB3	11	5.2
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB1	11	5.2
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB2	11	5.2
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB3	11	5.2
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB1	11	5.2
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB2	11	5.2
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB3	11	5.2
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD11	14	5.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD12	14	5.18
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD13	14	5.18
(2,3)	1:A:661:LEU:HD11	1:B:680:TRP:HE1	5	5.14
(2,3)	1:A:661:LEU:HD12	1:B:680:TRP:HE1	5	5.14
(2,3)	1:A:661:LEU:HD13	1:B:680:TRP:HE1	5	5.14
(2,3)	1:A:661:LEU:HD21	1:B:680:TRP:HE1	5	5.14
(2,3)	1:A:661:LEU:HD22	1:B:680:TRP:HE1	5	5.14
(2,3)	1:A:661:LEU:HD23	1:B:680:TRP:HE1	5	5.14
(2,3)	1:A:661:LEU:HD11	1:B:680:TRP:HE1	9	5.13
(2,3)	1:A:661:LEU:HD12	1:B:680:TRP:HE1	9	5.13
(2,3)	1:A:661:LEU:HD13	1:B:680:TRP:HE1	9	5.13
(2,3)	1:A:661:LEU:HD21	1:B:680:TRP:HE1	9	5.13
(2,3)	1:A:661:LEU:HD22	1:B:680:TRP:HE1	9	5.13
(2,3)	1:A:661:LEU:HD23	1:B:680:TRP:HE1	9	5.13
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD1	4	5.12
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD2	4	5.12
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD1	4	5.12
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD2	4	5.12
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD1	4	5.12
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD2	4	5.12
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD1	4	5.12
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD2	4	5.12
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH21	11	5.12
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH22	11	5.12
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH21	11	5.12
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH22	11	5.12
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH21	11	5.12
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH22	11	5.12
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	6	5.08
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	6	5.08
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	6	5.08
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	6	5.08
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	6	5.08
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	6	5.08
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	6	5.08
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	6	5.08
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	6	5.08
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	6	5.08
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	6	5.08
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	6	5.08
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	6	5.08
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	6	5.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	6	5.08
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	6	5.08
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	1	5.07
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	1	5.07
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	1	5.07
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	1	5.07
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	1	5.07
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	1	5.07
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	1	5.07
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	1	5.07
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	1	5.07
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	1	5.07
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	1	5.07
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	1	5.07
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	1	5.07
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	1	5.07
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	1	5.07
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	1	5.07
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH21	8	5.06
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH22	8	5.06
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH21	8	5.06
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH22	8	5.06
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH21	8	5.06
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH22	8	5.06
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD1	13	5.03
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD2	13	5.03
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD1	13	5.03
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD2	13	5.03
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD1	13	5.03
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD2	13	5.03
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD1	13	5.03
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD2	13	5.03
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD1	12	5.03
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD2	12	5.03
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD1	12	5.03
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD2	12	5.03
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD1	12	5.03
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD2	12	5.03
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD1	12	5.03
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD2	12	5.03
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG21	13	5.03
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG22	13	5.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG23	13	5.03
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG21	13	5.03
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG22	13	5.03
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG23	13	5.03
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG21	13	5.03
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG22	13	5.03
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG23	13	5.03
(2,3)	1:A:661:LEU:HD11	1:B:680:TRP:HE1	3	5.03
(2,3)	1:A:661:LEU:HD12	1:B:680:TRP:HE1	3	5.03
(2,3)	1:A:661:LEU:HD13	1:B:680:TRP:HE1	3	5.03
(2,3)	1:A:661:LEU:HD21	1:B:680:TRP:HE1	3	5.03
(2,3)	1:A:661:LEU:HD22	1:B:680:TRP:HE1	3	5.03
(2,3)	1:A:661:LEU:HD23	1:B:680:TRP:HE1	3	5.03
(2,3)	1:A:661:LEU:HD11	1:B:680:TRP:HE1	13	5.03
(2,3)	1:A:661:LEU:HD12	1:B:680:TRP:HE1	13	5.03
(2,3)	1:A:661:LEU:HD13	1:B:680:TRP:HE1	13	5.03
(2,3)	1:A:661:LEU:HD21	1:B:680:TRP:HE1	13	5.03
(2,3)	1:A:661:LEU:HD22	1:B:680:TRP:HE1	13	5.03
(2,3)	1:A:661:LEU:HD23	1:B:680:TRP:HE1	13	5.03
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD21	4	5.02
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD22	4	5.02
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD23	4	5.02
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG21	3	5.0
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG22	3	5.0
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG23	3	5.0
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG21	3	5.0
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG22	3	5.0
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG23	3	5.0
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG21	3	5.0
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG22	3	5.0
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG23	3	5.0
(2,3)	1:A:661:LEU:HD11	1:B:680:TRP:HE1	2	4.99
(2,3)	1:A:661:LEU:HD12	1:B:680:TRP:HE1	2	4.99
(2,3)	1:A:661:LEU:HD13	1:B:680:TRP:HE1	2	4.99
(2,3)	1:A:661:LEU:HD21	1:B:680:TRP:HE1	2	4.99
(2,3)	1:A:661:LEU:HD22	1:B:680:TRP:HE1	2	4.99
(2,3)	1:A:661:LEU:HD23	1:B:680:TRP:HE1	2	4.99
(2,3)	1:A:661:LEU:HD11	1:B:680:TRP:HE1	6	4.98
(2,3)	1:A:661:LEU:HD12	1:B:680:TRP:HE1	6	4.98
(2,3)	1:A:661:LEU:HD13	1:B:680:TRP:HE1	6	4.98
(2,3)	1:A:661:LEU:HD21	1:B:680:TRP:HE1	6	4.98
(2,3)	1:A:661:LEU:HD22	1:B:680:TRP:HE1	6	4.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:A:661:LEU:HD23	1:B:680:TRP:HE1	6	4.98
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB1	4	4.97
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB2	4	4.97
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB3	4	4.97
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB1	4	4.97
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB2	4	4.97
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB3	4	4.97
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB1	4	4.97
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB2	4	4.97
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB3	4	4.97
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD1	11	4.97
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD2	11	4.97
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD1	11	4.97
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD2	11	4.97
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD1	11	4.97
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD2	11	4.97
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD1	11	4.97
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD2	11	4.97
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA2	8	4.97
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA3	8	4.97
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD2	4	4.96
(2,77)	1:A:708:VAL:HG21	1:A:714:PRO:HD3	4	4.96
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD2	4	4.96
(2,77)	1:A:708:VAL:HG22	1:A:714:PRO:HD3	4	4.96
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD2	4	4.96
(2,77)	1:A:708:VAL:HG23	1:A:714:PRO:HD3	4	4.96
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB2	12	4.96
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB3	12	4.96
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB2	12	4.96
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB3	12	4.96
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB2	12	4.96
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB3	12	4.96
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH21	12	4.95
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH22	12	4.95
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH21	12	4.95
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH22	12	4.95
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH21	12	4.95
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH22	12	4.95
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	14	4.95
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	14	4.95
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	14	4.95
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	14	4.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	14	4.95
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	14	4.95
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	14	4.95
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	14	4.95
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	14	4.95
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	14	4.95
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	14	4.95
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	14	4.95
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	14	4.95
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	14	4.95
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	14	4.95
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	14	4.95
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD1	2	4.94
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD2	2	4.94
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD1	2	4.94
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD2	2	4.94
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD1	2	4.94
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD2	2	4.94
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD1	2	4.94
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD2	2	4.94
(2,3)	1:A:661:LEU:HD11	1:B:680:TRP:HE1	8	4.92
(2,3)	1:A:661:LEU:HD12	1:B:680:TRP:HE1	8	4.92
(2,3)	1:A:661:LEU:HD13	1:B:680:TRP:HE1	8	4.92
(2,3)	1:A:661:LEU:HD21	1:B:680:TRP:HE1	8	4.92
(2,3)	1:A:661:LEU:HD22	1:B:680:TRP:HE1	8	4.92
(2,3)	1:A:661:LEU:HD23	1:B:680:TRP:HE1	8	4.92
(2,3)	1:A:661:LEU:HD11	1:B:680:TRP:HE1	14	4.92
(2,3)	1:A:661:LEU:HD12	1:B:680:TRP:HE1	14	4.92
(2,3)	1:A:661:LEU:HD13	1:B:680:TRP:HE1	14	4.92
(2,3)	1:A:661:LEU:HD21	1:B:680:TRP:HE1	14	4.92
(2,3)	1:A:661:LEU:HD22	1:B:680:TRP:HE1	14	4.92
(2,3)	1:A:661:LEU:HD23	1:B:680:TRP:HE1	14	4.92
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB1	14	4.91
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB2	14	4.91
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB3	14	4.91
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB1	14	4.91
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB2	14	4.91
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB3	14	4.91
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB1	14	4.91
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB2	14	4.91
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB3	14	4.91
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD11	13	4.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD12	13	4.91
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD13	13	4.91
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG21	2	4.91
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG22	2	4.91
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG23	2	4.91
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG21	2	4.91
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG22	2	4.91
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG23	2	4.91
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG21	2	4.91
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG22	2	4.91
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG23	2	4.91
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD11	1	4.9
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD12	1	4.9
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD13	1	4.9
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD11	12	4.9
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD12	12	4.9
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD13	12	4.9
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	3	4.9
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	3	4.9
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	3	4.9
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	3	4.9
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	3	4.9
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	3	4.9
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	3	4.9
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	3	4.9
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	3	4.9
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	3	4.9
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	3	4.9
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	3	4.9
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	3	4.9
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	3	4.9
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	3	4.9
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	3	4.9
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB1	10	4.89
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB2	10	4.89
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB3	10	4.89
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB1	10	4.89
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB2	10	4.89
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB3	10	4.89
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB1	10	4.89
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB2	10	4.89
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB3	10	4.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH21	10	4.89
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH22	10	4.89
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH21	10	4.89
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH22	10	4.89
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH21	10	4.89
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH22	10	4.89
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG21	12	4.88
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG22	12	4.88
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG23	12	4.88
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG21	12	4.88
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG22	12	4.88
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG23	12	4.88
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG21	12	4.88
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG22	12	4.88
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG23	12	4.88
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG21	14	4.88
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG22	14	4.88
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG23	14	4.88
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG21	14	4.88
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG22	14	4.88
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG23	14	4.88
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG21	14	4.88
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG22	14	4.88
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG23	14	4.88
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG21	10	4.86
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG22	10	4.86
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG23	10	4.86
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE1	1	4.86
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE2	1	4.86
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE1	1	4.86
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE2	1	4.86
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE1	1	4.86
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE2	1	4.86
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD11	8	4.86
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD12	8	4.86
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD13	8	4.86
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB1	5	4.85
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB2	5	4.85
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB3	5	4.85
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB1	5	4.85
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB2	5	4.85
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB3	5	4.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB1	5	4.85
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB2	5	4.85
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB3	5	4.85
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG21	5	4.85
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG22	5	4.85
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG23	5	4.85
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG21	5	4.85
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG22	5	4.85
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG23	5	4.85
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG21	5	4.85
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG22	5	4.85
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG23	5	4.85
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG21	4	4.83
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG22	4	4.83
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG23	4	4.83
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG21	4	4.83
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG22	4	4.83
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG23	4	4.83
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG21	4	4.83
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG22	4	4.83
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG23	4	4.83
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH21	7	4.81
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH22	7	4.81
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH21	7	4.81
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH22	7	4.81
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH21	7	4.81
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH22	7	4.81
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG11	6	4.79
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG12	6	4.79
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG13	6	4.79
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG21	8	4.77
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG22	8	4.77
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG23	8	4.77
(2,2)	1:A:661:LEU:HD11	1:A:680:TRP:HE1	14	4.74
(2,2)	1:A:661:LEU:HD12	1:A:680:TRP:HE1	14	4.74
(2,2)	1:A:661:LEU:HD13	1:A:680:TRP:HE1	14	4.74
(2,2)	1:A:661:LEU:HD21	1:A:680:TRP:HE1	14	4.74
(2,2)	1:A:661:LEU:HD22	1:A:680:TRP:HE1	14	4.74
(2,2)	1:A:661:LEU:HD23	1:A:680:TRP:HE1	14	4.74
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG21	14	4.73
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG22	14	4.73
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG23	14	4.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	8	4.73
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	8	4.73
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	8	4.73
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	8	4.73
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	8	4.73
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	8	4.73
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	8	4.73
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	8	4.73
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	8	4.73
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	8	4.73
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	8	4.73
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	8	4.73
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	8	4.73
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	8	4.73
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	8	4.73
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	8	4.73
(2,2)	1:A:661:LEU:HD11	1:A:680:TRP:HE1	9	4.7
(2,2)	1:A:661:LEU:HD12	1:A:680:TRP:HE1	9	4.7
(2,2)	1:A:661:LEU:HD13	1:A:680:TRP:HE1	9	4.7
(2,2)	1:A:661:LEU:HD21	1:A:680:TRP:HE1	9	4.7
(2,2)	1:A:661:LEU:HD22	1:A:680:TRP:HE1	9	4.7
(2,2)	1:A:661:LEU:HD23	1:A:680:TRP:HE1	9	4.7
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG21	9	4.68
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG22	9	4.68
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG23	9	4.68
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG21	9	4.68
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG22	9	4.68
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG23	9	4.68
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG21	9	4.68
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG22	9	4.68
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG23	9	4.68
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	9	4.67
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	9	4.67
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	9	4.67
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	9	4.67
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	9	4.67
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	9	4.67
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	9	4.67
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	9	4.67
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	9	4.67
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	9	4.67
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	9	4.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	9	4.67
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	9	4.67
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	9	4.67
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	9	4.67
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	9	4.67
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD11	11	4.66
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD12	11	4.66
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD13	11	4.66
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG21	1	4.63
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG22	1	4.63
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG23	1	4.63
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG21	1	4.63
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG22	1	4.63
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG23	1	4.63
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG21	1	4.63
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG22	1	4.63
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG23	1	4.63
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG21	7	4.61
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG22	7	4.61
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG23	7	4.61
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD1	5	4.61
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD2	5	4.61
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD1	5	4.61
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD2	5	4.61
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD1	5	4.61
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD2	5	4.61
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD1	5	4.61
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD2	5	4.61
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG21	15	4.59
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG22	15	4.59
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG23	15	4.59
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB1	2	4.57
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB2	2	4.57
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB3	2	4.57
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB1	2	4.57
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB2	2	4.57
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB3	2	4.57
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB1	2	4.57
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB2	2	4.57
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB3	2	4.57
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA2	11	4.57
(2,57)	1:A:696:ARG:HE	1:B:694:GLY:HA3	11	4.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:A:661:LEU:HD11	1:A:680:TRP:HE1	15	4.57
(2,2)	1:A:661:LEU:HD12	1:A:680:TRP:HE1	15	4.57
(2,2)	1:A:661:LEU:HD13	1:A:680:TRP:HE1	15	4.57
(2,2)	1:A:661:LEU:HD21	1:A:680:TRP:HE1	15	4.57
(2,2)	1:A:661:LEU:HD22	1:A:680:TRP:HE1	15	4.57
(2,2)	1:A:661:LEU:HD23	1:A:680:TRP:HE1	15	4.57
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD11	5	4.56
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD12	5	4.56
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD13	5	4.56
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG21	11	4.56
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG22	11	4.56
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG23	11	4.56
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG21	11	4.56
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG22	11	4.56
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG23	11	4.56
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG21	11	4.56
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG22	11	4.56
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG23	11	4.56
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB1	8	4.55
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB2	8	4.55
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB3	8	4.55
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB1	8	4.55
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB2	8	4.55
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB3	8	4.55
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB1	8	4.55
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB2	8	4.55
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB3	8	4.55
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD11	4	4.54
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD12	4	4.54
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD13	4	4.54
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG21	6	4.53
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG22	6	4.53
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG23	6	4.53
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD1	8	4.5
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD2	8	4.5
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD1	8	4.5
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD2	8	4.5
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD1	8	4.5
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD2	8	4.5
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD1	8	4.5
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD2	8	4.5
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD11	2	4.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD12	2	4.5
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD13	2	4.5
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG21	1	4.48
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG22	1	4.48
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG23	1	4.48
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG21	11	4.47
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG22	11	4.47
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG23	11	4.47
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB1	3	4.47
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB2	3	4.47
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB3	3	4.47
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB1	3	4.47
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB2	3	4.47
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB3	3	4.47
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB1	3	4.47
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB2	3	4.47
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB3	3	4.47
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD1	1	4.45
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD2	1	4.45
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD1	1	4.45
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD2	1	4.45
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD1	1	4.45
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD2	1	4.45
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD1	1	4.45
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD2	1	4.45
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB2	9	4.43
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB3	9	4.43
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD1	9	4.41
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD2	9	4.41
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD1	9	4.41
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD2	9	4.41
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD1	9	4.41
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD2	9	4.41
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD1	9	4.41
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD2	9	4.41
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD1	6	4.38
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD2	6	4.38
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD1	6	4.38
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD2	6	4.38
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD1	6	4.38
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD2	6	4.38
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD1	6	4.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD2	6	4.38
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG11	10	4.38
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG12	10	4.38
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG13	10	4.38
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE1	10	4.37
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE2	10	4.37
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE1	10	4.37
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE2	10	4.37
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE1	10	4.37
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE2	10	4.37
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG21	12	4.33
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG22	12	4.33
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG23	12	4.33
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD11	7	4.31
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD12	7	4.31
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD13	7	4.31
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB2	11	4.3
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB3	11	4.3
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB2	11	4.3
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB3	11	4.3
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB2	11	4.3
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB3	11	4.3
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB2	12	4.28
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB3	12	4.28
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG21	2	4.26
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG22	2	4.26
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG23	2	4.26
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG11	8	4.25
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG12	8	4.25
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG13	8	4.25
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD1	12	4.23
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD2	12	4.23
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD1	12	4.23
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD2	12	4.23
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD1	12	4.23
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD2	12	4.23
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD1	12	4.23
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD2	12	4.23
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH21	9	4.23
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH22	9	4.23
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH21	9	4.23
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH22	9	4.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH21	9	4.23
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH22	9	4.23
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE1	6	4.22
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE2	6	4.22
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE1	6	4.22
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE2	6	4.22
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE1	6	4.22
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE2	6	4.22
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD1	12	4.21
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD2	12	4.21
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD1	12	4.21
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD2	12	4.21
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD1	12	4.21
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD2	12	4.21
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG21	13	4.2
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG22	13	4.2
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG23	13	4.2
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD1	3	4.19
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD2	3	4.19
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD1	3	4.19
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD2	3	4.19
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD1	3	4.19
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD2	3	4.19
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD1	3	4.19
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD2	3	4.19
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD11	14	4.18
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD12	14	4.18
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD13	14	4.18
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG21	3	4.15
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG22	3	4.15
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG23	3	4.15
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH21	4	4.15
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH22	4	4.15
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH21	4	4.15
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH22	4	4.15
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH21	4	4.15
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH22	4	4.15
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD11	12	4.15
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD12	12	4.15
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD13	12	4.15
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB2	9	4.14
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB3	9	4.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB2	9	4.14
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB3	9	4.14
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB2	9	4.14
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB3	9	4.14
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE1	15	4.12
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE2	15	4.12
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE1	15	4.12
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE2	15	4.12
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE1	15	4.12
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE2	15	4.12
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE1	15	4.12
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE2	15	4.12
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB2	8	4.11
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB3	8	4.11
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB2	8	4.11
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB3	8	4.11
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB2	8	4.11
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB3	8	4.11
(2,2)	1:A:661:LEU:HD11	1:A:680:TRP:HE1	6	4.11
(2,2)	1:A:661:LEU:HD12	1:A:680:TRP:HE1	6	4.11
(2,2)	1:A:661:LEU:HD13	1:A:680:TRP:HE1	6	4.11
(2,2)	1:A:661:LEU:HD21	1:A:680:TRP:HE1	6	4.11
(2,2)	1:A:661:LEU:HD22	1:A:680:TRP:HE1	6	4.11
(2,2)	1:A:661:LEU:HD23	1:A:680:TRP:HE1	6	4.11
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	11	4.11
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	11	4.11
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	11	4.11
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	11	4.11
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	11	4.11
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	11	4.11
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	11	4.11
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	11	4.11
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	11	4.11
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	11	4.11
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	11	4.11
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	11	4.11
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	11	4.11
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	11	4.11
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	11	4.11
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	11	4.11
(2,39)	1:A:692:LEU:HD21	1:B:694:GLY:H	8	4.1
(2,39)	1:A:692:LEU:HD22	1:B:694:GLY:H	8	4.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,39)	1:A:692:LEU:HD23	1:B:694:GLY:H	8	4.1
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH21	3	4.06
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH22	3	4.06
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH21	3	4.06
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH22	3	4.06
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH21	3	4.06
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH22	3	4.06
(2,3)	1:A:661:LEU:HD11	1:B:680:TRP:HE1	15	4.06
(2,3)	1:A:661:LEU:HD12	1:B:680:TRP:HE1	15	4.06
(2,3)	1:A:661:LEU:HD13	1:B:680:TRP:HE1	15	4.06
(2,3)	1:A:661:LEU:HD21	1:B:680:TRP:HE1	15	4.06
(2,3)	1:A:661:LEU:HD22	1:B:680:TRP:HE1	15	4.06
(2,3)	1:A:661:LEU:HD23	1:B:680:TRP:HE1	15	4.06
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	15	4.05
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	15	4.05
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	15	4.05
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	15	4.05
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	15	4.05
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	15	4.05
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	15	4.05
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	15	4.05
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	15	4.05
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	15	4.05
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	15	4.05
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	15	4.05
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	15	4.05
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	15	4.05
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	15	4.05
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	15	4.05
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB2	15	4.04
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB3	15	4.04
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB2	15	4.04
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB3	15	4.04
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB2	15	4.04
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB3	15	4.04
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH21	4	4.03
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH22	4	4.03
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH21	4	4.03
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH22	4	4.03
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH21	4	4.03
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH22	4	4.03
(2,2)	1:A:661:LEU:HD11	1:A:680:TRP:HE1	4	4.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:A:661:LEU:HD12	1:A:680:TRP:HE1	4	4.03
(2,2)	1:A:661:LEU:HD13	1:A:680:TRP:HE1	4	4.03
(2,2)	1:A:661:LEU:HD21	1:A:680:TRP:HE1	4	4.03
(2,2)	1:A:661:LEU:HD22	1:A:680:TRP:HE1	4	4.03
(2,2)	1:A:661:LEU:HD23	1:A:680:TRP:HE1	4	4.03
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	15	4.02
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	15	4.02
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	15	4.02
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	15	4.02
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	15	4.02
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	15	4.02
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	15	4.02
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	15	4.02
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	15	4.02
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	15	4.02
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	15	4.02
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	15	4.02
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	15	4.02
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	15	4.02
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	15	4.02
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	15	4.02
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB2	13	4.01
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB3	13	4.01
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB2	13	4.01
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB3	13	4.01
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB2	13	4.01
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB3	13	4.01
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG21	7	4.0
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG22	7	4.0
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG23	7	4.0
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG21	7	4.0
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG22	7	4.0
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG23	7	4.0
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG21	7	4.0
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG22	7	4.0
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG23	7	4.0
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG21	15	4.0
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG22	15	4.0
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG23	15	4.0
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG21	15	4.0
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG22	15	4.0
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG23	15	4.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG21	15	4.0
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG22	15	4.0
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG23	15	4.0
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB2	5	3.98
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB3	5	3.98
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD11	3	3.98
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD12	3	3.98
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD13	3	3.98
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB2	7	3.97
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB3	7	3.97
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB2	7	3.97
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB3	7	3.97
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB2	7	3.97
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB3	7	3.97
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE1	13	3.95
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE2	13	3.95
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE1	13	3.95
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE2	13	3.95
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE1	13	3.95
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE2	13	3.95
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE1	13	3.95
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE2	13	3.95
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD11	9	3.95
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD12	9	3.95
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD13	9	3.95
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD1	15	3.94
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD2	15	3.94
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD1	15	3.94
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD2	15	3.94
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD1	15	3.94
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD2	15	3.94
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD1	15	3.94
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD2	15	3.94
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD11	13	3.92
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD12	13	3.92
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD13	13	3.92
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG21	9	3.91
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG22	9	3.91
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG23	9	3.91
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD11	1	3.91
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD12	1	3.91
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD13	1	3.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH21	5	3.9
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH22	5	3.9
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH21	5	3.9
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH22	5	3.9
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH21	5	3.9
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH22	5	3.9
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD11	15	3.89
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD12	15	3.89
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD13	15	3.89
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB2	3	3.88
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB3	3	3.88
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB2	3	3.88
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB3	3	3.88
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB2	3	3.88
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB3	3	3.88
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD11	2	3.88
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD12	2	3.88
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD13	2	3.88
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD11	5	3.86
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD12	5	3.86
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD13	5	3.86
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH21	2	3.85
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH22	2	3.85
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH21	2	3.85
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH22	2	3.85
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH21	2	3.85
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH22	2	3.85
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE1	3	3.84
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE2	3	3.84
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE1	3	3.84
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE2	3	3.84
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE1	3	3.84
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE2	3	3.84
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH21	8	3.82
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH22	8	3.82
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH21	8	3.82
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH22	8	3.82
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH21	8	3.82
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH22	8	3.82
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG21	6	3.81
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG22	6	3.81
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG23	6	3.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG21	6	3.81
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG22	6	3.81
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG23	6	3.81
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG21	6	3.81
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG22	6	3.81
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG23	6	3.81
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD11	7	3.8
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD12	7	3.8
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD13	7	3.8
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB2	5	3.79
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB3	5	3.79
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB2	5	3.79
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB3	5	3.79
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB2	5	3.79
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB3	5	3.79
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	5	3.79
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	5	3.79
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	5	3.79
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	5	3.79
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	5	3.79
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	5	3.79
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	5	3.79
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	5	3.79
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	5	3.79
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	5	3.79
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	5	3.79
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	5	3.79
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	5	3.79
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	5	3.79
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	5	3.79
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	5	3.79
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH21	15	3.78
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH22	15	3.78
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH21	15	3.78
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH22	15	3.78
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH21	15	3.78
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH22	15	3.78
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB2	6	3.76
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB3	6	3.76
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB2	6	3.76
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB3	6	3.76
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB2	6	3.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB3	6	3.76
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB2	2	3.76
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB3	2	3.76
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB2	6	3.75
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB3	6	3.75
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE1	4	3.75
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE2	4	3.75
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE1	4	3.75
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE2	4	3.75
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE1	4	3.75
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE2	4	3.75
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE1	2	3.74
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE2	2	3.74
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE1	2	3.74
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE2	2	3.74
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE1	2	3.74
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE2	2	3.74
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH21	10	3.74
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH22	10	3.74
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH21	10	3.74
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH22	10	3.74
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH21	10	3.74
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH22	10	3.74
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB2	13	3.73
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB3	13	3.73
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB2	10	3.73
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB3	10	3.73
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB2	10	3.73
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB3	10	3.73
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB2	10	3.73
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB3	10	3.73
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH21	9	3.72
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH22	9	3.72
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH21	9	3.72
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH22	9	3.72
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH21	9	3.72
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH22	9	3.72
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB2	10	3.69
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB3	10	3.69
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB2	10	3.69
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB3	10	3.69
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB2	10	3.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB3	10	3.69
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB2	14	3.69
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB3	14	3.69
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB2	14	3.69
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB3	14	3.69
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB2	14	3.69
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB3	14	3.69
(2,2)	1:A:661:LEU:HD11	1:A:680:TRP:HE1	11	3.68
(2,2)	1:A:661:LEU:HD12	1:A:680:TRP:HE1	11	3.68
(2,2)	1:A:661:LEU:HD13	1:A:680:TRP:HE1	11	3.68
(2,2)	1:A:661:LEU:HD21	1:A:680:TRP:HE1	11	3.68
(2,2)	1:A:661:LEU:HD22	1:A:680:TRP:HE1	11	3.68
(2,2)	1:A:661:LEU:HD23	1:A:680:TRP:HE1	11	3.68
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG21	8	3.67
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG22	8	3.67
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG23	8	3.67
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG21	8	3.67
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG22	8	3.67
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG23	8	3.67
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG21	8	3.67
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG22	8	3.67
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG23	8	3.67
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE1	14	3.65
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE2	14	3.65
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE1	14	3.65
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE2	14	3.65
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE1	14	3.65
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE2	14	3.65
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD11	15	3.65
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD12	15	3.65
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD13	15	3.65
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE1	8	3.64
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE2	8	3.64
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE1	8	3.64
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE2	8	3.64
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE1	8	3.64
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE2	8	3.64
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE1	8	3.64
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE2	8	3.64
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD11	4	3.63
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD12	4	3.63
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD13	4	3.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD1	10	3.61
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD2	10	3.61
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD1	10	3.61
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD2	10	3.61
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD1	10	3.61
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD2	10	3.61
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD1	10	3.61
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD2	10	3.61
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD21	8	3.6
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD22	8	3.6
(2,49)	1:B:694:GLY:H	1:A:692:LEU:HD23	8	3.6
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH21	3	3.6
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH22	3	3.6
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH21	3	3.6
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH22	3	3.6
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH21	3	3.6
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH22	3	3.6
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	2	3.6
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	2	3.6
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	2	3.6
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	2	3.6
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	2	3.6
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	2	3.6
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	2	3.6
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	2	3.6
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	2	3.6
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	2	3.6
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	2	3.6
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	2	3.6
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	2	3.6
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	2	3.6
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	2	3.6
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	2	3.6
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB2	4	3.58
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB3	4	3.58
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB2	4	3.57
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB3	4	3.57
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB2	4	3.57
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB3	4	3.57
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB2	4	3.57
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB3	4	3.57
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG21	5	3.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG22	5	3.54
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG23	5	3.54
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG21	4	3.52
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG22	4	3.52
(2,88)	1:A:713:SER:H	1:A:708:VAL:HG23	4	3.52
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD11	11	3.51
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD12	11	3.51
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD13	11	3.51
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB2	6	3.5
(2,67)	1:B:704:LEU:HD21	1:A:706:ASN:HB3	6	3.5
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB2	6	3.5
(2,67)	1:B:704:LEU:HD22	1:A:706:ASN:HB3	6	3.5
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB2	6	3.5
(2,67)	1:B:704:LEU:HD23	1:A:706:ASN:HB3	6	3.5
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB2	14	3.48
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB3	14	3.48
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB2	14	3.48
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB3	14	3.48
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB2	14	3.48
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB3	14	3.48
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH21	2	3.48
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH22	2	3.48
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH21	2	3.48
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH22	2	3.48
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH21	2	3.48
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH22	2	3.48
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG21	15	3.47
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG22	15	3.47
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG23	15	3.47
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB2	3	3.46
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB3	3	3.46
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD11	14	3.46
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD12	14	3.46
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD13	14	3.46
(2,3)	1:A:661:LEU:HD11	1:B:680:TRP:HE1	10	3.42
(2,3)	1:A:661:LEU:HD12	1:B:680:TRP:HE1	10	3.42
(2,3)	1:A:661:LEU:HD13	1:B:680:TRP:HE1	10	3.42
(2,3)	1:A:661:LEU:HD21	1:B:680:TRP:HE1	10	3.42
(2,3)	1:A:661:LEU:HD22	1:B:680:TRP:HE1	10	3.42
(2,3)	1:A:661:LEU:HD23	1:B:680:TRP:HE1	10	3.42
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB2	6	3.41
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB3	6	3.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB2	6	3.41
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB3	6	3.41
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB2	6	3.41
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB3	6	3.41
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB2	9	3.41
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB3	9	3.41
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB2	9	3.41
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB3	9	3.41
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB2	9	3.41
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB3	9	3.41
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD1	7	3.4
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD2	7	3.4
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD1	7	3.4
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD2	7	3.4
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD1	7	3.4
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD2	7	3.4
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD1	7	3.4
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD2	7	3.4
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB2	5	3.39
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB3	5	3.39
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB2	5	3.39
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB3	5	3.39
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB2	5	3.39
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB3	5	3.39
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH21	7	3.39
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH22	7	3.39
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH21	7	3.39
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH22	7	3.39
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH21	7	3.39
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH22	7	3.39
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB2	1	3.38
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB3	1	3.38
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE1	5	3.38
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE2	5	3.38
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE1	5	3.38
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE2	5	3.38
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE1	5	3.38
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE2	5	3.38
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD11	8	3.35
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD12	8	3.35
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD13	8	3.35
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB1	7	3.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB2	7	3.34
(2,66)	1:A:702:LEU:HD21	1:B:700:ALA:HB3	7	3.34
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB1	7	3.34
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB2	7	3.34
(2,66)	1:A:702:LEU:HD22	1:B:700:ALA:HB3	7	3.34
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB1	7	3.34
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB2	7	3.34
(2,66)	1:A:702:LEU:HD23	1:B:700:ALA:HB3	7	3.34
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG21	10	3.33
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG22	10	3.33
(2,31)	1:B:687:ILE:HG21	1:A:689:VAL:HG23	10	3.33
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG21	10	3.33
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG22	10	3.33
(2,31)	1:B:687:ILE:HG22	1:A:689:VAL:HG23	10	3.33
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG21	10	3.33
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG22	10	3.33
(2,31)	1:B:687:ILE:HG23	1:A:689:VAL:HG23	10	3.33
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG21	12	3.32
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG22	12	3.32
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG23	12	3.32
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE1	12	3.31
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE2	12	3.31
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE1	12	3.31
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE2	12	3.31
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE1	12	3.31
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE2	12	3.31
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE1	9	3.3
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE2	9	3.3
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE1	9	3.3
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE2	9	3.3
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE1	9	3.3
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE2	9	3.3
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB2	1	3.3
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB3	1	3.3
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB2	1	3.3
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB3	1	3.3
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB2	1	3.3
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB3	1	3.3
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD1	13	3.27
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD2	13	3.27
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD1	13	3.27
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD2	13	3.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD1	13	3.27
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD2	13	3.27
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB2	2	3.26
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB3	2	3.26
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB2	2	3.26
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB3	2	3.26
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB2	2	3.26
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB3	2	3.26
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB2	15	3.26
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB3	15	3.26
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD1	15	3.24
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD2	15	3.24
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD1	15	3.24
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD2	15	3.24
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD1	15	3.24
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD2	15	3.24
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD1	15	3.24
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD2	15	3.24
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD11	9	3.24
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD12	9	3.24
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD13	9	3.24
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB2	8	3.22
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB3	8	3.22
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB2	8	3.22
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB3	8	3.22
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB2	8	3.22
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB3	8	3.22
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE1	11	3.21
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE2	11	3.21
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE1	11	3.21
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE2	11	3.21
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE1	11	3.21
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE2	11	3.21
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB2	7	3.21
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB3	7	3.21
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB2	7	3.21
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB3	7	3.21
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB2	7	3.21
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB3	7	3.21
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE1	8	3.2
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE2	8	3.2
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE1	8	3.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE2	8	3.2
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE1	8	3.2
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE2	8	3.2
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD1	7	3.19
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD2	7	3.19
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD1	7	3.19
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD2	7	3.19
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD1	7	3.19
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD2	7	3.19
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB2	3	3.18
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB3	3	3.18
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB2	3	3.18
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB3	3	3.18
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB2	3	3.18
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB3	3	3.18
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD11	15	3.18
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD12	15	3.18
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD13	15	3.18
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB2	10	3.17
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB3	10	3.17
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE1	15	3.15
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE2	15	3.15
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE1	15	3.15
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE2	15	3.15
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE1	15	3.15
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE2	15	3.15
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE1	7	3.14
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE2	7	3.14
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE1	7	3.14
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE2	7	3.14
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE1	7	3.14
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE2	7	3.14
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE1	7	3.14
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE2	7	3.14
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD1	15	3.14
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD2	15	3.14
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD1	15	3.14
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD2	15	3.14
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD1	15	3.14
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD2	15	3.14
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB2	13	3.11
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB3	13	3.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB2	13	3.11
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB3	13	3.11
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB2	13	3.11
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB3	13	3.11
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD1	11	3.11
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD2	11	3.11
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD1	11	3.11
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD2	11	3.11
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD1	11	3.11
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD2	11	3.11
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG11	15	3.1
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG12	15	3.1
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG13	15	3.1
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD1	14	3.09
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD2	14	3.09
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD1	14	3.09
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD2	14	3.09
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD1	14	3.09
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD2	14	3.09
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD1	14	3.09
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD2	14	3.09
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB2	2	3.08
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB3	2	3.08
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD11	12	3.08
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD12	12	3.08
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD13	12	3.08
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD1	10	3.06
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD2	10	3.06
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD1	10	3.06
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD2	10	3.06
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD1	10	3.06
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD2	10	3.06
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD11	7	3.05
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD12	7	3.05
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD13	7	3.05
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	1	3.04
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	1	3.04
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	1	3.04
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	1	3.04
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	1	3.04
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	1	3.04
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	1	3.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	1	3.04
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	1	3.04
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	1	3.04
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	1	3.04
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	1	3.04
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	1	3.04
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	1	3.04
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	1	3.04
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	1	3.04
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE1	13	3.02
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE2	13	3.02
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE1	13	3.02
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE2	13	3.02
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE1	13	3.02
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE2	13	3.02
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB2	1	3.01
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB3	1	3.01
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB2	1	3.01
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB3	1	3.01
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB2	1	3.01
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB3	1	3.01
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG12	13	3.01
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG13	13	3.01
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB1	15	3.0
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB2	15	3.0
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB3	15	3.0
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB1	15	3.0
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB2	15	3.0
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB3	15	3.0
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB1	15	3.0
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB2	15	3.0
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB3	15	3.0
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB1	9	2.99
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB2	9	2.99
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB3	9	2.99
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB1	9	2.99
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB2	9	2.99
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB3	9	2.99
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB1	9	2.99
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB2	9	2.99
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB3	9	2.99
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG12	12	2.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG13	12	2.99
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE1	11	2.98
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE2	11	2.98
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE1	11	2.98
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE2	11	2.98
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE1	11	2.98
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE2	11	2.98
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE1	11	2.98
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE2	11	2.98
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB2	3	2.97
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB3	3	2.97
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB2	3	2.97
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB3	3	2.97
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB2	3	2.97
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB3	3	2.97
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB2	1	2.97
(2,61)	1:B:700:ALA:HB1	1:A:702:LEU:HB3	1	2.97
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB2	1	2.97
(2,61)	1:B:700:ALA:HB2	1:A:702:LEU:HB3	1	2.97
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB2	1	2.97
(2,61)	1:B:700:ALA:HB3	1:A:702:LEU:HB3	1	2.97
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD1	1	2.97
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD2	1	2.97
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD1	1	2.97
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD2	1	2.97
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD1	1	2.97
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD2	1	2.97
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB2	15	2.94
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB3	15	2.94
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB2	15	2.94
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB3	15	2.94
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB2	15	2.94
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB3	15	2.94
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB1	1	2.94
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB2	1	2.94
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB3	1	2.94
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB1	1	2.94
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB2	1	2.94
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB3	1	2.94
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB1	1	2.94
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB2	1	2.94
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB3	1	2.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE1	10	2.93
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE2	10	2.93
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE1	10	2.93
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE2	10	2.93
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE1	10	2.93
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE2	10	2.93
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE1	6	2.93
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE2	6	2.93
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE1	6	2.93
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE2	6	2.93
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE1	6	2.93
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE2	6	2.93
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE1	6	2.93
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE2	6	2.93
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD1	2	2.92
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD2	2	2.92
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD1	2	2.92
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD2	2	2.92
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD1	2	2.92
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD2	2	2.92
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD1	2	2.92
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD2	2	2.92
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD1	14	2.92
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD2	14	2.92
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD1	14	2.92
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD2	14	2.92
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD1	14	2.92
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD2	14	2.92
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH21	11	2.92
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH22	11	2.92
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH21	11	2.92
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH22	11	2.92
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH21	11	2.92
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH22	11	2.92
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB2	12	2.91
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB3	12	2.91
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB2	12	2.91
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB3	12	2.91
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB2	12	2.91
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB3	12	2.91
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB2	7	2.91
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB3	7	2.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB2	7	2.91
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB3	7	2.91
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB2	7	2.91
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB3	7	2.91
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG12	2	2.91
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG13	2	2.91
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB2	15	2.89
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB3	15	2.89
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB2	15	2.89
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB3	15	2.89
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB2	15	2.89
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB3	15	2.89
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB2	7	2.86
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB3	7	2.86
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG12	5	2.86
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG13	5	2.86
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD11	13	2.86
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD12	13	2.86
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD13	13	2.86
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB2	13	2.84
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB3	13	2.84
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB2	13	2.84
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB3	13	2.84
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB2	13	2.84
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB3	13	2.84
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD11	3	2.84
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD12	3	2.84
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD13	3	2.84
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG21	3	2.84
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG22	3	2.84
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG23	3	2.84
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	8	2.84
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	8	2.84
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	8	2.84
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	8	2.84
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	8	2.84
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	8	2.84
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	8	2.84
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	8	2.84
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	8	2.84
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	8	2.84
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	8	2.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	8	2.84
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	8	2.84
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	8	2.84
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	8	2.84
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	8	2.84
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB2	4	2.83
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB3	4	2.83
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB2	4	2.83
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB3	4	2.83
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB2	4	2.83
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB3	4	2.83
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB2	2	2.82
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB3	2	2.82
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB2	2	2.82
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB3	2	2.82
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB2	2	2.82
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB3	2	2.82
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH21	6	2.82
(2,46)	1:B:693:ILE:HD11	1:A:696:ARG:HH22	6	2.82
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH21	6	2.82
(2,46)	1:B:693:ILE:HD12	1:A:696:ARG:HH22	6	2.82
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH21	6	2.82
(2,46)	1:B:693:ILE:HD13	1:A:696:ARG:HH22	6	2.82
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG12	14	2.82
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG13	14	2.82
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE1	6	2.81
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE2	6	2.81
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE1	6	2.81
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE2	6	2.81
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE1	6	2.81
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE2	6	2.81
(2,3)	1:A:661:LEU:HD11	1:B:680:TRP:HE1	4	2.81
(2,3)	1:A:661:LEU:HD12	1:B:680:TRP:HE1	4	2.81
(2,3)	1:A:661:LEU:HD13	1:B:680:TRP:HE1	4	2.81
(2,3)	1:A:661:LEU:HD21	1:B:680:TRP:HE1	4	2.81
(2,3)	1:A:661:LEU:HD22	1:B:680:TRP:HE1	4	2.81
(2,3)	1:A:661:LEU:HD23	1:B:680:TRP:HE1	4	2.81
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	10	2.81
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	10	2.81
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	10	2.81
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	10	2.81
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	10	2.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	10	2.81
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	10	2.81
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	10	2.81
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	10	2.81
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	10	2.81
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	10	2.81
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	10	2.81
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	10	2.81
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	10	2.81
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	10	2.81
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	10	2.81
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD1	8	2.79
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD2	8	2.79
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD1	8	2.79
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD2	8	2.79
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD1	8	2.79
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD2	8	2.79
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	9	2.79
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	9	2.79
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	9	2.79
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	9	2.79
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	9	2.79
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	9	2.79
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	9	2.79
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	9	2.79
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	9	2.79
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	9	2.79
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	9	2.79
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	9	2.79
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	9	2.79
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	9	2.79
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	9	2.79
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	9	2.79
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD1	5	2.78
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD2	5	2.78
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD1	5	2.78
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD2	5	2.78
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD1	5	2.78
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD2	5	2.78
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB2	11	2.77
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB3	11	2.77
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB2	11	2.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB3	11	2.77
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB2	11	2.77
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB3	11	2.77
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB2	11	2.77
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB3	11	2.77
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB1	6	2.77
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB2	6	2.77
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB3	6	2.77
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB1	6	2.77
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB2	6	2.77
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB3	6	2.77
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB1	6	2.77
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB2	6	2.77
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB3	6	2.77
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD1	11	2.76
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD2	11	2.76
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD1	11	2.76
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD2	11	2.76
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD1	11	2.76
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD2	11	2.76
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD1	11	2.76
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD2	11	2.76
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD1	4	2.76
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD2	4	2.76
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD1	4	2.76
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD2	4	2.76
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD1	4	2.76
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD2	4	2.76
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB1	4	2.75
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB2	4	2.75
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB3	4	2.75
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB1	4	2.75
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB2	4	2.75
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB3	4	2.75
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB1	4	2.75
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB2	4	2.75
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB3	4	2.75
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB2	11	2.74
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB3	11	2.74
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG21	14	2.73
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG22	14	2.73
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG23	14	2.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE1	13	2.72
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE2	13	2.72
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE1	13	2.72
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE2	13	2.72
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE1	13	2.72
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE2	13	2.72
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD1	9	2.72
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD2	9	2.72
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD1	9	2.72
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD2	9	2.72
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD1	9	2.72
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD2	9	2.72
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG12	15	2.72
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG13	15	2.72
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD11	10	2.71
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD12	10	2.71
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD13	10	2.71
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB2	3	2.71
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB3	3	2.71
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB2	9	2.7
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB3	9	2.7
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB2	9	2.7
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB3	9	2.7
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB2	9	2.7
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB3	9	2.7
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD1	6	2.7
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD2	6	2.7
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD1	6	2.7
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD2	6	2.7
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD1	6	2.7
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD2	6	2.7
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG12	7	2.68
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG13	7	2.68
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD11	10	2.64
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD12	10	2.64
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD13	10	2.64
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD1	8	2.63
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD2	8	2.63
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD1	8	2.63
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD2	8	2.63
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD1	8	2.63
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD2	8	2.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD1	8	2.63
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD2	8	2.63
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD1	13	2.63
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD2	13	2.63
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD1	13	2.63
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD2	13	2.63
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD1	13	2.63
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD2	13	2.63
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD1	13	2.63
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD2	13	2.63
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	3	2.62
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	3	2.62
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	3	2.62
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	3	2.62
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	3	2.62
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	3	2.62
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	3	2.62
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	3	2.62
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	3	2.62
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	3	2.62
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	3	2.62
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	3	2.62
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	3	2.62
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	3	2.62
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	3	2.62
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	3	2.62
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	6	2.61
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	6	2.61
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	6	2.61
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	6	2.61
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	6	2.61
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	6	2.61
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	6	2.61
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	6	2.61
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	6	2.61
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	6	2.61
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	6	2.61
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	6	2.61
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	6	2.61
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	6	2.61
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	6	2.61
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	6	2.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD1	5	2.6
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD2	5	2.6
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD1	5	2.6
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD2	5	2.6
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD1	5	2.6
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD2	5	2.6
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD1	5	2.6
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD2	5	2.6
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB2	5	2.6
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB3	5	2.6
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB1	2	2.58
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB2	2	2.58
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB3	2	2.58
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB1	2	2.58
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB2	2	2.58
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB3	2	2.58
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB1	2	2.58
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB2	2	2.58
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB3	2	2.58
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB1	10	2.58
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB2	10	2.58
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB3	10	2.58
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB1	10	2.58
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB2	10	2.58
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB3	10	2.58
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB1	10	2.58
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB2	10	2.58
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB3	10	2.58
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG12	4	2.58
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG13	4	2.58
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG21	7	2.57
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG22	7	2.57
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG23	7	2.57
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB2	14	2.56
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB3	14	2.56
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD1	8	2.56
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD2	8	2.56
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD1	8	2.56
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD2	8	2.56
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD1	8	2.56
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD2	8	2.56
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD1	8	2.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD2	8	2.56
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA2	6	2.56
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA3	6	2.56
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA2	15	2.56
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA3	15	2.56
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	8	2.56
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	8	2.56
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	8	2.56
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	8	2.56
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	8	2.56
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	8	2.56
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	8	2.56
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	8	2.56
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	8	2.56
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	8	2.56
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	8	2.56
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	8	2.56
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	8	2.56
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	8	2.56
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	8	2.56
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	8	2.56
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH21	12	2.55
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH22	12	2.55
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH21	12	2.55
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH22	12	2.55
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH21	12	2.55
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH22	12	2.55
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB2	13	2.53
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB3	13	2.53
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD11	4	2.53
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD12	4	2.53
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD13	4	2.53
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	12	2.53
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	12	2.53
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	12	2.53
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	12	2.53
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	12	2.53
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	12	2.53
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	12	2.53
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	12	2.53
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	12	2.53
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	12	2.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	12	2.53
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	12	2.53
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	12	2.53
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	12	2.53
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	12	2.53
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	12	2.53
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD1	2	2.52
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD2	2	2.52
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD1	2	2.52
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD2	2	2.52
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD1	2	2.52
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD2	2	2.52
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD1	11	2.51
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD2	11	2.51
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD1	11	2.51
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD2	11	2.51
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD1	11	2.51
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD2	11	2.51
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD1	11	2.51
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD2	11	2.51
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD1	10	2.51
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD2	10	2.51
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD1	10	2.51
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD2	10	2.51
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD1	10	2.51
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD2	10	2.51
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD1	10	2.51
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD2	10	2.51
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	7	2.51
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	7	2.51
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	7	2.51
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	7	2.51
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	7	2.51
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	7	2.51
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	7	2.51
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	7	2.51
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	5	2.51
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	5	2.51
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	5	2.51
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	5	2.51
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	5	2.51
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	5	2.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	5	2.51
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	5	2.51
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	7	2.51
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	7	2.51
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	7	2.51
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	7	2.51
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	7	2.51
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	7	2.51
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	7	2.51
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	7	2.51
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	5	2.51
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	5	2.51
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	5	2.51
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	5	2.51
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	5	2.51
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	5	2.51
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	5	2.51
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	5	2.51
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB2	7	2.5
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB3	7	2.5
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG21	4	2.5
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG22	4	2.5
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG23	4	2.5
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	3	2.49
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	3	2.49
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	3	2.49
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	3	2.49
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	3	2.49
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	3	2.49
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	3	2.49
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	3	2.49
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	3	2.49
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	3	2.49
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	3	2.49
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	3	2.49
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	3	2.49
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	3	2.49
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	3	2.49
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	3	2.49
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB1	3	2.48
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB2	3	2.48
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB3	3	2.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB1	3	2.48
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB2	3	2.48
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB3	3	2.48
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB1	3	2.48
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB2	3	2.48
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB3	3	2.48
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB1	14	2.48
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB2	14	2.48
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB3	14	2.48
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB1	14	2.48
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB2	14	2.48
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB3	14	2.48
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB1	14	2.48
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB2	14	2.48
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB3	14	2.48
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG12	11	2.48
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG13	11	2.48
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD1	6	2.47
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD2	6	2.47
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD1	6	2.47
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD2	6	2.47
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD1	6	2.47
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD2	6	2.47
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD1	6	2.47
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD2	6	2.47
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB2	14	2.47
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB3	14	2.47
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD1	15	2.46
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD2	15	2.46
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD1	15	2.46
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD2	15	2.46
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD1	15	2.46
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD2	15	2.46
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD1	15	2.46
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD2	15	2.46
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD1	2	2.45
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD2	2	2.45
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD1	2	2.45
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD2	2	2.45
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD1	2	2.45
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD2	2	2.45
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD1	2	2.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD2	2	2.45
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH21	14	2.44
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH22	14	2.44
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH21	14	2.44
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH22	14	2.44
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH21	14	2.44
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH22	14	2.44
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG12	1	2.44
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG13	1	2.44
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB1	11	2.43
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB2	11	2.43
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB3	11	2.43
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB1	11	2.43
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB2	11	2.43
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB3	11	2.43
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB1	11	2.43
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB2	11	2.43
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB3	11	2.43
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG21	2	2.43
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG22	2	2.43
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG23	2	2.43
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD1	8	2.42
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD2	8	2.42
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD1	8	2.42
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD2	8	2.42
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD1	8	2.42
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD2	8	2.42
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD1	8	2.42
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD2	8	2.42
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD11	2	2.42
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD12	2	2.42
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD13	2	2.42
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	13	2.42
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	13	2.42
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	13	2.42
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	13	2.42
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	13	2.42
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	13	2.42
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	13	2.42
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	13	2.42
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	13	2.42
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	13	2.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	13	2.42
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	13	2.42
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	13	2.42
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	13	2.42
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	13	2.42
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	13	2.42
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB1	12	2.41
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB2	12	2.41
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB3	12	2.41
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB1	12	2.41
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB2	12	2.41
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB3	12	2.41
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB1	12	2.41
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB2	12	2.41
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB3	12	2.41
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD1	9	2.41
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD2	9	2.41
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD1	9	2.41
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD2	9	2.41
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD1	9	2.41
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD2	9	2.41
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD1	9	2.41
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD2	9	2.41
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB1	5	2.4
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB2	5	2.4
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB3	5	2.4
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB1	5	2.4
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB2	5	2.4
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB3	5	2.4
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB1	5	2.4
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB2	5	2.4
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB3	5	2.4
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD11	3	2.39
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD12	3	2.39
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD13	3	2.39
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	2	2.39
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	2	2.39
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	2	2.39
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	2	2.39
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	2	2.39
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	2	2.39
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	2	2.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	2	2.39
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	2	2.39
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	2	2.39
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	2	2.39
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	2	2.39
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	2	2.39
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	2	2.39
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	2	2.39
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	2	2.39
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE1	7	2.38
(2,73)	1:B:708:VAL:HG21	1:A:712:TYR:HE2	7	2.38
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE1	7	2.38
(2,73)	1:B:708:VAL:HG22	1:A:712:TYR:HE2	7	2.38
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE1	7	2.38
(2,73)	1:B:708:VAL:HG23	1:A:712:TYR:HE2	7	2.38
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD1	3	2.38
(2,58)	1:B:700:ALA:HB1	1:A:699:PHE:HD2	3	2.38
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD1	3	2.38
(2,58)	1:B:700:ALA:HB2	1:A:699:PHE:HD2	3	2.38
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD1	3	2.38
(2,58)	1:B:700:ALA:HB3	1:A:699:PHE:HD2	3	2.38
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD11	6	2.38
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD12	6	2.38
(2,54)	1:A:696:ARG:H	1:B:693:ILE:HD13	6	2.38
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE1	14	2.37
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE2	14	2.37
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE1	14	2.37
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE2	14	2.37
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE1	14	2.37
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE2	14	2.37
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH21	13	2.36
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH22	13	2.36
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH21	13	2.36
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH22	13	2.36
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH21	13	2.36
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH22	13	2.36
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD1	15	2.35
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD2	15	2.35
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD1	15	2.35
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD2	15	2.35
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD1	15	2.35
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD2	15	2.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD1	15	2.35
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD2	15	2.35
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB1	13	2.34
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB2	13	2.34
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB3	13	2.34
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB1	13	2.34
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB2	13	2.34
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB3	13	2.34
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB1	13	2.34
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB2	13	2.34
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB3	13	2.34
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	15	2.33
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	15	2.33
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	15	2.33
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	15	2.33
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	15	2.33
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	15	2.33
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	15	2.33
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	15	2.33
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	15	2.33
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	15	2.33
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	15	2.33
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	15	2.33
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	15	2.33
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	15	2.33
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	15	2.33
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	15	2.33
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD11	1	2.32
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD12	1	2.32
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD13	1	2.32
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG12	8	2.31
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG13	8	2.31
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG11	3	2.31
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG12	3	2.31
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG13	3	2.31
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE1	15	2.29
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE2	15	2.29
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE1	15	2.29
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE2	15	2.29
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE1	15	2.29
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE2	15	2.29
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD1	6	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD2	6	2.27
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD1	6	2.27
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD2	6	2.27
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD1	6	2.27
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD2	6	2.27
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD1	6	2.27
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD2	6	2.27
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG12	9	2.27
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG13	9	2.27
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA2	10	2.22
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA3	10	2.22
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB2	8	2.21
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB3	8	2.21
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE1	1	2.21
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE2	1	2.21
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE1	1	2.21
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE2	1	2.21
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE1	1	2.21
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE2	1	2.21
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	14	2.19
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	14	2.19
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	14	2.19
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	14	2.19
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	14	2.19
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	14	2.19
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	14	2.19
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	14	2.19
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	14	2.19
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	14	2.19
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	14	2.19
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	14	2.19
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	14	2.19
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	14	2.19
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	14	2.19
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	14	2.19
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE1	11	2.16
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE2	11	2.16
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE1	11	2.16
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE2	11	2.16
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE1	11	2.16
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE2	11	2.16
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD1	11	2.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD2	11	2.16
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD1	11	2.16
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD2	11	2.16
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD1	11	2.16
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD2	11	2.16
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD1	11	2.16
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD2	11	2.16
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD1	3	2.15
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD2	3	2.15
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD1	3	2.15
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD2	3	2.15
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD1	3	2.15
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD2	3	2.15
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD1	3	2.15
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD2	3	2.15
(2,38)	1:A:692:LEU:HD21	1:A:694:GLY:H	15	2.15
(2,38)	1:A:692:LEU:HD22	1:A:694:GLY:H	15	2.15
(2,38)	1:A:692:LEU:HD23	1:A:694:GLY:H	15	2.15
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	8	2.15
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	8	2.15
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	8	2.15
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	8	2.15
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	8	2.15
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	8	2.15
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	8	2.15
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	8	2.15
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	8	2.15
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	8	2.15
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	8	2.15
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	8	2.15
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	8	2.15
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	8	2.15
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	8	2.15
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	8	2.15
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	12	2.14
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	12	2.14
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	12	2.14
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	12	2.14
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	12	2.14
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	12	2.14
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	12	2.14
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	12	2.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	12	2.14
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	12	2.14
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	12	2.14
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	12	2.14
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	12	2.14
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	12	2.14
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	12	2.14
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	12	2.14
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD11	8	2.12
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD12	8	2.12
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD13	8	2.12
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB2	15	2.1
(2,8)	1:A:664:ASP:H	1:A:660:LEU:HB3	15	2.1
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB1	8	2.1
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB2	8	2.1
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB3	8	2.1
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB1	8	2.1
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB2	8	2.1
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB3	8	2.1
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB1	8	2.1
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB2	8	2.1
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB3	8	2.1
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA2	9	2.1
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA3	9	2.1
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE1	7	2.08
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE2	7	2.08
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE1	7	2.08
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE2	7	2.08
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE1	7	2.08
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE2	7	2.08
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD1	9	2.08
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD2	9	2.08
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD1	9	2.08
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD2	9	2.08
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD1	9	2.08
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD2	9	2.08
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD1	9	2.08
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD2	9	2.08
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA2	4	2.06
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA3	4	2.06
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG11	13	2.06
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG12	13	2.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG13	13	2.06
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	3	2.06
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	3	2.06
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	3	2.06
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	3	2.06
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	3	2.06
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	3	2.06
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	3	2.06
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	3	2.06
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	7	2.06
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	7	2.06
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	7	2.06
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	7	2.06
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	7	2.06
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	7	2.06
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	7	2.06
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	7	2.06
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	3	2.06
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	3	2.06
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	3	2.06
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	3	2.06
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	3	2.06
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	3	2.06
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	3	2.06
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	3	2.06
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	7	2.06
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	7	2.06
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	7	2.06
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	7	2.06
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	7	2.06
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	7	2.06
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	7	2.06
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	7	2.06
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG12	3	2.03
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG13	3	2.03
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE1	8	2.02
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE2	8	2.02
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE1	8	2.02
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE2	8	2.02
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE1	8	2.02
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE2	8	2.02
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD11	6	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD12	6	2.02
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD13	6	2.02
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG11	5	2.02
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG12	5	2.02
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG13	5	2.02
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG21	6	2.0
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG22	6	2.0
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG23	6	2.0
(2,38)	1:A:692:LEU:HD21	1:A:694:GLY:H	14	1.99
(2,38)	1:A:692:LEU:HD22	1:A:694:GLY:H	14	1.99
(2,38)	1:A:692:LEU:HD23	1:A:694:GLY:H	14	1.99
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG11	12	1.98
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG12	12	1.98
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG13	12	1.98
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB2	4	1.97
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB3	4	1.97
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB2	4	1.97
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB3	4	1.97
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB2	4	1.97
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB3	4	1.97
(2,38)	1:A:692:LEU:HD21	1:A:694:GLY:H	12	1.97
(2,38)	1:A:692:LEU:HD22	1:A:694:GLY:H	12	1.97
(2,38)	1:A:692:LEU:HD23	1:A:694:GLY:H	12	1.97
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE1	3	1.96
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE2	3	1.96
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE1	3	1.96
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE2	3	1.96
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE1	3	1.96
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE2	3	1.96
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH21	5	1.94
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH22	5	1.94
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH21	5	1.94
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH22	5	1.94
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH21	5	1.94
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH22	5	1.94
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG11	4	1.94
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG12	4	1.94
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG13	4	1.94
(2,38)	1:A:692:LEU:HD21	1:A:694:GLY:H	3	1.93
(2,38)	1:A:692:LEU:HD22	1:A:694:GLY:H	3	1.93
(2,38)	1:A:692:LEU:HD23	1:A:694:GLY:H	3	1.93
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD11	5	1.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD12	5	1.93
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD13	5	1.93
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA2	13	1.92
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA3	13	1.92
(2,38)	1:A:692:LEU:HD21	1:A:694:GLY:H	13	1.92
(2,38)	1:A:692:LEU:HD22	1:A:694:GLY:H	13	1.92
(2,38)	1:A:692:LEU:HD23	1:A:694:GLY:H	13	1.92
(2,38)	1:A:692:LEU:HD21	1:A:694:GLY:H	9	1.91
(2,38)	1:A:692:LEU:HD22	1:A:694:GLY:H	9	1.91
(2,38)	1:A:692:LEU:HD23	1:A:694:GLY:H	9	1.91
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE1	12	1.9
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE2	12	1.9
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE1	12	1.9
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE2	12	1.9
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE1	12	1.9
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE2	12	1.9
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD1	13	1.9
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD2	13	1.9
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD1	13	1.9
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD2	13	1.9
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD1	13	1.9
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD2	13	1.9
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD1	13	1.9
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD2	13	1.9
(2,38)	1:A:692:LEU:HD21	1:A:694:GLY:H	6	1.9
(2,38)	1:A:692:LEU:HD22	1:A:694:GLY:H	6	1.9
(2,38)	1:A:692:LEU:HD23	1:A:694:GLY:H	6	1.9
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB2	5	1.89
(2,71)	1:A:708:VAL:HG21	1:A:712:TYR:HB3	5	1.89
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB2	5	1.89
(2,71)	1:A:708:VAL:HG22	1:A:712:TYR:HB3	5	1.89
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB2	5	1.89
(2,71)	1:A:708:VAL:HG23	1:A:712:TYR:HB3	5	1.89
(2,38)	1:A:692:LEU:HD21	1:A:694:GLY:H	1	1.89
(2,38)	1:A:692:LEU:HD22	1:A:694:GLY:H	1	1.89
(2,38)	1:A:692:LEU:HD23	1:A:694:GLY:H	1	1.89
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB2	8	1.88
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB3	8	1.88
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH21	1	1.87
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH22	1	1.87
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH21	1	1.87
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH22	1	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH21	1	1.87
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH22	1	1.87
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB2	12	1.87
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB3	12	1.87
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD11	11	1.87
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD12	11	1.87
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD13	11	1.87
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB2	11	1.86
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB3	11	1.86
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB2	11	1.86
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB3	11	1.86
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB2	11	1.86
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB3	11	1.86
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD1	3	1.82
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD2	3	1.82
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD1	3	1.82
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD2	3	1.82
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD1	3	1.82
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD2	3	1.82
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD1	3	1.82
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD2	3	1.82
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB2	1	1.82
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB3	1	1.82
(2,38)	1:A:692:LEU:HD21	1:A:694:GLY:H	4	1.82
(2,38)	1:A:692:LEU:HD22	1:A:694:GLY:H	4	1.82
(2,38)	1:A:692:LEU:HD23	1:A:694:GLY:H	4	1.82
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	3	1.82
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	3	1.82
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	3	1.82
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	3	1.82
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	3	1.82
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	3	1.82
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	3	1.82
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	3	1.82
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	3	1.82
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	3	1.82
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	3	1.82
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	3	1.82
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	3	1.82
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	3	1.82
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	3	1.82
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	3	1.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD1	4	1.81
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD2	4	1.81
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD1	4	1.81
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD2	4	1.81
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD1	4	1.81
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD2	4	1.81
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD1	4	1.81
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD2	4	1.81
(2,38)	1:A:692:LEU:HD21	1:A:694:GLY:H	5	1.81
(2,38)	1:A:692:LEU:HD22	1:A:694:GLY:H	5	1.81
(2,38)	1:A:692:LEU:HD23	1:A:694:GLY:H	5	1.81
(2,38)	1:A:692:LEU:HD21	1:A:694:GLY:H	7	1.81
(2,38)	1:A:692:LEU:HD22	1:A:694:GLY:H	7	1.81
(2,38)	1:A:692:LEU:HD23	1:A:694:GLY:H	7	1.81
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD11	6	1.81
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD12	6	1.81
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD13	6	1.81
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA2	11	1.79
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA3	11	1.79
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB2	2	1.78
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB3	2	1.78
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB2	2	1.78
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB3	2	1.78
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB2	2	1.78
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB3	2	1.78
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD11	9	1.78
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD12	9	1.78
(2,28)	1:B:687:ILE:H	1:A:686:ILE:HD13	9	1.78
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG21	13	1.78
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG22	13	1.78
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG23	13	1.78
(2,38)	1:A:692:LEU:HD21	1:A:694:GLY:H	11	1.77
(2,38)	1:A:692:LEU:HD22	1:A:694:GLY:H	11	1.77
(2,38)	1:A:692:LEU:HD23	1:A:694:GLY:H	11	1.77
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	5	1.77
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	5	1.77
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	5	1.77
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	5	1.77
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	5	1.77
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	5	1.77
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	5	1.77
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	5	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	8	1.77
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	8	1.77
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	8	1.77
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	8	1.77
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	8	1.77
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	8	1.77
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	8	1.77
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	8	1.77
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	5	1.77
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	5	1.77
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	5	1.77
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	5	1.77
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	5	1.77
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	5	1.77
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	5	1.77
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	5	1.77
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	8	1.77
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	8	1.77
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	8	1.77
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	8	1.77
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	8	1.77
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	8	1.77
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	8	1.77
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	8	1.77
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG11	1	1.74
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG12	1	1.74
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG13	1	1.74
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB2	9	1.71
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB3	9	1.71
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB2	9	1.71
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB3	9	1.71
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB2	9	1.71
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB3	9	1.71
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB2	10	1.71
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB3	10	1.71
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB2	10	1.71
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB3	10	1.71
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB2	10	1.71
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB3	10	1.71
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA2	12	1.71
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA3	12	1.71
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD1	10	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD2	10	1.69
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD1	10	1.69
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD2	10	1.69
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD1	10	1.69
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD2	10	1.69
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD1	10	1.69
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD2	10	1.69
(2,38)	1:A:692:LEU:HD21	1:A:694:GLY:H	2	1.69
(2,38)	1:A:692:LEU:HD22	1:A:694:GLY:H	2	1.69
(2,38)	1:A:692:LEU:HD23	1:A:694:GLY:H	2	1.69
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB2	9	1.67
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB3	9	1.67
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	7	1.66
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	7	1.66
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	7	1.66
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	7	1.66
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	7	1.66
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	7	1.66
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	7	1.66
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	7	1.66
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	7	1.66
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	7	1.66
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	7	1.66
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	7	1.66
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	7	1.66
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	7	1.66
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	7	1.66
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	7	1.66
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD21	15	1.65
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD22	15	1.65
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD23	15	1.65
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG11	2	1.64
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG12	2	1.64
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG13	2	1.64
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	10	1.63
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	10	1.63
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	10	1.63
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	10	1.63
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	10	1.63
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	10	1.63
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	10	1.63
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	10	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	10	1.63
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	10	1.63
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	10	1.63
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	10	1.63
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	10	1.63
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	10	1.63
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	10	1.63
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	10	1.63
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	15	1.62
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	15	1.62
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	15	1.62
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	15	1.62
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	15	1.62
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	15	1.62
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	15	1.62
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	15	1.62
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	15	1.62
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	15	1.62
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	15	1.62
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	15	1.62
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	15	1.62
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	15	1.62
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	15	1.62
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	15	1.62
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA2	7	1.6
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA3	7	1.6
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD1	2	1.58
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD2	2	1.58
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD1	2	1.58
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD2	2	1.58
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD1	2	1.58
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD2	2	1.58
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD1	2	1.58
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD2	2	1.58
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	12	1.58
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	12	1.58
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	12	1.58
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	12	1.58
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	12	1.58
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	12	1.58
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	12	1.58
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	12	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	12	1.58
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	12	1.58
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	12	1.58
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	12	1.58
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	12	1.58
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	12	1.58
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	12	1.58
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	12	1.58
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG11	11	1.57
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG12	11	1.57
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG13	11	1.57
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG11	14	1.57
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG12	14	1.57
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG13	14	1.57
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB2	6	1.55
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB3	6	1.55
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB2	6	1.55
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB3	6	1.55
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB2	6	1.55
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB3	6	1.55
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE1	2	1.54
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE2	2	1.54
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE1	2	1.54
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE2	2	1.54
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE1	2	1.54
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE2	2	1.54
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA2	8	1.51
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA3	8	1.51
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD1	7	1.5
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD2	7	1.5
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD1	7	1.5
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD2	7	1.5
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD1	7	1.5
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD2	7	1.5
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD1	7	1.5
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD2	7	1.5
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA2	14	1.5
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA3	14	1.5
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG21	5	1.5
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG22	5	1.5
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG23	5	1.5
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	4	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	4	1.5
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	4	1.5
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	4	1.5
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	4	1.5
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	4	1.5
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	4	1.5
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	4	1.5
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	4	1.5
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	4	1.5
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	4	1.5
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	4	1.5
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	4	1.5
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	4	1.5
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	4	1.5
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	4	1.5
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD21	14	1.49
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD22	14	1.49
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD23	14	1.49
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB2	5	1.48
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB3	5	1.48
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB2	5	1.48
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB3	5	1.48
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB2	5	1.48
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB3	5	1.48
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA2	5	1.48
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA3	5	1.48
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG11	9	1.48
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG12	9	1.48
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG13	9	1.48
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD21	12	1.47
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD22	12	1.47
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD23	12	1.47
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	15	1.47
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	15	1.47
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	15	1.47
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	15	1.47
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	15	1.47
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	15	1.47
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	15	1.47
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	15	1.47
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	15	1.47
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	15	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	15	1.47
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	15	1.47
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	15	1.47
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	15	1.47
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	15	1.47
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	15	1.47
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA2	2	1.46
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA3	2	1.46
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH21	15	1.46
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH22	15	1.46
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH21	15	1.46
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH22	15	1.46
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH21	15	1.46
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH22	15	1.46
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG11	7	1.44
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG12	7	1.44
(2,34)	1:B:690:GLY:H	1:A:689:VAL:HG13	7	1.44
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD21	3	1.43
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD22	3	1.43
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD23	3	1.43
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD1	4	1.42
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD2	4	1.42
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD1	4	1.42
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD2	4	1.42
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD1	4	1.42
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD2	4	1.42
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD1	4	1.42
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD2	4	1.42
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD21	13	1.42
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD22	13	1.42
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD23	13	1.42
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD21	9	1.41
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD22	9	1.41
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD23	9	1.41
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD11	10	1.41
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD12	10	1.41
(2,45)	1:A:693:ILE:H	1:B:693:ILE:HD13	10	1.41
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD21	6	1.4
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD22	6	1.4
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD23	6	1.4
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD1	14	1.39
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD2	14	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD1	14	1.39
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD2	14	1.39
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD1	14	1.39
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD2	14	1.39
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD1	14	1.39
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD2	14	1.39
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD21	1	1.39
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD22	1	1.39
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD23	1	1.39
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE1	9	1.38
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE2	9	1.38
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE1	9	1.38
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE2	9	1.38
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE1	9	1.38
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE2	9	1.38
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB2	3	1.37
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB3	3	1.37
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB2	3	1.37
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB3	3	1.37
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB2	3	1.37
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB3	3	1.37
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB2	8	1.37
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB3	8	1.37
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB2	8	1.37
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB3	8	1.37
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB2	8	1.37
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB3	8	1.37
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	1	1.37
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	1	1.37
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	1	1.37
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	1	1.37
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	1	1.37
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	1	1.37
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	1	1.37
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	1	1.37
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	1	1.37
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	1	1.37
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	1	1.37
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	1	1.37
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	1	1.37
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	1	1.37
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	1	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	1	1.37
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE1	12	1.36
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE2	12	1.36
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE1	12	1.36
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE2	12	1.36
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE1	12	1.36
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE2	12	1.36
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE1	12	1.36
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE2	12	1.36
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD1	7	1.35
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD2	7	1.35
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD1	7	1.35
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD2	7	1.35
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD1	7	1.35
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD2	7	1.35
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD1	7	1.35
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD2	7	1.35
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	14	1.34
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	14	1.34
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	14	1.34
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	14	1.34
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	14	1.34
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	14	1.34
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	14	1.34
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	14	1.34
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	14	1.34
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	14	1.34
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	14	1.34
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	14	1.34
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	14	1.34
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	14	1.34
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	14	1.34
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	14	1.34
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	14	1.33
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	14	1.33
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	14	1.33
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	14	1.33
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	14	1.33
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	14	1.33
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	14	1.33
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	14	1.33
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	14	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	14	1.33
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	14	1.33
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	14	1.33
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	14	1.33
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	14	1.33
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	14	1.33
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	14	1.33
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD21	4	1.32
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD22	4	1.32
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD23	4	1.32
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD21	5	1.31
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD22	5	1.31
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD23	5	1.31
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD21	7	1.31
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD22	7	1.31
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD23	7	1.31
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB2	12	1.29
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB3	12	1.29
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB2	12	1.29
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB3	12	1.29
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB2	12	1.29
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB3	12	1.29
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA2	3	1.27
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA3	3	1.27
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD21	11	1.27
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD22	11	1.27
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD23	11	1.27
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH21	6	1.27
(2,47)	1:A:693:ILE:HD11	1:A:696:ARG:HH22	6	1.27
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH21	6	1.27
(2,47)	1:A:693:ILE:HD12	1:A:696:ARG:HH22	6	1.27
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH21	6	1.27
(2,47)	1:A:693:ILE:HD13	1:A:696:ARG:HH22	6	1.27
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	11	1.26
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	11	1.26
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	11	1.26
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	11	1.26
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	11	1.26
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	11	1.26
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	11	1.26
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	11	1.26
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD2	4	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD3	4	1.26
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	11	1.26
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	11	1.26
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	11	1.26
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	11	1.26
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	11	1.26
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	11	1.26
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	11	1.26
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	11	1.26
(2,41)	1:A:693:ILE:H	1:A:693:ILE:HG12	11	1.25
(2,41)	1:A:693:ILE:H	1:A:693:ILE:HG13	11	1.25
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB2	10	1.25
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB3	10	1.25
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	13	1.25
(2,1486)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	13	1.25
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	13	1.25
(2,1486)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	13	1.25
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	13	1.25
(2,1486)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	13	1.25
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	13	1.25
(2,1486)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	13	1.25
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD2	1	1.25
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD3	1	1.25
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD1	13	1.25
(2,1061)	1:A:761:ARG:HH11	1:A:758:ASP:OD2	13	1.25
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD1	13	1.25
(2,1061)	1:A:761:ARG:HH12	1:A:758:ASP:OD2	13	1.25
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD1	13	1.25
(2,1061)	1:A:761:ARG:HH21	1:A:758:ASP:OD2	13	1.25
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD1	13	1.25
(2,1061)	1:A:761:ARG:HH22	1:A:758:ASP:OD2	13	1.25
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	6	1.23
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	6	1.23
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	6	1.23
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	6	1.23
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	6	1.23
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	6	1.23
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	6	1.23
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	6	1.23
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	6	1.23
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	6	1.23
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	6	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	6	1.23
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	6	1.23
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	6	1.23
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	6	1.23
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	6	1.23
(2,15)	1:A:666:TRP:HE1	1:B:666:TRP:HD1	15	1.22
(2,38)	1:A:692:LEU:HD21	1:A:694:GLY:H	10	1.2
(2,38)	1:A:692:LEU:HD22	1:A:694:GLY:H	10	1.2
(2,38)	1:A:692:LEU:HD23	1:A:694:GLY:H	10	1.2
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE1	9	1.19
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE2	9	1.19
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE1	9	1.19
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE2	9	1.19
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE1	9	1.19
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE2	9	1.19
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE1	9	1.19
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE2	9	1.19
(2,622)	1:B:802:TYR:H	1:B:803:TRP:HH2	9	1.19
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD21	2	1.19
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD22	2	1.19
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD23	2	1.19
(2,15)	1:A:666:TRP:HE1	1:B:666:TRP:HD1	12	1.19
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE1	10	1.18
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE2	10	1.18
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE1	10	1.18
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE2	10	1.18
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE1	10	1.18
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE2	10	1.18
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE1	10	1.18
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE2	10	1.18
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD1	12	1.17
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD2	12	1.17
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD1	12	1.17
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD2	12	1.17
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD1	12	1.17
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD2	12	1.17
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD1	12	1.17
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD2	12	1.17
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD2	12	1.17
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD3	12	1.17
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB1	7	1.16
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB2	7	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,65)	1:A:702:LEU:HD21	1:A:700:ALA:HB3	7	1.16
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB1	7	1.16
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB2	7	1.16
(2,65)	1:A:702:LEU:HD22	1:A:700:ALA:HB3	7	1.16
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB1	7	1.16
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB2	7	1.16
(2,65)	1:A:702:LEU:HD23	1:A:700:ALA:HB3	7	1.16
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD1	14	1.16
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD2	14	1.16
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD1	14	1.16
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD2	14	1.16
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD1	14	1.16
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD2	14	1.16
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD1	14	1.16
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD2	14	1.16
(2,15)	1:A:666:TRP:HE1	1:B:666:TRP:HD1	14	1.16
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	13	1.14
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	13	1.14
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	13	1.14
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	13	1.14
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	13	1.14
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	13	1.14
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	13	1.14
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	13	1.14
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	13	1.14
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	13	1.14
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	13	1.14
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	13	1.14
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	13	1.14
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	13	1.14
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	13	1.14
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	13	1.14
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB2	14	1.13
(2,68)	1:A:704:LEU:HD21	1:A:706:ASN:HB3	14	1.13
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB2	14	1.13
(2,68)	1:A:704:LEU:HD22	1:A:706:ASN:HB3	14	1.13
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB2	14	1.13
(2,68)	1:A:704:LEU:HD23	1:A:706:ASN:HB3	14	1.13
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	1	1.13
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	1	1.13
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	1	1.13
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	1	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	1	1.13
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	1	1.13
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	1	1.13
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	1	1.13
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	1	1.13
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	1	1.13
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	1	1.13
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	1	1.13
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	1	1.13
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	1	1.13
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	1	1.13
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	1	1.13
(2,15)	1:A:666:TRP:HE1	1:B:666:TRP:HD1	10	1.12
(2,15)	1:A:666:TRP:HE1	1:B:666:TRP:HD1	5	1.11
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA2	1	1.1
(2,56)	1:A:696:ARG:HE	1:A:694:GLY:HA3	1	1.1
(2,15)	1:A:666:TRP:HE1	1:B:666:TRP:HD1	7	1.08
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE1	4	1.07
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE2	4	1.07
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE1	4	1.07
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE2	4	1.07
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE1	4	1.07
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE2	4	1.07
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE1	4	1.07
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE2	4	1.07
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD1	5	1.07
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD2	5	1.07
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD1	5	1.07
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD2	5	1.07
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD1	5	1.07
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD2	5	1.07
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD1	5	1.07
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD2	5	1.07
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB2	4	1.07
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB3	4	1.07
(2,15)	1:A:666:TRP:HE1	1:B:666:TRP:HD1	3	1.07
(2,15)	1:A:666:TRP:HE1	1:B:666:TRP:HD1	8	1.07
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	13	1.07
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	13	1.07
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	13	1.07
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	13	1.07
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	13	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	13	1.07
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	13	1.07
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	13	1.07
(2,135)	1:B:756:ILE:H	1:A:796:TRP:HE1	11	1.07
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	13	1.07
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	13	1.07
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	13	1.07
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	13	1.07
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	13	1.07
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	13	1.07
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	13	1.07
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	13	1.07
(2,1472)	1:A:802:TYR:H	1:A:803:TRP:HH2	9	1.05
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	6	1.05
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	6	1.05
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	6	1.05
(2,1047)	1:A:802:TYR:H	1:A:803:TRP:HH2	9	1.05
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	6	1.05
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	6	1.05
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	6	1.05
(2,41)	1:A:693:ILE:H	1:A:693:ILE:HG12	10	1.03
(2,41)	1:A:693:ILE:H	1:A:693:ILE:HG13	10	1.03
(2,15)	1:A:666:TRP:HE1	1:B:666:TRP:HD1	11	1.03
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD2	3	1.03
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD3	3	1.03
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	2	1.02
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	2	1.02
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	2	1.02
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	2	1.02
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	2	1.02
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	2	1.02
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	2	1.02
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	2	1.02
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	2	1.02
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	2	1.02
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	2	1.02
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	2	1.02
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	2	1.02
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	2	1.02
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	2	1.02
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	2	1.02
(2,15)	1:A:666:TRP:HE1	1:B:666:TRP:HD1	9	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD2	6	1.01
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD3	6	1.01
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	11	1.0
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	11	1.0
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	11	1.0
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	11	1.0
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	11	1.0
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	11	1.0
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	11	1.0
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	11	1.0
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	11	1.0
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	11	1.0
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	11	1.0
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	11	1.0
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	11	1.0
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	11	1.0
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	11	1.0
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	11	1.0
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB2	14	0.99
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB3	14	0.99
(2,15)	1:A:666:TRP:HE1	1:B:666:TRP:HD1	1	0.99
(2,778)	1:A:697:ILE:HG21	1:A:698:VAL:HA	9	0.97
(2,778)	1:A:697:ILE:HG22	1:A:698:VAL:HA	9	0.97
(2,778)	1:A:697:ILE:HG23	1:A:698:VAL:HA	9	0.97
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE1	7	0.97
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE2	7	0.97
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE1	7	0.97
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE2	7	0.97
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE1	7	0.97
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE2	7	0.97
(2,1203)	1:A:697:ILE:HG21	1:A:698:VAL:HA	9	0.97
(2,1203)	1:A:697:ILE:HG22	1:A:698:VAL:HA	9	0.97
(2,1203)	1:A:697:ILE:HG23	1:A:698:VAL:HA	9	0.97
(2,956)	1:A:773:ASP:H	1:A:770:ARG:HD2	13	0.96
(2,956)	1:A:773:ASP:H	1:A:770:ARG:HD3	13	0.96
(2,778)	1:A:697:ILE:HG21	1:A:698:VAL:HA	2	0.96
(2,778)	1:A:697:ILE:HG22	1:A:698:VAL:HA	2	0.96
(2,778)	1:A:697:ILE:HG23	1:A:698:VAL:HA	2	0.96
(2,1381)	1:A:773:ASP:H	1:A:770:ARG:HD2	13	0.96
(2,1381)	1:A:773:ASP:H	1:A:770:ARG:HD3	13	0.96
(2,1203)	1:A:697:ILE:HG21	1:A:698:VAL:HA	2	0.96
(2,1203)	1:A:697:ILE:HG22	1:A:698:VAL:HA	2	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1203)	1:A:697:ILE:HG23	1:A:698:VAL:HA	2	0.96
(2,536)	1:B:774:LEU:H	1:B:764:SER:HA	2	0.94
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG21	9	0.94
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG22	9	0.94
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG23	9	0.94
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG21	9	0.94
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG22	9	0.94
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG23	9	0.94
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG21	9	0.94
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG22	9	0.94
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG23	9	0.94
(2,778)	1:A:697:ILE:HG21	1:A:698:VAL:HA	15	0.93
(2,778)	1:A:697:ILE:HG22	1:A:698:VAL:HA	15	0.93
(2,778)	1:A:697:ILE:HG23	1:A:698:VAL:HA	15	0.93
(2,15)	1:A:666:TRP:HE1	1:B:666:TRP:HD1	2	0.93
(2,1203)	1:A:697:ILE:HG21	1:A:698:VAL:HA	15	0.93
(2,1203)	1:A:697:ILE:HG22	1:A:698:VAL:HA	15	0.93
(2,1203)	1:A:697:ILE:HG23	1:A:698:VAL:HA	15	0.93
(2,614)	1:B:793:LEU:H	1:B:790:TRP:HE3	14	0.91
(2,15)	1:A:666:TRP:HE1	1:B:666:TRP:HD1	6	0.91
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	5	0.91
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	5	0.91
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	5	0.91
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	5	0.91
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	5	0.91
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	5	0.91
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	5	0.91
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	5	0.91
(2,1472)	1:A:802:TYR:H	1:A:803:TRP:HH2	7	0.91
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	5	0.91
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	5	0.91
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	5	0.91
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG21	13	0.91
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG22	13	0.91
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG23	13	0.91
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	5	0.91
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	5	0.91
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	5	0.91
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	5	0.91
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	5	0.91
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	5	0.91
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	5	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	5	0.91
(2,1047)	1:A:802:TYR:H	1:A:803:TRP:HH2	7	0.91
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	5	0.91
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	5	0.91
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	5	0.91
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG12	12	0.9
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG13	12	0.9
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG12	12	0.9
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG13	12	0.9
(2,135)	1:B:756:ILE:H	1:A:796:TRP:HE1	7	0.9
(2,1472)	1:A:802:TYR:H	1:A:803:TRP:HH2	6	0.89
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	2	0.89
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	2	0.89
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	2	0.89
(2,1047)	1:A:802:TYR:H	1:A:803:TRP:HH2	6	0.89
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	2	0.89
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	2	0.89
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	2	0.89
(2,778)	1:A:697:ILE:HG21	1:A:698:VAL:HA	3	0.88
(2,778)	1:A:697:ILE:HG22	1:A:698:VAL:HA	3	0.88
(2,778)	1:A:697:ILE:HG23	1:A:698:VAL:HA	3	0.88
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD1	12	0.88
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD2	12	0.88
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD1	12	0.88
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD2	12	0.88
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD1	12	0.88
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD2	12	0.88
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD1	12	0.88
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD2	12	0.88
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB1	3	0.88
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB2	3	0.88
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB3	3	0.88
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD2	13	0.88
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD3	13	0.88
(2,135)	1:B:756:ILE:H	1:A:796:TRP:HE1	15	0.88
(2,1203)	1:A:697:ILE:HG21	1:A:698:VAL:HA	3	0.88
(2,1203)	1:A:697:ILE:HG22	1:A:698:VAL:HA	3	0.88
(2,1203)	1:A:697:ILE:HG23	1:A:698:VAL:HA	3	0.88
(2,778)	1:A:697:ILE:HG21	1:A:698:VAL:HA	4	0.87
(2,778)	1:A:697:ILE:HG22	1:A:698:VAL:HA	4	0.87
(2,778)	1:A:697:ILE:HG23	1:A:698:VAL:HA	4	0.87
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	3	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	3	0.87
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	3	0.87
(2,1203)	1:A:697:ILE:HG21	1:A:698:VAL:HA	4	0.87
(2,1203)	1:A:697:ILE:HG22	1:A:698:VAL:HA	4	0.87
(2,1203)	1:A:697:ILE:HG23	1:A:698:VAL:HA	4	0.87
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	3	0.87
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	3	0.87
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	3	0.87
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB2	1	0.86
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB3	1	0.86
(2,1472)	1:A:802:TYR:H	1:A:803:TRP:HH2	1	0.86
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	8	0.86
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	8	0.86
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	8	0.86
(2,1047)	1:A:802:TYR:H	1:A:803:TRP:HH2	1	0.86
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	8	0.86
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	8	0.86
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	8	0.86
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB2	11	0.85
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB3	11	0.85
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	10	0.85
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	10	0.85
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	10	0.85
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	10	0.85
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	10	0.85
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	10	0.85
(2,622)	1:B:802:TYR:H	1:B:803:TRP:HH2	6	0.85
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB1	13	0.85
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB2	13	0.85
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB3	13	0.85
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	10	0.85
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	10	0.85
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	10	0.85
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	10	0.85
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	10	0.85
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	10	0.85
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	1	0.84
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	1	0.84
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	1	0.84
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	1	0.84
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	1	0.84
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	1	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	1	0.84
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	1	0.84
(2,1472)	1:A:802:TYR:H	1:A:803:TRP:HH2	13	0.84
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	1	0.84
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	1	0.84
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	1	0.84
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	1	0.84
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	1	0.84
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	1	0.84
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	1	0.84
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	1	0.84
(2,1047)	1:A:802:TYR:H	1:A:803:TRP:HH2	13	0.84
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB1	1	0.83
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB2	1	0.83
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB3	1	0.83
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB1	6	0.83
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB2	6	0.83
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB3	6	0.83
(2,41)	1:A:693:ILE:H	1:A:693:ILE:HG12	8	0.83
(2,41)	1:A:693:ILE:H	1:A:693:ILE:HG13	8	0.83
(2,1472)	1:A:802:TYR:H	1:A:803:TRP:HH2	8	0.83
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	12	0.83
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	12	0.83
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	12	0.83
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	15	0.83
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	15	0.83
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	15	0.83
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD2	13	0.83
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD3	13	0.83
(2,1047)	1:A:802:TYR:H	1:A:803:TRP:HH2	8	0.83
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	12	0.83
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	12	0.83
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	12	0.83
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	15	0.83
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	15	0.83
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	15	0.83
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB2	9	0.82
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB3	9	0.82
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD2	11	0.82
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD3	11	0.82
(2,622)	1:B:802:TYR:H	1:B:803:TRP:HH2	1	0.82
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB1	4	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB2	4	0.82
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB3	4	0.82
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB1	15	0.82
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB2	15	0.82
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB3	15	0.82
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB2	6	0.82
(2,4)	1:B:663:LEU:H	1:A:661:LEU:HB3	6	0.82
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB2	7	0.81
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB3	7	0.81
(2,622)	1:B:802:TYR:H	1:B:803:TRP:HH2	11	0.81
(2,1472)	1:A:802:TYR:H	1:A:803:TRP:HH2	14	0.81
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	4	0.81
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	4	0.81
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	4	0.81
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD2	8	0.81
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD3	8	0.81
(2,135)	1:B:756:ILE:H	1:A:796:TRP:HE1	2	0.81
(2,1047)	1:A:802:TYR:H	1:A:803:TRP:HH2	14	0.81
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	4	0.81
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	4	0.81
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	4	0.81
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB1	2	0.8
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB2	2	0.8
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB3	2	0.8
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	7	0.8
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	7	0.8
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	7	0.8
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	7	0.8
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	7	0.8
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	7	0.8
(2,622)	1:B:802:TYR:H	1:B:803:TRP:HH2	5	0.79
(2,531)	1:B:773:ASP:H	1:B:770:ARG:HD2	8	0.79
(2,531)	1:B:773:ASP:H	1:B:770:ARG:HD3	8	0.79
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG21	11	0.79
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG22	11	0.79
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG23	11	0.79
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD2	4	0.78
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD3	4	0.78
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB2	15	0.78
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB3	15	0.78
(2,815)	1:A:704:LEU:H	1:A:704:LEU:HB3	14	0.78
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB1	12	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB2	12	0.78
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB3	12	0.78
(2,390)	1:B:704:LEU:H	1:B:704:LEU:HB3	3	0.78
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG21	3	0.78
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG22	3	0.78
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG23	3	0.78
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG21	3	0.78
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG22	3	0.78
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG23	3	0.78
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG21	3	0.78
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG22	3	0.78
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG23	3	0.78
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	9	0.78
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	9	0.78
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	9	0.78
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	11	0.78
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	11	0.78
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	11	0.78
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD2	4	0.78
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD3	4	0.78
(2,1240)	1:A:704:LEU:H	1:A:704:LEU:HB3	14	0.78
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG21	5	0.78
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG22	5	0.78
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG23	5	0.78
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	9	0.78
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	9	0.78
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	9	0.78
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	11	0.78
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	11	0.78
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	11	0.78
(2,961)	1:A:774:LEU:H	1:A:764:SER:HA	11	0.77
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB2	3	0.77
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB3	3	0.77
(2,622)	1:B:802:TYR:H	1:B:803:TRP:HH2	3	0.77
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB1	5	0.77
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB2	5	0.77
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB3	5	0.77
(2,402)	1:B:705:VAL:HG11	1:B:706:ASN:HA	12	0.77
(2,402)	1:B:705:VAL:HG12	1:B:706:ASN:HA	12	0.77
(2,402)	1:B:705:VAL:HG13	1:B:706:ASN:HA	12	0.77
(2,180)	1:A:806:GLU:H	1:B:771:LEU:HG	11	0.77
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	14	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	14	0.77
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	14	0.77
(2,1386)	1:A:774:LEU:H	1:A:764:SER:HA	11	0.77
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG21	4	0.77
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG22	4	0.77
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG23	4	0.77
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	14	0.77
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	14	0.77
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	14	0.77
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB2	10	0.76
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB3	10	0.76
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD2	13	0.76
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD3	13	0.76
(2,439)	1:B:710:GLN:H	1:B:708:VAL:HA	3	0.76
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	12	0.76
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	12	0.76
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	12	0.76
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	12	0.76
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	12	0.76
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	12	0.76
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	12	0.76
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	12	0.76
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	12	0.76
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	12	0.76
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	12	0.76
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	12	0.76
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	12	0.76
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	12	0.76
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	12	0.76
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	12	0.76
(2,888)	1:A:746:ILE:H	1:A:742:ARG:HA	15	0.75
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD2	15	0.75
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD3	15	0.75
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB1	9	0.75
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB2	9	0.75
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB3	9	0.75
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD11	10	0.75
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD12	10	0.75
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD13	10	0.75
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG21	5	0.75
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG22	5	0.75
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG23	5	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG21	5	0.75
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG22	5	0.75
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG23	5	0.75
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG21	5	0.75
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG22	5	0.75
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG23	5	0.75
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG21	12	0.75
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG22	12	0.75
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG23	12	0.75
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG21	12	0.75
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG22	12	0.75
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG23	12	0.75
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG21	12	0.75
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG22	12	0.75
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG23	12	0.75
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	1	0.75
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	1	0.75
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	1	0.75
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD2	2	0.75
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD3	2	0.75
(2,1313)	1:A:746:ILE:H	1:A:742:ARG:HA	15	0.75
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG21	7	0.75
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG22	7	0.75
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG23	7	0.75
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	1	0.75
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	1	0.75
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	1	0.75
(2,961)	1:A:774:LEU:H	1:A:764:SER:HA	6	0.74
(2,815)	1:A:704:LEU:H	1:A:704:LEU:HB3	3	0.74
(2,622)	1:B:802:TYR:H	1:B:803:TRP:HH2	4	0.74
(2,622)	1:B:802:TYR:H	1:B:803:TRP:HH2	8	0.74
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG21	9	0.74
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG22	9	0.74
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG23	9	0.74
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG12	13	0.74
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG13	13	0.74
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG12	13	0.74
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG13	13	0.74
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB2	7	0.74
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB3	7	0.74
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD2	6	0.74
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD3	6	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	10	0.74
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	10	0.74
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	10	0.74
(2,1386)	1:A:774:LEU:H	1:A:764:SER:HA	6	0.74
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD2	10	0.74
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD3	10	0.74
(2,1240)	1:A:704:LEU:H	1:A:704:LEU:HB3	3	0.74
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD2	6	0.74
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD3	6	0.74
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	10	0.74
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	10	0.74
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	10	0.74
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD2	8	0.73
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD3	8	0.73
(2,439)	1:B:710:GLN:H	1:B:708:VAL:HA	7	0.73
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG21	4	0.73
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG22	4	0.73
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG23	4	0.73
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG21	4	0.73
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG22	4	0.73
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG23	4	0.73
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG21	4	0.73
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG22	4	0.73
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG23	4	0.73
(2,1470)	1:A:802:TYR:H	1:A:802:TYR:HB3	15	0.73
(2,1045)	1:A:802:TYR:H	1:A:802:TYR:HB3	15	0.73
(2,888)	1:A:746:ILE:H	1:A:742:ARG:HA	13	0.72
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB2	4	0.72
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB3	4	0.72
(2,853)	1:A:708:VAL:HG11	1:A:705:VAL:HA	1	0.72
(2,853)	1:A:708:VAL:HG12	1:A:705:VAL:HA	1	0.72
(2,853)	1:A:708:VAL:HG13	1:A:705:VAL:HA	1	0.72
(2,783)	1:A:698:VAL:HG11	1:A:702:LEU:HB2	13	0.72
(2,783)	1:A:698:VAL:HG11	1:A:702:LEU:HB3	13	0.72
(2,783)	1:A:698:VAL:HG12	1:A:702:LEU:HB2	13	0.72
(2,783)	1:A:698:VAL:HG12	1:A:702:LEU:HB3	13	0.72
(2,783)	1:A:698:VAL:HG13	1:A:702:LEU:HB2	13	0.72
(2,783)	1:A:698:VAL:HG13	1:A:702:LEU:HB3	13	0.72
(2,536)	1:B:774:LEU:H	1:B:764:SER:HA	14	0.72
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	10	0.72
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	10	0.72
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	10	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	10	0.72
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	10	0.72
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	10	0.72
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	10	0.72
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	10	0.72
(2,1313)	1:A:746:ILE:H	1:A:742:ARG:HA	13	0.72
(2,1278)	1:A:708:VAL:HG11	1:A:705:VAL:HA	1	0.72
(2,1278)	1:A:708:VAL:HG12	1:A:705:VAL:HA	1	0.72
(2,1278)	1:A:708:VAL:HG13	1:A:705:VAL:HA	1	0.72
(2,1208)	1:A:698:VAL:HG11	1:A:702:LEU:HB2	13	0.72
(2,1208)	1:A:698:VAL:HG11	1:A:702:LEU:HB3	13	0.72
(2,1208)	1:A:698:VAL:HG12	1:A:702:LEU:HB2	13	0.72
(2,1208)	1:A:698:VAL:HG12	1:A:702:LEU:HB3	13	0.72
(2,1208)	1:A:698:VAL:HG13	1:A:702:LEU:HB2	13	0.72
(2,1208)	1:A:698:VAL:HG13	1:A:702:LEU:HB3	13	0.72
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG21	3	0.72
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG22	3	0.72
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG23	3	0.72
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	10	0.72
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	10	0.72
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	10	0.72
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	10	0.72
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	10	0.72
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	10	0.72
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	10	0.72
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	10	0.72
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB1	8	0.71
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB2	8	0.71
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB3	8	0.71
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB1	11	0.71
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB2	11	0.71
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB3	11	0.71
(2,1472)	1:A:802:TYR:H	1:A:803:TRP:HH2	4	0.71
(2,1047)	1:A:802:TYR:H	1:A:803:TRP:HH2	4	0.71
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD2	7	0.7
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD3	7	0.7
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD2	8	0.7
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD3	8	0.7
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB1	7	0.7
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB2	7	0.7
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB3	7	0.7
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD21	10	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD22	10	0.7
(2,50)	1:A:694:GLY:H	1:A:692:LEU:HD23	10	0.7
(2,439)	1:B:710:GLN:H	1:B:708:VAL:HA	15	0.7
(2,180)	1:A:806:GLU:H	1:B:771:LEU:HG	3	0.7
(2,135)	1:B:756:ILE:H	1:A:796:TRP:HE1	12	0.7
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD1	4	0.69
(2,636)	1:B:761:ARG:HH11	1:B:758:ASP:OD2	4	0.69
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD1	4	0.69
(2,636)	1:B:761:ARG:HH12	1:B:758:ASP:OD2	4	0.69
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD1	4	0.69
(2,636)	1:B:761:ARG:HH21	1:B:758:ASP:OD2	4	0.69
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD1	4	0.69
(2,636)	1:B:761:ARG:HH22	1:B:758:ASP:OD2	4	0.69
(2,428)	1:B:708:VAL:HG11	1:B:705:VAL:HA	11	0.69
(2,428)	1:B:708:VAL:HG12	1:B:705:VAL:HA	11	0.69
(2,428)	1:B:708:VAL:HG13	1:B:705:VAL:HA	11	0.69
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG21	11	0.69
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG22	11	0.69
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG23	11	0.69
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG21	11	0.69
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG22	11	0.69
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG23	11	0.69
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG21	11	0.69
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG22	11	0.69
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG23	11	0.69
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG21	14	0.69
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG22	14	0.69
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG23	14	0.69
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG21	14	0.69
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG22	14	0.69
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG23	14	0.69
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG21	14	0.69
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG22	14	0.69
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG23	14	0.69
(2,220)	1:B:663:LEU:H	1:B:665:LYS:H	11	0.69
(2,888)	1:A:746:ILE:H	1:A:742:ARG:HA	6	0.68
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	4	0.68
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	4	0.68
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	4	0.68
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	4	0.68
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	4	0.68
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	4	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	4	0.68
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	4	0.68
(2,1470)	1:A:802:TYR:H	1:A:802:TYR:HB3	2	0.68
(2,1470)	1:A:802:TYR:H	1:A:802:TYR:HB3	5	0.68
(2,1313)	1:A:746:ILE:H	1:A:742:ARG:HA	6	0.68
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	4	0.68
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	4	0.68
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	4	0.68
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	4	0.68
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	4	0.68
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	4	0.68
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	4	0.68
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	4	0.68
(2,1045)	1:A:802:TYR:H	1:A:802:TYR:HB3	2	0.68
(2,1045)	1:A:802:TYR:H	1:A:802:TYR:HB3	5	0.68
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB2	8	0.67
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB3	8	0.67
(2,620)	1:B:802:TYR:H	1:B:802:TYR:HB3	14	0.67
(2,513)	1:B:759:ASP:H	1:B:759:ASP:HB2	1	0.67
(2,180)	1:A:806:GLU:H	1:B:771:LEU:HG	14	0.67
(2,15)	1:A:666:TRP:HE1	1:B:666:TRP:HD1	4	0.67
(2,1472)	1:A:802:TYR:H	1:A:803:TRP:HH2	3	0.67
(2,1470)	1:A:802:TYR:H	1:A:802:TYR:HB3	4	0.67
(2,1470)	1:A:802:TYR:H	1:A:802:TYR:HB3	9	0.67
(2,1470)	1:A:802:TYR:H	1:A:802:TYR:HB3	12	0.67
(2,1047)	1:A:802:TYR:H	1:A:803:TRP:HH2	3	0.67
(2,1045)	1:A:802:TYR:H	1:A:802:TYR:HB3	4	0.67
(2,1045)	1:A:802:TYR:H	1:A:802:TYR:HB3	9	0.67
(2,1045)	1:A:802:TYR:H	1:A:802:TYR:HB3	12	0.67
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD2	7	0.66
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD3	7	0.66
(2,783)	1:A:698:VAL:HG11	1:A:702:LEU:HB2	8	0.66
(2,783)	1:A:698:VAL:HG11	1:A:702:LEU:HB3	8	0.66
(2,783)	1:A:698:VAL:HG12	1:A:702:LEU:HB2	8	0.66
(2,783)	1:A:698:VAL:HG12	1:A:702:LEU:HB3	8	0.66
(2,783)	1:A:698:VAL:HG13	1:A:702:LEU:HB2	8	0.66
(2,783)	1:A:698:VAL:HG13	1:A:702:LEU:HB3	8	0.66
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD1	5	0.66
(2,635)	1:B:744:ARG:HH11	1:B:741:ASP:OD2	5	0.66
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD1	5	0.66
(2,635)	1:B:744:ARG:HH12	1:B:741:ASP:OD2	5	0.66
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD1	5	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,635)	1:B:744:ARG:HH21	1:B:741:ASP:OD2	5	0.66
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD1	5	0.66
(2,635)	1:B:744:ARG:HH22	1:B:741:ASP:OD2	5	0.66
(2,622)	1:B:802:TYR:H	1:B:803:TRP:HH2	13	0.66
(2,620)	1:B:802:TYR:H	1:B:802:TYR:HB3	7	0.66
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB1	10	0.66
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB2	10	0.66
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB3	10	0.66
(2,439)	1:B:710:GLN:H	1:B:708:VAL:HA	9	0.66
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG21	10	0.66
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG22	10	0.66
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG23	10	0.66
(2,1470)	1:A:802:TYR:H	1:A:802:TYR:HB3	8	0.66
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD2	7	0.66
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD3	7	0.66
(2,1208)	1:A:698:VAL:HG11	1:A:702:LEU:HB2	8	0.66
(2,1208)	1:A:698:VAL:HG11	1:A:702:LEU:HB3	8	0.66
(2,1208)	1:A:698:VAL:HG12	1:A:702:LEU:HB2	8	0.66
(2,1208)	1:A:698:VAL:HG12	1:A:702:LEU:HB3	8	0.66
(2,1208)	1:A:698:VAL:HG13	1:A:702:LEU:HB2	8	0.66
(2,1208)	1:A:698:VAL:HG13	1:A:702:LEU:HB3	8	0.66
(2,1045)	1:A:802:TYR:H	1:A:802:TYR:HB3	8	0.66
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB2	2	0.65
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB3	2	0.65
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD11	9	0.65
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD12	9	0.65
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD13	9	0.65
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD21	9	0.65
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD22	9	0.65
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD23	9	0.65
(2,620)	1:B:802:TYR:H	1:B:802:TYR:HB3	12	0.65
(2,439)	1:B:710:GLN:H	1:B:708:VAL:HA	10	0.65
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG12	9	0.65
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG13	9	0.65
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG12	9	0.65
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG13	9	0.65
(2,1470)	1:A:802:TYR:H	1:A:802:TYR:HB3	6	0.65
(2,1470)	1:A:802:TYR:H	1:A:802:TYR:HB3	10	0.65
(2,1470)	1:A:802:TYR:H	1:A:802:TYR:HB3	11	0.65
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD2	11	0.65
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD3	11	0.65
(2,135)	1:B:756:ILE:H	1:A:796:TRP:HE1	13	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1045)	1:A:802:TYR:H	1:A:802:TYR:HB3	6	0.65
(2,1045)	1:A:802:TYR:H	1:A:802:TYR:HB3	10	0.65
(2,1045)	1:A:802:TYR:H	1:A:802:TYR:HB3	11	0.65
(2,888)	1:A:746:ILE:H	1:A:742:ARG:HA	1	0.64
(2,540)	1:B:775:LEU:H	1:B:772:ARG:HA	3	0.64
(2,445)	1:B:710:GLN:H	1:B:710:GLN:HB2	15	0.64
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD2	15	0.64
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD3	15	0.64
(2,1470)	1:A:802:TYR:H	1:A:802:TYR:HB3	13	0.64
(2,1470)	1:A:802:TYR:H	1:A:802:TYR:HB3	14	0.64
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	13	0.64
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	13	0.64
(2,1462)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	13	0.64
(2,1313)	1:A:746:ILE:H	1:A:742:ARG:HA	1	0.64
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG21	1	0.64
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG22	1	0.64
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG23	1	0.64
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD2	15	0.64
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD3	15	0.64
(2,1045)	1:A:802:TYR:H	1:A:802:TYR:HB3	13	0.64
(2,1045)	1:A:802:TYR:H	1:A:802:TYR:HB3	14	0.64
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB1	13	0.64
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB2	13	0.64
(2,1037)	1:A:790:TRP:HE1	1:A:792:ALA:HB3	13	0.64
(2,984)	1:A:778:VAL:H	1:A:775:LEU:HA	6	0.63
(2,961)	1:A:774:LEU:H	1:A:764:SER:HA	13	0.63
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	15	0.63
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	15	0.63
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	15	0.63
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	15	0.63
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	15	0.63
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	15	0.63
(2,853)	1:A:708:VAL:HG11	1:A:705:VAL:HA	12	0.63
(2,853)	1:A:708:VAL:HG12	1:A:705:VAL:HA	12	0.63
(2,853)	1:A:708:VAL:HG13	1:A:705:VAL:HA	12	0.63
(2,620)	1:B:802:TYR:H	1:B:802:TYR:HB3	2	0.63
(2,620)	1:B:802:TYR:H	1:B:802:TYR:HB3	10	0.63
(2,536)	1:B:774:LEU:H	1:B:764:SER:HA	9	0.63
(2,445)	1:B:710:GLN:H	1:B:710:GLN:HB2	10	0.63
(2,1409)	1:A:778:VAL:H	1:A:775:LEU:HA	6	0.63
(2,1386)	1:A:774:LEU:H	1:A:764:SER:HA	13	0.63
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD2	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD3	5	0.63
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD2	9	0.63
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD3	9	0.63
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	15	0.63
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	15	0.63
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	15	0.63
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	15	0.63
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	15	0.63
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	15	0.63
(2,1278)	1:A:708:VAL:HG11	1:A:705:VAL:HA	12	0.63
(2,1278)	1:A:708:VAL:HG12	1:A:705:VAL:HA	12	0.63
(2,1278)	1:A:708:VAL:HG13	1:A:705:VAL:HA	12	0.63
(2,99)	1:A:758:ASP:H	1:B:715:LEU:HD21	9	0.62
(2,99)	1:A:758:ASP:H	1:B:715:LEU:HD22	9	0.62
(2,99)	1:A:758:ASP:H	1:B:715:LEU:HD23	9	0.62
(2,815)	1:A:704:LEU:H	1:A:704:LEU:HB3	12	0.62
(2,622)	1:B:802:TYR:H	1:B:803:TRP:HH2	12	0.62
(2,620)	1:B:802:TYR:H	1:B:802:TYR:HB3	15	0.62
(2,536)	1:B:774:LEU:H	1:B:764:SER:HA	7	0.62
(2,536)	1:B:774:LEU:H	1:B:764:SER:HA	12	0.62
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG21	2	0.62
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG22	2	0.62
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG23	2	0.62
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG21	2	0.62
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG22	2	0.62
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG23	2	0.62
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG21	2	0.62
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG22	2	0.62
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG23	2	0.62
(2,169)	1:B:797:TRP:HE1	1:B:848:ARG:HB2	3	0.62
(2,169)	1:B:797:TRP:HE1	1:B:848:ARG:HB3	3	0.62
(2,1464)	1:A:793:LEU:H	1:A:790:TRP:HE3	5	0.62
(2,1240)	1:A:704:LEU:H	1:A:704:LEU:HB3	12	0.62
(2,1039)	1:A:793:LEU:H	1:A:790:TRP:HE3	5	0.62
(2,961)	1:A:774:LEU:H	1:A:764:SER:HA	4	0.61
(2,870)	1:A:710:GLN:H	1:A:710:GLN:HB2	13	0.61
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD2	3	0.61
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD3	3	0.61
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD2	9	0.61
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD3	9	0.61
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH21	15	0.61
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH22	15	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH21	15	0.61
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH22	15	0.61
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH21	15	0.61
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH22	15	0.61
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB2	2	0.61
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB3	2	0.61
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB2	2	0.61
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB3	2	0.61
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB2	2	0.61
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB3	2	0.61
(2,428)	1:B:708:VAL:HG11	1:B:705:VAL:HA	12	0.61
(2,428)	1:B:708:VAL:HG12	1:B:705:VAL:HA	12	0.61
(2,428)	1:B:708:VAL:HG13	1:B:705:VAL:HA	12	0.61
(2,1386)	1:A:774:LEU:H	1:A:764:SER:HA	4	0.61
(2,1295)	1:A:710:GLN:H	1:A:710:GLN:HB2	13	0.61
(2,99)	1:A:758:ASP:H	1:B:715:LEU:HD21	6	0.6
(2,99)	1:A:758:ASP:H	1:B:715:LEU:HD22	6	0.6
(2,99)	1:A:758:ASP:H	1:B:715:LEU:HD23	6	0.6
(2,983)	1:A:777:ILE:HG21	1:A:780:ARG:HD2	7	0.6
(2,983)	1:A:777:ILE:HG21	1:A:780:ARG:HD3	7	0.6
(2,983)	1:A:777:ILE:HG22	1:A:780:ARG:HD2	7	0.6
(2,983)	1:A:777:ILE:HG22	1:A:780:ARG:HD3	7	0.6
(2,983)	1:A:777:ILE:HG23	1:A:780:ARG:HD2	7	0.6
(2,983)	1:A:777:ILE:HG23	1:A:780:ARG:HD3	7	0.6
(2,888)	1:A:746:ILE:H	1:A:742:ARG:HA	12	0.6
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB2	5	0.6
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB3	5	0.6
(2,864)	1:A:710:GLN:H	1:A:708:VAL:HA	1	0.6
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	2	0.6
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	2	0.6
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	2	0.6
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	2	0.6
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	2	0.6
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	2	0.6
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB1	4	0.6
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB2	4	0.6
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB3	4	0.6
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB1	4	0.6
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB2	4	0.6
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB3	4	0.6
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB1	4	0.6
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB2	4	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB3	4	0.6
(2,540)	1:B:775:LEU:H	1:B:772:ARG:HA	1	0.6
(2,444)	1:B:710:GLN:H	1:B:710:GLN:HB3	11	0.6
(2,428)	1:B:708:VAL:HG11	1:B:705:VAL:HA	10	0.6
(2,428)	1:B:708:VAL:HG12	1:B:705:VAL:HA	10	0.6
(2,428)	1:B:708:VAL:HG13	1:B:705:VAL:HA	10	0.6
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD2	11	0.6
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD3	11	0.6
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD2	11	0.6
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD3	11	0.6
(2,1472)	1:A:802:TYR:H	1:A:803:TRP:HH2	15	0.6
(2,1464)	1:A:793:LEU:H	1:A:790:TRP:HE3	8	0.6
(2,1408)	1:A:777:ILE:HG21	1:A:780:ARG:HD2	7	0.6
(2,1408)	1:A:777:ILE:HG21	1:A:780:ARG:HD3	7	0.6
(2,1408)	1:A:777:ILE:HG22	1:A:780:ARG:HD2	7	0.6
(2,1408)	1:A:777:ILE:HG22	1:A:780:ARG:HD3	7	0.6
(2,1408)	1:A:777:ILE:HG23	1:A:780:ARG:HD2	7	0.6
(2,1408)	1:A:777:ILE:HG23	1:A:780:ARG:HD3	7	0.6
(2,1313)	1:A:746:ILE:H	1:A:742:ARG:HA	12	0.6
(2,1289)	1:A:710:GLN:H	1:A:708:VAL:HA	1	0.6
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	2	0.6
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	2	0.6
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	2	0.6
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	2	0.6
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	2	0.6
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	2	0.6
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG21	11	0.6
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG22	11	0.6
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG23	11	0.6
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD2	11	0.6
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD3	11	0.6
(2,1047)	1:A:802:TYR:H	1:A:803:TRP:HH2	15	0.6
(2,1039)	1:A:793:LEU:H	1:A:790:TRP:HE3	8	0.6
(1,87)	1:B:790:TRP:O	1:B:794:LYS:H	14	0.6
(1,173)	1:B:790:TRP:O	1:B:794:LYS:H	14	0.6
(1,1)	1:B:790:TRP:O	1:B:794:LYS:H	14	0.6
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB2	6	0.59
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB3	6	0.59
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB2	12	0.59
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB3	12	0.59
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB2	12	0.59
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB3	12	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB2	12	0.59
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB3	12	0.59
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	1	0.59
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	1	0.59
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	1	0.59
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	1	0.59
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	1	0.59
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	1	0.59
(2,622)	1:B:802:TYR:H	1:B:803:TRP:HH2	14	0.59
(2,620)	1:B:802:TYR:H	1:B:802:TYR:HB3	9	0.59
(2,463)	1:B:746:ILE:H	1:B:742:ARG:HA	5	0.59
(2,444)	1:B:710:GLN:H	1:B:710:GLN:HB3	5	0.59
(2,439)	1:B:710:GLN:H	1:B:708:VAL:HA	11	0.59
(2,428)	1:B:708:VAL:HG11	1:B:705:VAL:HA	8	0.59
(2,428)	1:B:708:VAL:HG12	1:B:705:VAL:HA	8	0.59
(2,428)	1:B:708:VAL:HG13	1:B:705:VAL:HA	8	0.59
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG21	13	0.59
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG22	13	0.59
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG23	13	0.59
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG21	13	0.59
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG22	13	0.59
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG23	13	0.59
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG21	13	0.59
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG22	13	0.59
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG23	13	0.59
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD2	8	0.59
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD3	8	0.59
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG12	3	0.59
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG13	3	0.59
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG12	3	0.59
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG13	3	0.59
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB2	2	0.59
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB3	2	0.59
(2,1477)	1:A:819:ALA:H	1:A:820:ILE:HD11	11	0.59
(2,1477)	1:A:819:ALA:H	1:A:820:ILE:HD12	11	0.59
(2,1477)	1:A:819:ALA:H	1:A:820:ILE:HD13	11	0.59
(2,1472)	1:A:802:TYR:H	1:A:803:TRP:HH2	10	0.59
(2,1470)	1:A:802:TYR:H	1:A:802:TYR:HB3	7	0.59
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB2	12	0.59
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB3	12	0.59
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB2	12	0.59
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB3	12	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB2	12	0.59
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB3	12	0.59
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	1	0.59
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	1	0.59
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	1	0.59
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	1	0.59
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	1	0.59
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	1	0.59
(2,1052)	1:A:819:ALA:H	1:A:820:ILE:HD11	11	0.59
(2,1052)	1:A:819:ALA:H	1:A:820:ILE:HD12	11	0.59
(2,1052)	1:A:819:ALA:H	1:A:820:ILE:HD13	11	0.59
(2,1047)	1:A:802:TYR:H	1:A:803:TRP:HH2	10	0.59
(2,1045)	1:A:802:TYR:H	1:A:802:TYR:HB3	7	0.59
(2,853)	1:A:708:VAL:HG11	1:A:705:VAL:HA	8	0.58
(2,853)	1:A:708:VAL:HG12	1:A:705:VAL:HA	8	0.58
(2,853)	1:A:708:VAL:HG13	1:A:705:VAL:HA	8	0.58
(2,815)	1:A:704:LEU:H	1:A:704:LEU:HB3	8	0.58
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD2	2	0.58
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD3	2	0.58
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD2	2	0.58
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD3	2	0.58
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD2	2	0.58
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD3	2	0.58
(2,536)	1:B:774:LEU:H	1:B:764:SER:HA	10	0.58
(2,536)	1:B:774:LEU:H	1:B:764:SER:HA	15	0.58
(2,492)	1:B:753:LEU:HD21	1:B:750:ASN:HB2	15	0.58
(2,492)	1:B:753:LEU:HD21	1:B:750:ASN:HB3	15	0.58
(2,492)	1:B:753:LEU:HD22	1:B:750:ASN:HB2	15	0.58
(2,492)	1:B:753:LEU:HD22	1:B:750:ASN:HB3	15	0.58
(2,492)	1:B:753:LEU:HD23	1:B:750:ASN:HB2	15	0.58
(2,492)	1:B:753:LEU:HD23	1:B:750:ASN:HB3	15	0.58
(2,463)	1:B:746:ILE:H	1:B:742:ARG:HA	6	0.58
(2,463)	1:B:746:ILE:H	1:B:742:ARG:HA	12	0.58
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG21	1	0.58
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG22	1	0.58
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG23	1	0.58
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG21	1	0.58
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG22	1	0.58
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG23	1	0.58
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG21	1	0.58
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG22	1	0.58
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG23	1	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG12	10	0.58
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG13	10	0.58
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG12	11	0.58
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG13	11	0.58
(2,183)	1:A:806:GLU:H	1:B:772:ARG:HE	5	0.58
(2,1464)	1:A:793:LEU:H	1:A:790:TRP:HE3	6	0.58
(2,1278)	1:A:708:VAL:HG11	1:A:705:VAL:HA	8	0.58
(2,1278)	1:A:708:VAL:HG12	1:A:705:VAL:HA	8	0.58
(2,1278)	1:A:708:VAL:HG13	1:A:705:VAL:HA	8	0.58
(2,1240)	1:A:704:LEU:H	1:A:704:LEU:HB3	8	0.58
(2,1039)	1:A:793:LEU:H	1:A:790:TRP:HE3	6	0.58
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD2	8	0.57
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD3	8	0.57
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB2	12	0.57
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB3	12	0.57
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB2	13	0.57
(2,87)	1:B:711:GLY:H	1:A:758:ASP:HB3	13	0.57
(2,869)	1:A:710:GLN:H	1:A:710:GLN:HB3	2	0.57
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD2	12	0.57
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD3	12	0.57
(2,764)	1:A:693:ILE:HG21	1:A:694:GLY:H	13	0.57
(2,764)	1:A:693:ILE:HG22	1:A:694:GLY:H	13	0.57
(2,764)	1:A:693:ILE:HG23	1:A:694:GLY:H	13	0.57
(2,620)	1:B:802:TYR:H	1:B:802:TYR:HB3	11	0.57
(2,405)	1:B:705:VAL:HG21	1:B:702:LEU:HG	12	0.57
(2,405)	1:B:705:VAL:HG22	1:B:702:LEU:HG	12	0.57
(2,405)	1:B:705:VAL:HG23	1:B:702:LEU:HG	12	0.57
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB2	3	0.57
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB3	3	0.57
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	11	0.57
(2,1484)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	11	0.57
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	11	0.57
(2,1484)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	11	0.57
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	11	0.57
(2,1484)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	11	0.57
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	11	0.57
(2,1484)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	11	0.57
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD2	12	0.57
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD3	12	0.57
(2,1472)	1:A:802:TYR:H	1:A:803:TRP:HH2	5	0.57
(2,135)	1:B:756:ILE:H	1:A:796:TRP:HE1	14	0.57
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD2	8	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD3	8	0.57
(2,1294)	1:A:710:GLN:H	1:A:710:GLN:HB3	2	0.57
(2,1189)	1:A:693:ILE:HG21	1:A:694:GLY:H	13	0.57
(2,1189)	1:A:693:ILE:HG22	1:A:694:GLY:H	13	0.57
(2,1189)	1:A:693:ILE:HG23	1:A:694:GLY:H	13	0.57
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD1	11	0.57
(2,1059)	1:A:740:ARG:HH11	1:A:743:ASP:OD2	11	0.57
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD1	11	0.57
(2,1059)	1:A:740:ARG:HH12	1:A:743:ASP:OD2	11	0.57
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD1	11	0.57
(2,1059)	1:A:740:ARG:HH21	1:A:743:ASP:OD2	11	0.57
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD1	11	0.57
(2,1059)	1:A:740:ARG:HH22	1:A:743:ASP:OD2	11	0.57
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD2	12	0.57
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD3	12	0.57
(2,1047)	1:A:802:TYR:H	1:A:803:TRP:HH2	5	0.57
(2,961)	1:A:774:LEU:H	1:A:764:SER:HA	1	0.56
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD2	5	0.56
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD3	5	0.56
(2,783)	1:A:698:VAL:HG11	1:A:702:LEU:HB2	6	0.56
(2,783)	1:A:698:VAL:HG11	1:A:702:LEU:HB3	6	0.56
(2,783)	1:A:698:VAL:HG12	1:A:702:LEU:HB2	6	0.56
(2,783)	1:A:698:VAL:HG12	1:A:702:LEU:HB3	6	0.56
(2,783)	1:A:698:VAL:HG13	1:A:702:LEU:HB2	6	0.56
(2,783)	1:A:698:VAL:HG13	1:A:702:LEU:HB3	6	0.56
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD2	8	0.56
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD3	8	0.56
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD2	8	0.56
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD3	8	0.56
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD2	8	0.56
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD3	8	0.56
(2,764)	1:A:693:ILE:HG21	1:A:694:GLY:H	14	0.56
(2,764)	1:A:693:ILE:HG22	1:A:694:GLY:H	14	0.56
(2,764)	1:A:693:ILE:HG23	1:A:694:GLY:H	14	0.56
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB1	3	0.56
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB2	3	0.56
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB3	3	0.56
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB1	3	0.56
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB2	3	0.56
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB3	3	0.56
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB1	3	0.56
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB2	3	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB3	3	0.56
(2,622)	1:B:802:TYR:H	1:B:803:TRP:HH2	10	0.56
(2,536)	1:B:774:LEU:H	1:B:764:SER:HA	8	0.56
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE1	3	0.56
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE2	3	0.56
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE1	3	0.56
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE2	3	0.56
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE1	3	0.56
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE2	3	0.56
(2,463)	1:B:746:ILE:H	1:B:742:ARG:HA	13	0.56
(2,444)	1:B:710:GLN:H	1:B:710:GLN:HB3	8	0.56
(2,439)	1:B:710:GLN:H	1:B:708:VAL:HA	1	0.56
(2,421)	1:B:707:ARG:H	1:B:707:ARG:HD2	5	0.56
(2,421)	1:B:707:ARG:H	1:B:707:ARG:HD3	5	0.56
(2,1386)	1:A:774:LEU:H	1:A:764:SER:HA	1	0.56
(2,135)	1:B:756:ILE:H	1:A:796:TRP:HE1	5	0.56
(2,1208)	1:A:698:VAL:HG11	1:A:702:LEU:HB2	6	0.56
(2,1208)	1:A:698:VAL:HG11	1:A:702:LEU:HB3	6	0.56
(2,1208)	1:A:698:VAL:HG12	1:A:702:LEU:HB2	6	0.56
(2,1208)	1:A:698:VAL:HG12	1:A:702:LEU:HB3	6	0.56
(2,1208)	1:A:698:VAL:HG13	1:A:702:LEU:HB2	6	0.56
(2,1208)	1:A:698:VAL:HG13	1:A:702:LEU:HB3	6	0.56
(2,1189)	1:A:693:ILE:HG21	1:A:694:GLY:H	14	0.56
(2,1189)	1:A:693:ILE:HG22	1:A:694:GLY:H	14	0.56
(2,1189)	1:A:693:ILE:HG23	1:A:694:GLY:H	14	0.56
(2,114)	1:A:781:ILE:HD11	1:B:743:ASP:HA	7	0.56
(2,114)	1:A:781:ILE:HD12	1:B:743:ASP:HA	7	0.56
(2,114)	1:A:781:ILE:HD13	1:B:743:ASP:HA	7	0.56
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG21	15	0.56
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG22	15	0.56
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG23	15	0.56
(2,888)	1:A:746:ILE:H	1:A:742:ARG:HA	7	0.55
(2,853)	1:A:708:VAL:HG11	1:A:705:VAL:HA	9	0.55
(2,853)	1:A:708:VAL:HG12	1:A:705:VAL:HA	9	0.55
(2,853)	1:A:708:VAL:HG13	1:A:705:VAL:HA	9	0.55
(2,815)	1:A:704:LEU:H	1:A:704:LEU:HB3	5	0.55
(2,759)	1:A:692:LEU:HD21	1:A:696:ARG:HH11	10	0.55
(2,759)	1:A:692:LEU:HD21	1:A:696:ARG:HH12	10	0.55
(2,759)	1:A:692:LEU:HD21	1:A:696:ARG:HH21	10	0.55
(2,759)	1:A:692:LEU:HD21	1:A:696:ARG:HH22	10	0.55
(2,759)	1:A:692:LEU:HD22	1:A:696:ARG:HH11	10	0.55
(2,759)	1:A:692:LEU:HD22	1:A:696:ARG:HH12	10	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,759)	1:A:692:LEU:HD22	1:A:696:ARG:HH21	10	0.55
(2,759)	1:A:692:LEU:HD22	1:A:696:ARG:HH22	10	0.55
(2,759)	1:A:692:LEU:HD23	1:A:696:ARG:HH11	10	0.55
(2,759)	1:A:692:LEU:HD23	1:A:696:ARG:HH12	10	0.55
(2,759)	1:A:692:LEU:HD23	1:A:696:ARG:HH21	10	0.55
(2,759)	1:A:692:LEU:HD23	1:A:696:ARG:HH22	10	0.55
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE1	5	0.55
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE2	5	0.55
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE1	5	0.55
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE2	5	0.55
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE1	5	0.55
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE2	5	0.55
(2,620)	1:B:802:TYR:H	1:B:802:TYR:HB3	8	0.55
(2,491)	1:B:753:LEU:HD11	1:B:757:TRP:HB2	11	0.55
(2,491)	1:B:753:LEU:HD11	1:B:757:TRP:HB3	11	0.55
(2,491)	1:B:753:LEU:HD12	1:B:757:TRP:HB2	11	0.55
(2,491)	1:B:753:LEU:HD12	1:B:757:TRP:HB3	11	0.55
(2,491)	1:B:753:LEU:HD13	1:B:757:TRP:HB2	11	0.55
(2,491)	1:B:753:LEU:HD13	1:B:757:TRP:HB3	11	0.55
(2,470)	1:B:746:ILE:HD11	1:B:743:ASP:HA	7	0.55
(2,470)	1:B:746:ILE:HD12	1:B:743:ASP:HA	7	0.55
(2,470)	1:B:746:ILE:HD13	1:B:743:ASP:HA	7	0.55
(2,463)	1:B:746:ILE:H	1:B:742:ARG:HA	14	0.55
(2,444)	1:B:710:GLN:H	1:B:710:GLN:HB3	1	0.55
(2,444)	1:B:710:GLN:H	1:B:710:GLN:HB3	7	0.55
(2,432)	1:B:709:ARG:H	1:B:707:ARG:H	2	0.55
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG12	6	0.55
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG13	6	0.55
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB2	13	0.55
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB3	13	0.55
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	12	0.55
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	12	0.55
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	12	0.55
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	12	0.55
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	14	0.55
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	14	0.55
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	14	0.55
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	14	0.55
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	14	0.55
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	14	0.55
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	14	0.55
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	14	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	13	0.55
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	13	0.55
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	13	0.55
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	13	0.55
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	13	0.55
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	13	0.55
(2,1472)	1:A:802:TYR:H	1:A:803:TRP:HH2	12	0.55
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG12	7	0.55
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG13	7	0.55
(2,1313)	1:A:746:ILE:H	1:A:742:ARG:HA	7	0.55
(2,1278)	1:A:708:VAL:HG11	1:A:705:VAL:HA	9	0.55
(2,1278)	1:A:708:VAL:HG12	1:A:705:VAL:HA	9	0.55
(2,1278)	1:A:708:VAL:HG13	1:A:705:VAL:HA	9	0.55
(2,1240)	1:A:704:LEU:H	1:A:704:LEU:HB3	5	0.55
(2,1184)	1:A:692:LEU:HD21	1:A:696:ARG:HH11	10	0.55
(2,1184)	1:A:692:LEU:HD21	1:A:696:ARG:HH12	10	0.55
(2,1184)	1:A:692:LEU:HD21	1:A:696:ARG:HH21	10	0.55
(2,1184)	1:A:692:LEU:HD21	1:A:696:ARG:HH22	10	0.55
(2,1184)	1:A:692:LEU:HD22	1:A:696:ARG:HH11	10	0.55
(2,1184)	1:A:692:LEU:HD22	1:A:696:ARG:HH12	10	0.55
(2,1184)	1:A:692:LEU:HD22	1:A:696:ARG:HH21	10	0.55
(2,1184)	1:A:692:LEU:HD22	1:A:696:ARG:HH22	10	0.55
(2,1184)	1:A:692:LEU:HD23	1:A:696:ARG:HH11	10	0.55
(2,1184)	1:A:692:LEU:HD23	1:A:696:ARG:HH12	10	0.55
(2,1184)	1:A:692:LEU:HD23	1:A:696:ARG:HH21	10	0.55
(2,1184)	1:A:692:LEU:HD23	1:A:696:ARG:HH22	10	0.55
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	14	0.55
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	14	0.55
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	14	0.55
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	14	0.55
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	14	0.55
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	14	0.55
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	14	0.55
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	14	0.55
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	13	0.55
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	13	0.55
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	13	0.55
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	13	0.55
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	13	0.55
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	13	0.55
(2,1047)	1:A:802:TYR:H	1:A:803:TRP:HH2	12	0.55
(2,965)	1:A:775:LEU:H	1:A:772:ARG:HA	4	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,961)	1:A:774:LEU:H	1:A:764:SER:HA	14	0.54
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB2	10	0.54
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB3	10	0.54
(2,888)	1:A:746:ILE:H	1:A:742:ARG:HA	5	0.54
(2,869)	1:A:710:GLN:H	1:A:710:GLN:HB3	10	0.54
(2,853)	1:A:708:VAL:HG11	1:A:705:VAL:HA	2	0.54
(2,853)	1:A:708:VAL:HG12	1:A:705:VAL:HA	2	0.54
(2,853)	1:A:708:VAL:HG13	1:A:705:VAL:HA	2	0.54
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD2	4	0.54
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD3	4	0.54
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD2	4	0.54
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD3	4	0.54
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD2	4	0.54
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD3	4	0.54
(2,778)	1:A:697:ILE:HG21	1:A:698:VAL:HA	6	0.54
(2,778)	1:A:697:ILE:HG22	1:A:698:VAL:HA	6	0.54
(2,778)	1:A:697:ILE:HG23	1:A:698:VAL:HA	6	0.54
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	6	0.54
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	6	0.54
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	6	0.54
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	6	0.54
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	6	0.54
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	6	0.54
(2,622)	1:B:802:TYR:H	1:B:803:TRP:HH2	2	0.54
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE1	4	0.54
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE2	4	0.54
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE1	4	0.54
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE2	4	0.54
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE1	4	0.54
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE2	4	0.54
(2,444)	1:B:710:GLN:H	1:B:710:GLN:HB3	13	0.54
(2,403)	1:B:705:VAL:HG11	1:B:709:ARG:HD2	12	0.54
(2,403)	1:B:705:VAL:HG11	1:B:709:ARG:HD3	12	0.54
(2,403)	1:B:705:VAL:HG12	1:B:709:ARG:HD2	12	0.54
(2,403)	1:B:705:VAL:HG12	1:B:709:ARG:HD3	12	0.54
(2,403)	1:B:705:VAL:HG13	1:B:709:ARG:HD2	12	0.54
(2,403)	1:B:705:VAL:HG13	1:B:709:ARG:HD3	12	0.54
(2,1472)	1:A:802:TYR:H	1:A:803:TRP:HH2	2	0.54
(2,1390)	1:A:775:LEU:H	1:A:772:ARG:HA	4	0.54
(2,1386)	1:A:774:LEU:H	1:A:764:SER:HA	14	0.54
(2,1313)	1:A:746:ILE:H	1:A:742:ARG:HA	5	0.54
(2,1294)	1:A:710:GLN:H	1:A:710:GLN:HB3	10	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1278)	1:A:708:VAL:HG11	1:A:705:VAL:HA	2	0.54
(2,1278)	1:A:708:VAL:HG12	1:A:705:VAL:HA	2	0.54
(2,1278)	1:A:708:VAL:HG13	1:A:705:VAL:HA	2	0.54
(2,1203)	1:A:697:ILE:HG21	1:A:698:VAL:HA	6	0.54
(2,1203)	1:A:697:ILE:HG22	1:A:698:VAL:HA	6	0.54
(2,1203)	1:A:697:ILE:HG23	1:A:698:VAL:HA	6	0.54
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	6	0.54
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	6	0.54
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	6	0.54
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	6	0.54
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	6	0.54
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	6	0.54
(2,114)	1:A:781:ILE:HD11	1:B:743:ASP:HA	3	0.54
(2,114)	1:A:781:ILE:HD12	1:B:743:ASP:HA	3	0.54
(2,114)	1:A:781:ILE:HD13	1:B:743:ASP:HA	3	0.54
(2,1047)	1:A:802:TYR:H	1:A:803:TRP:HH2	2	0.54
(2,983)	1:A:777:ILE:HG21	1:A:780:ARG:HD2	10	0.53
(2,983)	1:A:777:ILE:HG21	1:A:780:ARG:HD3	10	0.53
(2,983)	1:A:777:ILE:HG22	1:A:780:ARG:HD2	10	0.53
(2,983)	1:A:777:ILE:HG22	1:A:780:ARG:HD3	10	0.53
(2,983)	1:A:777:ILE:HG23	1:A:780:ARG:HD2	10	0.53
(2,983)	1:A:777:ILE:HG23	1:A:780:ARG:HD3	10	0.53
(2,888)	1:A:746:ILE:H	1:A:742:ARG:HA	14	0.53
(2,864)	1:A:710:GLN:H	1:A:708:VAL:HA	13	0.53
(2,863)	1:A:709:ARG:HE	1:A:709:ARG:H	6	0.53
(2,853)	1:A:708:VAL:HG11	1:A:705:VAL:HA	7	0.53
(2,853)	1:A:708:VAL:HG12	1:A:705:VAL:HA	7	0.53
(2,853)	1:A:708:VAL:HG13	1:A:705:VAL:HA	7	0.53
(2,815)	1:A:704:LEU:H	1:A:704:LEU:HB3	2	0.53
(2,764)	1:A:693:ILE:HG21	1:A:694:GLY:H	5	0.53
(2,764)	1:A:693:ILE:HG22	1:A:694:GLY:H	5	0.53
(2,764)	1:A:693:ILE:HG23	1:A:694:GLY:H	5	0.53
(2,764)	1:A:693:ILE:HG21	1:A:694:GLY:H	12	0.53
(2,764)	1:A:693:ILE:HG22	1:A:694:GLY:H	12	0.53
(2,764)	1:A:693:ILE:HG23	1:A:694:GLY:H	12	0.53
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	12	0.53
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	12	0.53
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	12	0.53
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	12	0.53
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	12	0.53
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	12	0.53
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	14	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	14	0.53
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	14	0.53
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	14	0.53
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	14	0.53
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	14	0.53
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD2	15	0.53
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD3	15	0.53
(2,536)	1:B:774:LEU:H	1:B:764:SER:HA	5	0.53
(2,444)	1:B:710:GLN:H	1:B:710:GLN:HB3	6	0.53
(2,439)	1:B:710:GLN:H	1:B:708:VAL:HA	5	0.53
(2,393)	1:B:704:LEU:HD11	1:B:707:ARG:HD2	13	0.53
(2,393)	1:B:704:LEU:HD11	1:B:707:ARG:HD3	13	0.53
(2,393)	1:B:704:LEU:HD12	1:B:707:ARG:HD2	13	0.53
(2,393)	1:B:704:LEU:HD12	1:B:707:ARG:HD3	13	0.53
(2,393)	1:B:704:LEU:HD13	1:B:707:ARG:HD2	13	0.53
(2,393)	1:B:704:LEU:HD13	1:B:707:ARG:HD3	13	0.53
(2,339)	1:B:693:ILE:HG21	1:B:694:GLY:H	6	0.53
(2,339)	1:B:693:ILE:HG22	1:B:694:GLY:H	6	0.53
(2,339)	1:B:693:ILE:HG23	1:B:694:GLY:H	6	0.53
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD11	8	0.53
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD12	8	0.53
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD13	8	0.53
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD21	8	0.53
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD22	8	0.53
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD23	8	0.53
(2,180)	1:A:806:GLU:H	1:B:771:LEU:HG	2	0.53
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD2	5	0.53
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD3	5	0.53
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	7	0.53
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	7	0.53
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	7	0.53
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	7	0.53
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	7	0.53
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	7	0.53
(2,1408)	1:A:777:ILE:HG21	1:A:780:ARG:HD2	10	0.53
(2,1408)	1:A:777:ILE:HG21	1:A:780:ARG:HD3	10	0.53
(2,1408)	1:A:777:ILE:HG22	1:A:780:ARG:HD2	10	0.53
(2,1408)	1:A:777:ILE:HG22	1:A:780:ARG:HD3	10	0.53
(2,1408)	1:A:777:ILE:HG23	1:A:780:ARG:HD2	10	0.53
(2,1408)	1:A:777:ILE:HG23	1:A:780:ARG:HD3	10	0.53
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD2	7	0.53
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD3	7	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD2	14	0.53
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD3	14	0.53
(2,1313)	1:A:746:ILE:H	1:A:742:ARG:HA	14	0.53
(2,1289)	1:A:710:GLN:H	1:A:708:VAL:HA	13	0.53
(2,1288)	1:A:709:ARG:HE	1:A:709:ARG:H	6	0.53
(2,1278)	1:A:708:VAL:HG11	1:A:705:VAL:HA	7	0.53
(2,1278)	1:A:708:VAL:HG12	1:A:705:VAL:HA	7	0.53
(2,1278)	1:A:708:VAL:HG13	1:A:705:VAL:HA	7	0.53
(2,1240)	1:A:704:LEU:H	1:A:704:LEU:HB3	2	0.53
(2,1189)	1:A:693:ILE:HG21	1:A:694:GLY:H	5	0.53
(2,1189)	1:A:693:ILE:HG22	1:A:694:GLY:H	5	0.53
(2,1189)	1:A:693:ILE:HG23	1:A:694:GLY:H	5	0.53
(2,1189)	1:A:693:ILE:HG21	1:A:694:GLY:H	12	0.53
(2,1189)	1:A:693:ILE:HG22	1:A:694:GLY:H	12	0.53
(2,1189)	1:A:693:ILE:HG23	1:A:694:GLY:H	12	0.53
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	12	0.53
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	12	0.53
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	12	0.53
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	12	0.53
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	12	0.53
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	12	0.53
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	14	0.53
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	14	0.53
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	14	0.53
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	14	0.53
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	14	0.53
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	14	0.53
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG21	9	0.53
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG22	9	0.53
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG23	9	0.53
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD2	5	0.53
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD3	5	0.53
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	7	0.53
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	7	0.53
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	7	0.53
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	7	0.53
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	7	0.53
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	7	0.53
(2,888)	1:A:746:ILE:H	1:A:742:ARG:HA	3	0.52
(2,853)	1:A:708:VAL:HG11	1:A:705:VAL:HA	14	0.52
(2,853)	1:A:708:VAL:HG12	1:A:705:VAL:HA	14	0.52
(2,853)	1:A:708:VAL:HG13	1:A:705:VAL:HA	14	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,782)	1:A:698:VAL:HG11	1:A:699:PHE:HD1	8	0.52
(2,782)	1:A:698:VAL:HG11	1:A:699:PHE:HD2	8	0.52
(2,782)	1:A:698:VAL:HG12	1:A:699:PHE:HD1	8	0.52
(2,782)	1:A:698:VAL:HG12	1:A:699:PHE:HD2	8	0.52
(2,782)	1:A:698:VAL:HG13	1:A:699:PHE:HD1	8	0.52
(2,782)	1:A:698:VAL:HG13	1:A:699:PHE:HD2	8	0.52
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD2	15	0.52
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD3	15	0.52
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD2	15	0.52
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD3	15	0.52
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD2	15	0.52
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD3	15	0.52
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE1	5	0.52
(2,74)	1:A:708:VAL:HG21	1:A:712:TYR:HE2	5	0.52
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE1	5	0.52
(2,74)	1:A:708:VAL:HG22	1:A:712:TYR:HE2	5	0.52
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE1	5	0.52
(2,74)	1:A:708:VAL:HG23	1:A:712:TYR:HE2	5	0.52
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	15	0.52
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	15	0.52
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	15	0.52
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	15	0.52
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	15	0.52
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	15	0.52
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD1	1	0.52
(2,634)	1:B:740:ARG:HH11	1:B:743:ASP:OD2	1	0.52
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD1	1	0.52
(2,634)	1:B:740:ARG:HH12	1:B:743:ASP:OD2	1	0.52
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD1	1	0.52
(2,634)	1:B:740:ARG:HH21	1:B:743:ASP:OD2	1	0.52
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD1	1	0.52
(2,634)	1:B:740:ARG:HH22	1:B:743:ASP:OD2	1	0.52
(2,620)	1:B:802:TYR:H	1:B:802:TYR:HB3	4	0.52
(2,614)	1:B:793:LEU:H	1:B:790:TRP:HE3	6	0.52
(2,536)	1:B:774:LEU:H	1:B:764:SER:HA	1	0.52
(2,439)	1:B:710:GLN:H	1:B:708:VAL:HA	14	0.52
(2,432)	1:B:709:ARG:H	1:B:707:ARG:H	12	0.52
(2,421)	1:B:707:ARG:H	1:B:707:ARG:HD2	7	0.52
(2,421)	1:B:707:ARG:H	1:B:707:ARG:HD3	7	0.52
(2,339)	1:B:693:ILE:HG21	1:B:694:GLY:H	10	0.52
(2,339)	1:B:693:ILE:HG22	1:B:694:GLY:H	10	0.52
(2,339)	1:B:693:ILE:HG23	1:B:694:GLY:H	10	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG12	8	0.52
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG13	8	0.52
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG12	13	0.52
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG13	13	0.52
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB2	11	0.52
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB3	11	0.52
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD2	14	0.52
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD3	14	0.52
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD2	15	0.52
(2,138)	1:B:756:ILE:H	1:A:794:LYS:HD3	15	0.52
(2,135)	1:B:756:ILE:H	1:A:796:TRP:HE1	6	0.52
(2,135)	1:B:756:ILE:H	1:A:796:TRP:HE1	8	0.52
(2,1313)	1:A:746:ILE:H	1:A:742:ARG:HA	3	0.52
(2,1278)	1:A:708:VAL:HG11	1:A:705:VAL:HA	14	0.52
(2,1278)	1:A:708:VAL:HG12	1:A:705:VAL:HA	14	0.52
(2,1278)	1:A:708:VAL:HG13	1:A:705:VAL:HA	14	0.52
(2,1207)	1:A:698:VAL:HG11	1:A:699:PHE:HD1	8	0.52
(2,1207)	1:A:698:VAL:HG11	1:A:699:PHE:HD2	8	0.52
(2,1207)	1:A:698:VAL:HG12	1:A:699:PHE:HD1	8	0.52
(2,1207)	1:A:698:VAL:HG12	1:A:699:PHE:HD2	8	0.52
(2,1207)	1:A:698:VAL:HG13	1:A:699:PHE:HD1	8	0.52
(2,1207)	1:A:698:VAL:HG13	1:A:699:PHE:HD2	8	0.52
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	15	0.52
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	15	0.52
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	15	0.52
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	15	0.52
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	15	0.52
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	15	0.52
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD2	14	0.52
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD3	14	0.52
(2,965)	1:A:775:LEU:H	1:A:772:ARG:HA	12	0.51
(2,888)	1:A:746:ILE:H	1:A:742:ARG:HA	8	0.51
(2,857)	1:A:709:ARG:H	1:A:707:ARG:H	4	0.51
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD2	5	0.51
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD3	5	0.51
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD2	5	0.51
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD3	5	0.51
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD2	5	0.51
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD3	5	0.51
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD2	9	0.51
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD3	9	0.51
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD2	9	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD3	9	0.51
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD2	9	0.51
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD3	9	0.51
(2,778)	1:A:697:ILE:HG21	1:A:698:VAL:HA	12	0.51
(2,778)	1:A:697:ILE:HG22	1:A:698:VAL:HA	12	0.51
(2,778)	1:A:697:ILE:HG23	1:A:698:VAL:HA	12	0.51
(2,764)	1:A:693:ILE:HG21	1:A:694:GLY:H	9	0.51
(2,764)	1:A:693:ILE:HG22	1:A:694:GLY:H	9	0.51
(2,764)	1:A:693:ILE:HG23	1:A:694:GLY:H	9	0.51
(2,647)	1:A:663:LEU:HD21	1:A:667:ALA:HB1	12	0.51
(2,647)	1:A:663:LEU:HD21	1:A:667:ALA:HB2	12	0.51
(2,647)	1:A:663:LEU:HD21	1:A:667:ALA:HB3	12	0.51
(2,647)	1:A:663:LEU:HD22	1:A:667:ALA:HB1	12	0.51
(2,647)	1:A:663:LEU:HD22	1:A:667:ALA:HB2	12	0.51
(2,647)	1:A:663:LEU:HD22	1:A:667:ALA:HB3	12	0.51
(2,647)	1:A:663:LEU:HD23	1:A:667:ALA:HB1	12	0.51
(2,647)	1:A:663:LEU:HD23	1:A:667:ALA:HB2	12	0.51
(2,647)	1:A:663:LEU:HD23	1:A:667:ALA:HB3	12	0.51
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD2	4	0.51
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD3	4	0.51
(2,614)	1:B:793:LEU:H	1:B:790:TRP:HE3	5	0.51
(2,457)	1:B:740:ARG:H	1:B:739:GLU:HA	14	0.51
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB2	3	0.51
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB3	3	0.51
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB2	3	0.51
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB3	3	0.51
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB2	3	0.51
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB3	3	0.51
(2,228)	1:B:665:LYS:H	1:B:662:GLU:HA	11	0.51
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ1	11	0.51
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ2	11	0.51
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ3	11	0.51
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG12	6	0.51
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG13	6	0.51
(2,1470)	1:A:802:TYR:H	1:A:802:TYR:HB3	1	0.51
(2,1464)	1:A:793:LEU:H	1:A:790:TRP:HE3	3	0.51
(2,1464)	1:A:793:LEU:H	1:A:790:TRP:HE3	10	0.51
(2,1443)	1:A:784:LEU:H	1:A:781:ILE:HA	7	0.51
(2,1390)	1:A:775:LEU:H	1:A:772:ARG:HA	12	0.51
(2,1313)	1:A:746:ILE:H	1:A:742:ARG:HA	8	0.51
(2,1282)	1:A:709:ARG:H	1:A:707:ARG:H	4	0.51
(2,1203)	1:A:697:ILE:HG21	1:A:698:VAL:HA	12	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1203)	1:A:697:ILE:HG22	1:A:698:VAL:HA	12	0.51
(2,1203)	1:A:697:ILE:HG23	1:A:698:VAL:HA	12	0.51
(2,12)	1:A:666:TRP:HE1	1:B:666:TRP:HZ2	1	0.51
(2,1189)	1:A:693:ILE:HG21	1:A:694:GLY:H	9	0.51
(2,1189)	1:A:693:ILE:HG22	1:A:694:GLY:H	9	0.51
(2,1189)	1:A:693:ILE:HG23	1:A:694:GLY:H	9	0.51
(2,1072)	1:A:663:LEU:HD21	1:A:667:ALA:HB1	12	0.51
(2,1072)	1:A:663:LEU:HD21	1:A:667:ALA:HB2	12	0.51
(2,1072)	1:A:663:LEU:HD21	1:A:667:ALA:HB3	12	0.51
(2,1072)	1:A:663:LEU:HD22	1:A:667:ALA:HB1	12	0.51
(2,1072)	1:A:663:LEU:HD22	1:A:667:ALA:HB2	12	0.51
(2,1072)	1:A:663:LEU:HD22	1:A:667:ALA:HB3	12	0.51
(2,1072)	1:A:663:LEU:HD23	1:A:667:ALA:HB1	12	0.51
(2,1072)	1:A:663:LEU:HD23	1:A:667:ALA:HB2	12	0.51
(2,1072)	1:A:663:LEU:HD23	1:A:667:ALA:HB3	12	0.51
(2,1045)	1:A:802:TYR:H	1:A:802:TYR:HB3	1	0.51
(2,1039)	1:A:793:LEU:H	1:A:790:TRP:HE3	3	0.51
(2,1039)	1:A:793:LEU:H	1:A:790:TRP:HE3	10	0.51
(2,1018)	1:A:784:LEU:H	1:A:781:ILE:HA	7	0.51
(2,984)	1:A:778:VAL:H	1:A:775:LEU:HA	15	0.5
(2,976)	1:A:776:LEU:HD11	1:A:773:ASP:HB2	2	0.5
(2,976)	1:A:776:LEU:HD11	1:A:773:ASP:HB3	2	0.5
(2,976)	1:A:776:LEU:HD12	1:A:773:ASP:HB2	2	0.5
(2,976)	1:A:776:LEU:HD12	1:A:773:ASP:HB3	2	0.5
(2,976)	1:A:776:LEU:HD13	1:A:773:ASP:HB2	2	0.5
(2,976)	1:A:776:LEU:HD13	1:A:773:ASP:HB3	2	0.5
(2,961)	1:A:774:LEU:H	1:A:764:SER:HA	10	0.5
(2,888)	1:A:746:ILE:H	1:A:742:ARG:HA	10	0.5
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD2	2	0.5
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD3	2	0.5
(2,622)	1:B:802:TYR:H	1:B:803:TRP:HH2	15	0.5
(2,620)	1:B:802:TYR:H	1:B:802:TYR:HB3	3	0.5
(2,614)	1:B:793:LEU:H	1:B:790:TRP:HE3	11	0.5
(2,536)	1:B:774:LEU:H	1:B:764:SER:HA	13	0.5
(2,525)	1:B:771:LEU:HD11	1:B:764:SER:HA	2	0.5
(2,525)	1:B:771:LEU:HD12	1:B:764:SER:HA	2	0.5
(2,525)	1:B:771:LEU:HD13	1:B:764:SER:HA	2	0.5
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD2	13	0.5
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD3	13	0.5
(2,457)	1:B:740:ARG:H	1:B:739:GLU:HA	10	0.5
(2,428)	1:B:708:VAL:HG11	1:B:705:VAL:HA	2	0.5
(2,428)	1:B:708:VAL:HG12	1:B:705:VAL:HA	2	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,428)	1:B:708:VAL:HG13	1:B:705:VAL:HA	2	0.5
(2,428)	1:B:708:VAL:HG11	1:B:705:VAL:HA	3	0.5
(2,428)	1:B:708:VAL:HG12	1:B:705:VAL:HA	3	0.5
(2,428)	1:B:708:VAL:HG13	1:B:705:VAL:HA	3	0.5
(2,180)	1:A:806:GLU:H	1:B:771:LEU:HG	13	0.5
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB2	12	0.5
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB3	12	0.5
(2,1409)	1:A:778:VAL:H	1:A:775:LEU:HA	15	0.5
(2,1401)	1:A:776:LEU:HD11	1:A:773:ASP:HB2	2	0.5
(2,1401)	1:A:776:LEU:HD11	1:A:773:ASP:HB3	2	0.5
(2,1401)	1:A:776:LEU:HD12	1:A:773:ASP:HB2	2	0.5
(2,1401)	1:A:776:LEU:HD12	1:A:773:ASP:HB3	2	0.5
(2,1401)	1:A:776:LEU:HD13	1:A:773:ASP:HB2	2	0.5
(2,1401)	1:A:776:LEU:HD13	1:A:773:ASP:HB3	2	0.5
(2,1386)	1:A:774:LEU:H	1:A:764:SER:HA	10	0.5
(2,1313)	1:A:746:ILE:H	1:A:742:ARG:HA	10	0.5
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	13	0.49
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	13	0.49
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	13	0.49
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	13	0.49
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	13	0.49
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	13	0.49
(2,698)	1:A:675:ILE:H	1:A:674:ASP:H	11	0.49
(2,614)	1:B:793:LEU:H	1:B:790:TRP:HE3	8	0.49
(2,457)	1:B:740:ARG:H	1:B:739:GLU:HA	4	0.49
(2,457)	1:B:740:ARG:H	1:B:739:GLU:HA	9	0.49
(2,457)	1:B:740:ARG:H	1:B:739:GLU:HA	15	0.49
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG21	1	0.49
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG22	1	0.49
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG23	1	0.49
(2,204)	1:A:827:ASP:H	1:A:820:ILE:HG12	11	0.49
(2,204)	1:A:827:ASP:H	1:A:820:ILE:HG13	11	0.49
(2,203)	1:A:827:ASP:H	1:A:820:ILE:HG12	11	0.49
(2,203)	1:A:827:ASP:H	1:A:820:ILE:HG13	11	0.49
(2,180)	1:A:806:GLU:H	1:B:771:LEU:HG	12	0.49
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG12	6	0.49
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG13	6	0.49
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG12	6	0.49
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG13	6	0.49
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG12	8	0.49
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG13	8	0.49
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG12	13	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG13	13	0.49
(2,1464)	1:A:793:LEU:H	1:A:790:TRP:HE3	2	0.49
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	13	0.49
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	13	0.49
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	13	0.49
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	13	0.49
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	13	0.49
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	13	0.49
(2,1123)	1:A:675:ILE:H	1:A:674:ASP:H	11	0.49
(2,1039)	1:A:793:LEU:H	1:A:790:TRP:HE3	2	0.49
(1,88)	1:B:790:TRP:O	1:B:794:LYS:N	14	0.49
(1,2)	1:B:790:TRP:O	1:B:794:LYS:N	14	0.49
(1,174)	1:B:790:TRP:O	1:B:794:LYS:N	14	0.49
(2,961)	1:A:774:LEU:H	1:A:764:SER:HA	5	0.48
(2,961)	1:A:774:LEU:H	1:A:764:SER:HA	8	0.48
(2,882)	1:A:740:ARG:H	1:A:739:GLU:HA	8	0.48
(2,815)	1:A:704:LEU:H	1:A:704:LEU:HB3	6	0.48
(2,764)	1:A:693:ILE:HG21	1:A:694:GLY:H	6	0.48
(2,764)	1:A:693:ILE:HG22	1:A:694:GLY:H	6	0.48
(2,764)	1:A:693:ILE:HG23	1:A:694:GLY:H	6	0.48
(2,764)	1:A:693:ILE:HG21	1:A:694:GLY:H	7	0.48
(2,764)	1:A:693:ILE:HG22	1:A:694:GLY:H	7	0.48
(2,764)	1:A:693:ILE:HG23	1:A:694:GLY:H	7	0.48
(2,620)	1:B:802:TYR:H	1:B:802:TYR:HB3	13	0.48
(2,614)	1:B:793:LEU:H	1:B:790:TRP:HE3	10	0.48
(2,457)	1:B:740:ARG:H	1:B:739:GLU:HA	1	0.48
(2,457)	1:B:740:ARG:H	1:B:739:GLU:HA	2	0.48
(2,457)	1:B:740:ARG:H	1:B:739:GLU:HA	6	0.48
(2,457)	1:B:740:ARG:H	1:B:739:GLU:HA	8	0.48
(2,457)	1:B:740:ARG:H	1:B:739:GLU:HA	12	0.48
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB2	14	0.48
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB3	14	0.48
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB2	14	0.48
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB3	14	0.48
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB2	14	0.48
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB3	14	0.48
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ1	8	0.48
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ2	8	0.48
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ3	8	0.48
(2,1386)	1:A:774:LEU:H	1:A:764:SER:HA	5	0.48
(2,1386)	1:A:774:LEU:H	1:A:764:SER:HA	8	0.48
(2,135)	1:B:756:ILE:H	1:A:796:TRP:HE1	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1307)	1:A:740:ARG:H	1:A:739:GLU:HA	8	0.48
(2,1240)	1:A:704:LEU:H	1:A:704:LEU:HB3	6	0.48
(2,1189)	1:A:693:ILE:HG21	1:A:694:GLY:H	6	0.48
(2,1189)	1:A:693:ILE:HG22	1:A:694:GLY:H	6	0.48
(2,1189)	1:A:693:ILE:HG23	1:A:694:GLY:H	6	0.48
(2,1189)	1:A:693:ILE:HG21	1:A:694:GLY:H	7	0.48
(2,1189)	1:A:693:ILE:HG22	1:A:694:GLY:H	7	0.48
(2,1189)	1:A:693:ILE:HG23	1:A:694:GLY:H	7	0.48
(2,965)	1:A:775:LEU:H	1:A:772:ARG:HA	3	0.47
(2,888)	1:A:746:ILE:H	1:A:742:ARG:HA	4	0.47
(2,853)	1:A:708:VAL:HG11	1:A:705:VAL:HA	13	0.47
(2,853)	1:A:708:VAL:HG12	1:A:705:VAL:HA	13	0.47
(2,853)	1:A:708:VAL:HG13	1:A:705:VAL:HA	13	0.47
(2,764)	1:A:693:ILE:HG21	1:A:694:GLY:H	2	0.47
(2,764)	1:A:693:ILE:HG22	1:A:694:GLY:H	2	0.47
(2,764)	1:A:693:ILE:HG23	1:A:694:GLY:H	2	0.47
(2,721)	1:A:682:ILE:HD11	1:A:681:TYR:H	9	0.47
(2,721)	1:A:682:ILE:HD12	1:A:681:TYR:H	9	0.47
(2,721)	1:A:682:ILE:HD13	1:A:681:TYR:H	9	0.47
(2,559)	1:B:778:VAL:H	1:B:775:LEU:HA	13	0.47
(2,536)	1:B:774:LEU:H	1:B:764:SER:HA	4	0.47
(2,536)	1:B:774:LEU:H	1:B:764:SER:HA	6	0.47
(2,482)	1:B:749:VAL:H	1:B:746:ILE:HA	3	0.47
(2,463)	1:B:746:ILE:H	1:B:742:ARG:HA	11	0.47
(2,457)	1:B:740:ARG:H	1:B:739:GLU:HA	13	0.47
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB2	11	0.47
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB3	11	0.47
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB2	11	0.47
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB3	11	0.47
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB2	11	0.47
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB3	11	0.47
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB2	7	0.47
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB3	7	0.47
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB2	7	0.47
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB3	7	0.47
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB2	7	0.47
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB3	7	0.47
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG12	1	0.47
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG13	1	0.47
(2,183)	1:A:806:GLU:H	1:B:772:ARG:HE	7	0.47
(2,15)	1:A:666:TRP:HE1	1:B:666:TRP:HD1	13	0.47
(2,1390)	1:A:775:LEU:H	1:A:772:ARG:HA	3	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1313)	1:A:746:ILE:H	1:A:742:ARG:HA	4	0.47
(2,1278)	1:A:708:VAL:HG11	1:A:705:VAL:HA	13	0.47
(2,1278)	1:A:708:VAL:HG12	1:A:705:VAL:HA	13	0.47
(2,1278)	1:A:708:VAL:HG13	1:A:705:VAL:HA	13	0.47
(2,1189)	1:A:693:ILE:HG21	1:A:694:GLY:H	2	0.47
(2,1189)	1:A:693:ILE:HG22	1:A:694:GLY:H	2	0.47
(2,1189)	1:A:693:ILE:HG23	1:A:694:GLY:H	2	0.47
(2,1146)	1:A:682:ILE:HD11	1:A:681:TYR:H	9	0.47
(2,1146)	1:A:682:ILE:HD12	1:A:681:TYR:H	9	0.47
(2,1146)	1:A:682:ILE:HD13	1:A:681:TYR:H	9	0.47
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG21	12	0.47
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG22	12	0.47
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG23	12	0.47
(1,87)	1:B:790:TRP:O	1:B:794:LYS:H	4	0.47
(1,87)	1:B:790:TRP:O	1:B:794:LYS:H	7	0.47
(1,173)	1:B:790:TRP:O	1:B:794:LYS:H	4	0.47
(1,173)	1:B:790:TRP:O	1:B:794:LYS:H	7	0.47
(1,1)	1:B:790:TRP:O	1:B:794:LYS:H	4	0.47
(1,1)	1:B:790:TRP:O	1:B:794:LYS:H	7	0.47
(2,984)	1:A:778:VAL:H	1:A:775:LEU:HA	2	0.46
(2,869)	1:A:710:GLN:H	1:A:710:GLN:HB3	5	0.46
(2,854)	1:A:708:VAL:HG21	1:A:707:ARG:HD2	7	0.46
(2,854)	1:A:708:VAL:HG21	1:A:707:ARG:HD3	7	0.46
(2,854)	1:A:708:VAL:HG22	1:A:707:ARG:HD2	7	0.46
(2,854)	1:A:708:VAL:HG22	1:A:707:ARG:HD3	7	0.46
(2,854)	1:A:708:VAL:HG23	1:A:707:ARG:HD2	7	0.46
(2,854)	1:A:708:VAL:HG23	1:A:707:ARG:HD3	7	0.46
(2,853)	1:A:708:VAL:HG11	1:A:705:VAL:HA	4	0.46
(2,853)	1:A:708:VAL:HG12	1:A:705:VAL:HA	4	0.46
(2,853)	1:A:708:VAL:HG13	1:A:705:VAL:HA	4	0.46
(2,765)	1:A:693:ILE:HG21	1:A:696:ARG:HG2	1	0.46
(2,765)	1:A:693:ILE:HG21	1:A:696:ARG:HG3	1	0.46
(2,765)	1:A:693:ILE:HG22	1:A:696:ARG:HG2	1	0.46
(2,765)	1:A:693:ILE:HG22	1:A:696:ARG:HG3	1	0.46
(2,765)	1:A:693:ILE:HG23	1:A:696:ARG:HG2	1	0.46
(2,765)	1:A:693:ILE:HG23	1:A:696:ARG:HG3	1	0.46
(2,765)	1:A:693:ILE:HG21	1:A:696:ARG:HG2	3	0.46
(2,765)	1:A:693:ILE:HG21	1:A:696:ARG:HG3	3	0.46
(2,765)	1:A:693:ILE:HG22	1:A:696:ARG:HG2	3	0.46
(2,765)	1:A:693:ILE:HG22	1:A:696:ARG:HG3	3	0.46
(2,765)	1:A:693:ILE:HG23	1:A:696:ARG:HG2	3	0.46
(2,765)	1:A:693:ILE:HG23	1:A:696:ARG:HG3	3	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE1	4	0.46
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE2	4	0.46
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE1	4	0.46
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE2	4	0.46
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE1	4	0.46
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE2	4	0.46
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD11	5	0.46
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD12	5	0.46
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD13	5	0.46
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD21	5	0.46
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD22	5	0.46
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD23	5	0.46
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD2	9	0.46
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD3	9	0.46
(2,620)	1:B:802:TYR:H	1:B:802:TYR:HB3	1	0.46
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD11	7	0.46
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD12	7	0.46
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD13	7	0.46
(2,540)	1:B:775:LEU:H	1:B:772:ARG:HA	15	0.46
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA2	4	0.46
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA3	4	0.46
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA2	4	0.46
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA3	4	0.46
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA2	4	0.46
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA3	4	0.46
(2,463)	1:B:746:ILE:H	1:B:742:ARG:HA	2	0.46
(2,457)	1:B:740:ARG:H	1:B:739:GLU:HA	7	0.46
(2,457)	1:B:740:ARG:H	1:B:739:GLU:HA	11	0.46
(2,391)	1:B:704:LEU:H	1:B:704:LEU:HB2	1	0.46
(2,355)	1:B:698:VAL:HG11	1:B:695:LEU:HA	5	0.46
(2,355)	1:B:698:VAL:HG12	1:B:695:LEU:HA	5	0.46
(2,355)	1:B:698:VAL:HG13	1:B:695:LEU:HA	5	0.46
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG12	4	0.46
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG13	4	0.46
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG12	4	0.46
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG13	4	0.46
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB2	4	0.46
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB3	4	0.46
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB2	6	0.46
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB3	6	0.46
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG12	9	0.46
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG13	9	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1409)	1:A:778:VAL:H	1:A:775:LEU:HA	2	0.46
(2,1294)	1:A:710:GLN:H	1:A:710:GLN:HB3	5	0.46
(2,1279)	1:A:708:VAL:HG21	1:A:707:ARG:HD2	7	0.46
(2,1279)	1:A:708:VAL:HG21	1:A:707:ARG:HD3	7	0.46
(2,1279)	1:A:708:VAL:HG22	1:A:707:ARG:HD2	7	0.46
(2,1279)	1:A:708:VAL:HG22	1:A:707:ARG:HD3	7	0.46
(2,1279)	1:A:708:VAL:HG23	1:A:707:ARG:HD2	7	0.46
(2,1279)	1:A:708:VAL:HG23	1:A:707:ARG:HD3	7	0.46
(2,1278)	1:A:708:VAL:HG11	1:A:705:VAL:HA	4	0.46
(2,1278)	1:A:708:VAL:HG12	1:A:705:VAL:HA	4	0.46
(2,1278)	1:A:708:VAL:HG13	1:A:705:VAL:HA	4	0.46
(2,1190)	1:A:693:ILE:HG21	1:A:696:ARG:HG2	1	0.46
(2,1190)	1:A:693:ILE:HG21	1:A:696:ARG:HG3	1	0.46
(2,1190)	1:A:693:ILE:HG22	1:A:696:ARG:HG2	1	0.46
(2,1190)	1:A:693:ILE:HG22	1:A:696:ARG:HG3	1	0.46
(2,1190)	1:A:693:ILE:HG23	1:A:696:ARG:HG2	1	0.46
(2,1190)	1:A:693:ILE:HG23	1:A:696:ARG:HG3	1	0.46
(2,1190)	1:A:693:ILE:HG21	1:A:696:ARG:HG2	3	0.46
(2,1190)	1:A:693:ILE:HG21	1:A:696:ARG:HG3	3	0.46
(2,1190)	1:A:693:ILE:HG22	1:A:696:ARG:HG2	3	0.46
(2,1190)	1:A:693:ILE:HG22	1:A:696:ARG:HG3	3	0.46
(2,1190)	1:A:693:ILE:HG23	1:A:696:ARG:HG2	3	0.46
(2,1190)	1:A:693:ILE:HG23	1:A:696:ARG:HG3	3	0.46
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD11	5	0.46
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD12	5	0.46
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD13	5	0.46
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD21	5	0.46
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD22	5	0.46
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD23	5	0.46
(1,87)	1:B:790:TRP:O	1:B:794:LYS:H	10	0.46
(1,173)	1:B:790:TRP:O	1:B:794:LYS:H	10	0.46
(1,1)	1:B:790:TRP:O	1:B:794:LYS:H	10	0.46
(2,990)	1:A:779:THR:H	1:A:776:LEU:HA	11	0.45
(2,984)	1:A:778:VAL:H	1:A:775:LEU:HA	11	0.45
(2,956)	1:A:773:ASP:H	1:A:770:ARG:HD2	15	0.45
(2,956)	1:A:773:ASP:H	1:A:770:ARG:HD3	15	0.45
(2,869)	1:A:710:GLN:H	1:A:710:GLN:HB3	12	0.45
(2,826)	1:A:705:VAL:HG11	1:A:702:LEU:HA	2	0.45
(2,826)	1:A:705:VAL:HG12	1:A:702:LEU:HA	2	0.45
(2,826)	1:A:705:VAL:HG13	1:A:702:LEU:HA	2	0.45
(2,820)	1:A:704:LEU:HD11	1:A:708:VAL:HG21	9	0.45
(2,820)	1:A:704:LEU:HD11	1:A:708:VAL:HG22	9	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,820)	1:A:704:LEU:HD11	1:A:708:VAL:HG23	9	0.45
(2,820)	1:A:704:LEU:HD12	1:A:708:VAL:HG21	9	0.45
(2,820)	1:A:704:LEU:HD12	1:A:708:VAL:HG22	9	0.45
(2,820)	1:A:704:LEU:HD12	1:A:708:VAL:HG23	9	0.45
(2,820)	1:A:704:LEU:HD13	1:A:708:VAL:HG21	9	0.45
(2,820)	1:A:704:LEU:HD13	1:A:708:VAL:HG22	9	0.45
(2,820)	1:A:704:LEU:HD13	1:A:708:VAL:HG23	9	0.45
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD2	14	0.45
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD3	14	0.45
(2,614)	1:B:793:LEU:H	1:B:790:TRP:HE3	1	0.45
(2,614)	1:B:793:LEU:H	1:B:790:TRP:HE3	3	0.45
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB1	14	0.45
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB2	14	0.45
(2,612)	1:B:790:TRP:HE1	1:B:792:ALA:HB3	14	0.45
(2,499)	1:B:754:ALA:HB1	1:B:753:LEU:HD21	11	0.45
(2,499)	1:B:754:ALA:HB1	1:B:753:LEU:HD22	11	0.45
(2,499)	1:B:754:ALA:HB1	1:B:753:LEU:HD23	11	0.45
(2,499)	1:B:754:ALA:HB2	1:B:753:LEU:HD21	11	0.45
(2,499)	1:B:754:ALA:HB2	1:B:753:LEU:HD22	11	0.45
(2,499)	1:B:754:ALA:HB2	1:B:753:LEU:HD23	11	0.45
(2,499)	1:B:754:ALA:HB3	1:B:753:LEU:HD21	11	0.45
(2,499)	1:B:754:ALA:HB3	1:B:753:LEU:HD22	11	0.45
(2,499)	1:B:754:ALA:HB3	1:B:753:LEU:HD23	11	0.45
(2,463)	1:B:746:ILE:H	1:B:742:ARG:HA	10	0.45
(2,457)	1:B:740:ARG:H	1:B:739:GLU:HA	5	0.45
(2,432)	1:B:709:ARG:H	1:B:707:ARG:H	13	0.45
(2,401)	1:B:705:VAL:HG11	1:B:702:LEU:HA	14	0.45
(2,401)	1:B:705:VAL:HG12	1:B:702:LEU:HA	14	0.45
(2,401)	1:B:705:VAL:HG13	1:B:702:LEU:HA	14	0.45
(2,393)	1:B:704:LEU:HD11	1:B:707:ARG:HD2	11	0.45
(2,393)	1:B:704:LEU:HD11	1:B:707:ARG:HD3	11	0.45
(2,393)	1:B:704:LEU:HD12	1:B:707:ARG:HD2	11	0.45
(2,393)	1:B:704:LEU:HD12	1:B:707:ARG:HD3	11	0.45
(2,393)	1:B:704:LEU:HD13	1:B:707:ARG:HD2	11	0.45
(2,393)	1:B:704:LEU:HD13	1:B:707:ARG:HD3	11	0.45
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG12	12	0.45
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG13	12	0.45
(2,180)	1:A:806:GLU:H	1:B:771:LEU:HG	1	0.45
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG12	4	0.45
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG13	4	0.45
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG12	4	0.45
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG13	4	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	3	0.45
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	3	0.45
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	3	0.45
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	3	0.45
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	3	0.45
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	3	0.45
(2,1464)	1:A:793:LEU:H	1:A:790:TRP:HE3	15	0.45
(2,1415)	1:A:779:THR:H	1:A:776:LEU:HA	11	0.45
(2,1409)	1:A:778:VAL:H	1:A:775:LEU:HA	11	0.45
(2,1381)	1:A:773:ASP:H	1:A:770:ARG:HD2	15	0.45
(2,1381)	1:A:773:ASP:H	1:A:770:ARG:HD3	15	0.45
(2,1294)	1:A:710:GLN:H	1:A:710:GLN:HB3	12	0.45
(2,1251)	1:A:705:VAL:HG11	1:A:702:LEU:HA	2	0.45
(2,1251)	1:A:705:VAL:HG12	1:A:702:LEU:HA	2	0.45
(2,1251)	1:A:705:VAL:HG13	1:A:702:LEU:HA	2	0.45
(2,1245)	1:A:704:LEU:HD11	1:A:708:VAL:HG21	9	0.45
(2,1245)	1:A:704:LEU:HD11	1:A:708:VAL:HG22	9	0.45
(2,1245)	1:A:704:LEU:HD11	1:A:708:VAL:HG23	9	0.45
(2,1245)	1:A:704:LEU:HD12	1:A:708:VAL:HG21	9	0.45
(2,1245)	1:A:704:LEU:HD12	1:A:708:VAL:HG22	9	0.45
(2,1245)	1:A:704:LEU:HD12	1:A:708:VAL:HG23	9	0.45
(2,1245)	1:A:704:LEU:HD13	1:A:708:VAL:HG21	9	0.45
(2,1245)	1:A:704:LEU:HD13	1:A:708:VAL:HG22	9	0.45
(2,1245)	1:A:704:LEU:HD13	1:A:708:VAL:HG23	9	0.45
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	3	0.45
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	3	0.45
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	3	0.45
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	3	0.45
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	3	0.45
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	3	0.45
(2,1039)	1:A:793:LEU:H	1:A:790:TRP:HE3	15	0.45
(2,965)	1:A:775:LEU:H	1:A:772:ARG:HA	7	0.44
(2,961)	1:A:774:LEU:H	1:A:764:SER:HA	7	0.44
(2,93)	1:A:754:ALA:H	1:B:716:SER:HB2	7	0.44
(2,93)	1:A:754:ALA:H	1:B:716:SER:HB3	7	0.44
(2,857)	1:A:709:ARG:H	1:A:707:ARG:H	9	0.44
(2,857)	1:A:709:ARG:H	1:A:707:ARG:H	14	0.44
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB2	9	0.44
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB3	9	0.44
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB2	9	0.44
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB3	9	0.44
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB2	9	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB3	9	0.44
(2,853)	1:A:708:VAL:HG11	1:A:705:VAL:HA	15	0.44
(2,853)	1:A:708:VAL:HG12	1:A:705:VAL:HA	15	0.44
(2,853)	1:A:708:VAL:HG13	1:A:705:VAL:HA	15	0.44
(2,826)	1:A:705:VAL:HG11	1:A:702:LEU:HA	4	0.44
(2,826)	1:A:705:VAL:HG12	1:A:702:LEU:HA	4	0.44
(2,826)	1:A:705:VAL:HG13	1:A:702:LEU:HA	4	0.44
(2,826)	1:A:705:VAL:HG11	1:A:702:LEU:HA	11	0.44
(2,826)	1:A:705:VAL:HG12	1:A:702:LEU:HA	11	0.44
(2,826)	1:A:705:VAL:HG13	1:A:702:LEU:HA	11	0.44
(2,826)	1:A:705:VAL:HG11	1:A:702:LEU:HA	13	0.44
(2,826)	1:A:705:VAL:HG12	1:A:702:LEU:HA	13	0.44
(2,826)	1:A:705:VAL:HG13	1:A:702:LEU:HA	13	0.44
(2,81)	1:A:708:VAL:HG21	1:B:714:PRO:HA	5	0.44
(2,81)	1:A:708:VAL:HG22	1:B:714:PRO:HA	5	0.44
(2,81)	1:A:708:VAL:HG23	1:B:714:PRO:HA	5	0.44
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	8	0.44
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	8	0.44
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	8	0.44
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	8	0.44
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	8	0.44
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	8	0.44
(2,622)	1:B:802:TYR:H	1:B:803:TRP:HH2	7	0.44
(2,614)	1:B:793:LEU:H	1:B:790:TRP:HE3	13	0.44
(2,565)	1:B:779:THR:H	1:B:776:LEU:HA	10	0.44
(2,559)	1:B:778:VAL:H	1:B:775:LEU:HA	10	0.44
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE1	10	0.44
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE2	10	0.44
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE1	10	0.44
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE2	10	0.44
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE1	10	0.44
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE2	10	0.44
(2,473)	1:B:746:ILE:HG21	1:B:750:ASN:HD22	5	0.44
(2,473)	1:B:746:ILE:HG22	1:B:750:ASN:HD22	5	0.44
(2,473)	1:B:746:ILE:HG23	1:B:750:ASN:HD22	5	0.44
(2,471)	1:B:746:ILE:HD11	1:B:743:ASP:HB2	6	0.44
(2,471)	1:B:746:ILE:HD11	1:B:743:ASP:HB3	6	0.44
(2,471)	1:B:746:ILE:HD12	1:B:743:ASP:HB2	6	0.44
(2,471)	1:B:746:ILE:HD12	1:B:743:ASP:HB3	6	0.44
(2,471)	1:B:746:ILE:HD13	1:B:743:ASP:HB2	6	0.44
(2,471)	1:B:746:ILE:HD13	1:B:743:ASP:HB3	6	0.44
(2,439)	1:B:710:GLN:H	1:B:708:VAL:HA	2	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,432)	1:B:709:ARG:H	1:B:707:ARG:H	6	0.44
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD11	2	0.44
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD12	2	0.44
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD13	2	0.44
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD2	2	0.44
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD3	2	0.44
(2,169)	1:B:797:TRP:HE1	1:B:848:ARG:HB2	9	0.44
(2,169)	1:B:797:TRP:HE1	1:B:848:ARG:HB3	9	0.44
(2,148)	1:B:790:TRP:HE1	1:B:851:LEU:HD11	14	0.44
(2,148)	1:B:790:TRP:HE1	1:B:851:LEU:HD12	14	0.44
(2,148)	1:B:790:TRP:HE1	1:B:851:LEU:HD13	14	0.44
(2,148)	1:B:790:TRP:HE1	1:B:851:LEU:HD21	14	0.44
(2,148)	1:B:790:TRP:HE1	1:B:851:LEU:HD22	14	0.44
(2,148)	1:B:790:TRP:HE1	1:B:851:LEU:HD23	14	0.44
(2,1390)	1:A:775:LEU:H	1:A:772:ARG:HA	7	0.44
(2,1386)	1:A:774:LEU:H	1:A:764:SER:HA	7	0.44
(2,135)	1:B:756:ILE:H	1:A:796:TRP:HE1	9	0.44
(2,1282)	1:A:709:ARG:H	1:A:707:ARG:H	9	0.44
(2,1282)	1:A:709:ARG:H	1:A:707:ARG:H	14	0.44
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB2	9	0.44
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB3	9	0.44
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB2	9	0.44
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB3	9	0.44
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB2	9	0.44
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB3	9	0.44
(2,1278)	1:A:708:VAL:HG11	1:A:705:VAL:HA	15	0.44
(2,1278)	1:A:708:VAL:HG12	1:A:705:VAL:HA	15	0.44
(2,1278)	1:A:708:VAL:HG13	1:A:705:VAL:HA	15	0.44
(2,1251)	1:A:705:VAL:HG11	1:A:702:LEU:HA	4	0.44
(2,1251)	1:A:705:VAL:HG12	1:A:702:LEU:HA	4	0.44
(2,1251)	1:A:705:VAL:HG13	1:A:702:LEU:HA	4	0.44
(2,1251)	1:A:705:VAL:HG11	1:A:702:LEU:HA	11	0.44
(2,1251)	1:A:705:VAL:HG12	1:A:702:LEU:HA	11	0.44
(2,1251)	1:A:705:VAL:HG13	1:A:702:LEU:HA	11	0.44
(2,1251)	1:A:705:VAL:HG11	1:A:702:LEU:HA	13	0.44
(2,1251)	1:A:705:VAL:HG12	1:A:702:LEU:HA	13	0.44
(2,1251)	1:A:705:VAL:HG13	1:A:702:LEU:HA	13	0.44
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	8	0.44
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	8	0.44
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	8	0.44
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	8	0.44
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	8	0.44
(2,990)	1:A:779:THR:H	1:A:776:LEU:HA	15	0.43
(2,984)	1:A:778:VAL:H	1:A:775:LEU:HA	1	0.43
(2,965)	1:A:775:LEU:H	1:A:772:ARG:HA	14	0.43
(2,943)	1:A:763:LEU:HD11	1:A:759:ASP:HA	6	0.43
(2,943)	1:A:763:LEU:HD12	1:A:759:ASP:HA	6	0.43
(2,943)	1:A:763:LEU:HD13	1:A:759:ASP:HA	6	0.43
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	6	0.43
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	6	0.43
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	6	0.43
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	6	0.43
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	6	0.43
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	6	0.43
(2,907)	1:A:749:VAL:H	1:A:746:ILE:HA	4	0.43
(2,869)	1:A:710:GLN:H	1:A:710:GLN:HB3	4	0.43
(2,857)	1:A:709:ARG:H	1:A:707:ARG:H	1	0.43
(2,826)	1:A:705:VAL:HG11	1:A:702:LEU:HA	6	0.43
(2,826)	1:A:705:VAL:HG12	1:A:702:LEU:HA	6	0.43
(2,826)	1:A:705:VAL:HG13	1:A:702:LEU:HA	6	0.43
(2,826)	1:A:705:VAL:HG11	1:A:702:LEU:HA	8	0.43
(2,826)	1:A:705:VAL:HG12	1:A:702:LEU:HA	8	0.43
(2,826)	1:A:705:VAL:HG13	1:A:702:LEU:HA	8	0.43
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD11	8	0.43
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD12	8	0.43
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD13	8	0.43
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD21	8	0.43
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD22	8	0.43
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD23	8	0.43
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE1	2	0.43
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE2	2	0.43
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE1	2	0.43
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE2	2	0.43
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE1	2	0.43
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE2	2	0.43
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA2	3	0.43
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA3	3	0.43
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA2	3	0.43
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA3	3	0.43
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA2	3	0.43
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA3	3	0.43
(2,492)	1:B:753:LEU:HD21	1:B:750:ASN:HB2	7	0.43
(2,492)	1:B:753:LEU:HD21	1:B:750:ASN:HB3	7	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,492)	1:B:753:LEU:HD22	1:B:750:ASN:HB2	7	0.43
(2,492)	1:B:753:LEU:HD22	1:B:750:ASN:HB3	7	0.43
(2,492)	1:B:753:LEU:HD23	1:B:750:ASN:HB2	7	0.43
(2,492)	1:B:753:LEU:HD23	1:B:750:ASN:HB3	7	0.43
(2,471)	1:B:746:ILE:HD11	1:B:743:ASP:HB2	10	0.43
(2,471)	1:B:746:ILE:HD11	1:B:743:ASP:HB3	10	0.43
(2,471)	1:B:746:ILE:HD12	1:B:743:ASP:HB2	10	0.43
(2,471)	1:B:746:ILE:HD12	1:B:743:ASP:HB3	10	0.43
(2,471)	1:B:746:ILE:HD13	1:B:743:ASP:HB2	10	0.43
(2,471)	1:B:746:ILE:HD13	1:B:743:ASP:HB3	10	0.43
(2,463)	1:B:746:ILE:H	1:B:742:ARG:HA	3	0.43
(2,432)	1:B:709:ARG:H	1:B:707:ARG:H	14	0.43
(2,401)	1:B:705:VAL:HG11	1:B:702:LEU:HA	15	0.43
(2,401)	1:B:705:VAL:HG12	1:B:702:LEU:HA	15	0.43
(2,401)	1:B:705:VAL:HG13	1:B:702:LEU:HA	15	0.43
(2,355)	1:B:698:VAL:HG11	1:B:695:LEU:HA	12	0.43
(2,355)	1:B:698:VAL:HG12	1:B:695:LEU:HA	12	0.43
(2,355)	1:B:698:VAL:HG13	1:B:695:LEU:HA	12	0.43
(2,296)	1:B:682:ILE:HD11	1:B:681:TYR:H	13	0.43
(2,296)	1:B:682:ILE:HD12	1:B:681:TYR:H	13	0.43
(2,296)	1:B:682:ILE:HD13	1:B:681:TYR:H	13	0.43
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD11	13	0.43
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD12	13	0.43
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD13	13	0.43
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ1	9	0.43
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ2	9	0.43
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ3	9	0.43
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG12	1	0.43
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG13	1	0.43
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD2	7	0.43
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD3	7	0.43
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD2	9	0.43
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD3	9	0.43
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	13	0.43
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	13	0.43
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	13	0.43
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	13	0.43
(2,165)	1:A:796:TRP:HE1	1:B:755:LEU:HD21	7	0.43
(2,165)	1:A:796:TRP:HE1	1:B:755:LEU:HD22	7	0.43
(2,165)	1:A:796:TRP:HE1	1:B:755:LEU:HD23	7	0.43
(2,1472)	1:A:802:TYR:H	1:A:803:TRP:HH2	11	0.43
(2,1464)	1:A:793:LEU:H	1:A:790:TRP:HE3	11	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1464)	1:A:793:LEU:H	1:A:790:TRP:HE3	12	0.43
(2,1431)	1:A:782:VAL:H	1:A:779:THR:HA	3	0.43
(2,1415)	1:A:779:THR:H	1:A:776:LEU:HA	15	0.43
(2,1409)	1:A:778:VAL:H	1:A:775:LEU:HA	1	0.43
(2,1390)	1:A:775:LEU:H	1:A:772:ARG:HA	14	0.43
(2,1368)	1:A:763:LEU:HD11	1:A:759:ASP:HA	6	0.43
(2,1368)	1:A:763:LEU:HD12	1:A:759:ASP:HA	6	0.43
(2,1368)	1:A:763:LEU:HD13	1:A:759:ASP:HA	6	0.43
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	6	0.43
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	6	0.43
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	6	0.43
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	6	0.43
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	6	0.43
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	6	0.43
(2,1332)	1:A:749:VAL:H	1:A:746:ILE:HA	4	0.43
(2,1294)	1:A:710:GLN:H	1:A:710:GLN:HB3	4	0.43
(2,1282)	1:A:709:ARG:H	1:A:707:ARG:H	1	0.43
(2,1251)	1:A:705:VAL:HG11	1:A:702:LEU:HA	6	0.43
(2,1251)	1:A:705:VAL:HG12	1:A:702:LEU:HA	6	0.43
(2,1251)	1:A:705:VAL:HG13	1:A:702:LEU:HA	6	0.43
(2,1251)	1:A:705:VAL:HG11	1:A:702:LEU:HA	8	0.43
(2,1251)	1:A:705:VAL:HG12	1:A:702:LEU:HA	8	0.43
(2,1251)	1:A:705:VAL:HG13	1:A:702:LEU:HA	8	0.43
(2,1047)	1:A:802:TYR:H	1:A:803:TRP:HH2	11	0.43
(2,1039)	1:A:793:LEU:H	1:A:790:TRP:HE3	11	0.43
(2,1039)	1:A:793:LEU:H	1:A:790:TRP:HE3	12	0.43
(2,1006)	1:A:782:VAL:H	1:A:779:THR:HA	3	0.43
(1,87)	1:B:790:TRP:O	1:B:794:LYS:H	9	0.43
(1,173)	1:B:790:TRP:O	1:B:794:LYS:H	9	0.43
(1,1)	1:B:790:TRP:O	1:B:794:LYS:H	9	0.43
(2,965)	1:A:775:LEU:H	1:A:772:ARG:HA	15	0.42
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	2	0.42
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	2	0.42
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	2	0.42
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	2	0.42
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	2	0.42
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	2	0.42
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD2	11	0.42
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD3	11	0.42
(2,853)	1:A:708:VAL:HG11	1:A:705:VAL:HA	3	0.42
(2,853)	1:A:708:VAL:HG12	1:A:705:VAL:HA	3	0.42
(2,853)	1:A:708:VAL:HG13	1:A:705:VAL:HA	3	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD2	2	0.42
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD3	2	0.42
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD2	4	0.42
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD3	4	0.42
(2,81)	1:A:708:VAL:HG21	1:B:714:PRO:HA	11	0.42
(2,81)	1:A:708:VAL:HG22	1:B:714:PRO:HA	11	0.42
(2,81)	1:A:708:VAL:HG23	1:B:714:PRO:HA	11	0.42
(2,782)	1:A:698:VAL:HG11	1:A:699:PHE:HD1	6	0.42
(2,782)	1:A:698:VAL:HG11	1:A:699:PHE:HD2	6	0.42
(2,782)	1:A:698:VAL:HG12	1:A:699:PHE:HD1	6	0.42
(2,782)	1:A:698:VAL:HG12	1:A:699:PHE:HD2	6	0.42
(2,782)	1:A:698:VAL:HG13	1:A:699:PHE:HD1	6	0.42
(2,782)	1:A:698:VAL:HG13	1:A:699:PHE:HD2	6	0.42
(2,764)	1:A:693:ILE:HG21	1:A:694:GLY:H	1	0.42
(2,764)	1:A:693:ILE:HG22	1:A:694:GLY:H	1	0.42
(2,764)	1:A:693:ILE:HG23	1:A:694:GLY:H	1	0.42
(2,721)	1:A:682:ILE:HD11	1:A:681:TYR:H	1	0.42
(2,721)	1:A:682:ILE:HD12	1:A:681:TYR:H	1	0.42
(2,721)	1:A:682:ILE:HD13	1:A:681:TYR:H	1	0.42
(2,614)	1:B:793:LEU:H	1:B:790:TRP:HE3	2	0.42
(2,559)	1:B:778:VAL:H	1:B:775:LEU:HA	14	0.42
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA2	7	0.42
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA3	7	0.42
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA2	7	0.42
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA3	7	0.42
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA2	7	0.42
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA3	7	0.42
(2,492)	1:B:753:LEU:HD21	1:B:750:ASN:HB2	8	0.42
(2,492)	1:B:753:LEU:HD21	1:B:750:ASN:HB3	8	0.42
(2,492)	1:B:753:LEU:HD22	1:B:750:ASN:HB2	8	0.42
(2,492)	1:B:753:LEU:HD22	1:B:750:ASN:HB3	8	0.42
(2,492)	1:B:753:LEU:HD23	1:B:750:ASN:HB2	8	0.42
(2,492)	1:B:753:LEU:HD23	1:B:750:ASN:HB3	8	0.42
(2,482)	1:B:749:VAL:H	1:B:746:ILE:HA	5	0.42
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD2	3	0.42
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD3	3	0.42
(2,439)	1:B:710:GLN:H	1:B:708:VAL:HA	8	0.42
(2,432)	1:B:709:ARG:H	1:B:707:ARG:H	3	0.42
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB2	8	0.42
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB3	8	0.42
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB2	8	0.42
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB3	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB2	8	0.42
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB3	8	0.42
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB2	10	0.42
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB3	10	0.42
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB2	10	0.42
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB3	10	0.42
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB2	10	0.42
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB3	10	0.42
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB2	15	0.42
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB3	15	0.42
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB2	15	0.42
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB3	15	0.42
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB2	15	0.42
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB3	15	0.42
(2,401)	1:B:705:VAL:HG11	1:B:702:LEU:HA	2	0.42
(2,401)	1:B:705:VAL:HG12	1:B:702:LEU:HA	2	0.42
(2,401)	1:B:705:VAL:HG13	1:B:702:LEU:HA	2	0.42
(2,355)	1:B:698:VAL:HG11	1:B:695:LEU:HA	1	0.42
(2,355)	1:B:698:VAL:HG12	1:B:695:LEU:HA	1	0.42
(2,355)	1:B:698:VAL:HG13	1:B:695:LEU:HA	1	0.42
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG12	10	0.42
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG13	10	0.42
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG12	10	0.42
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG13	10	0.42
(2,165)	1:A:796:TRP:HE1	1:B:755:LEU:HD21	4	0.42
(2,165)	1:A:796:TRP:HE1	1:B:755:LEU:HD22	4	0.42
(2,165)	1:A:796:TRP:HE1	1:B:755:LEU:HD23	4	0.42
(2,1477)	1:A:819:ALA:H	1:A:820:ILE:HD11	6	0.42
(2,1477)	1:A:819:ALA:H	1:A:820:ILE:HD12	6	0.42
(2,1477)	1:A:819:ALA:H	1:A:820:ILE:HD13	6	0.42
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD11	1	0.42
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD12	1	0.42
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD13	1	0.42
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD21	1	0.42
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD22	1	0.42
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD23	1	0.42
(2,1390)	1:A:775:LEU:H	1:A:772:ARG:HA	15	0.42
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	2	0.42
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	2	0.42
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	2	0.42
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	2	0.42
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	2	0.42
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD2	11	0.42
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD3	11	0.42
(2,1278)	1:A:708:VAL:HG11	1:A:705:VAL:HA	3	0.42
(2,1278)	1:A:708:VAL:HG12	1:A:705:VAL:HA	3	0.42
(2,1278)	1:A:708:VAL:HG13	1:A:705:VAL:HA	3	0.42
(2,1207)	1:A:698:VAL:HG11	1:A:699:PHE:HD1	6	0.42
(2,1207)	1:A:698:VAL:HG11	1:A:699:PHE:HD2	6	0.42
(2,1207)	1:A:698:VAL:HG12	1:A:699:PHE:HD1	6	0.42
(2,1207)	1:A:698:VAL:HG12	1:A:699:PHE:HD2	6	0.42
(2,1207)	1:A:698:VAL:HG13	1:A:699:PHE:HD1	6	0.42
(2,1207)	1:A:698:VAL:HG13	1:A:699:PHE:HD2	6	0.42
(2,1189)	1:A:693:ILE:HG21	1:A:694:GLY:H	1	0.42
(2,1189)	1:A:693:ILE:HG22	1:A:694:GLY:H	1	0.42
(2,1189)	1:A:693:ILE:HG23	1:A:694:GLY:H	1	0.42
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB2	6	0.42
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB3	6	0.42
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB2	6	0.42
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB3	6	0.42
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB2	6	0.42
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB3	6	0.42
(2,1146)	1:A:682:ILE:HD11	1:A:681:TYR:H	1	0.42
(2,1146)	1:A:682:ILE:HD12	1:A:681:TYR:H	1	0.42
(2,1146)	1:A:682:ILE:HD13	1:A:681:TYR:H	1	0.42
(2,1052)	1:A:819:ALA:H	1:A:820:ILE:HD11	6	0.42
(2,1052)	1:A:819:ALA:H	1:A:820:ILE:HD12	6	0.42
(2,1052)	1:A:819:ALA:H	1:A:820:ILE:HD13	6	0.42
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD11	1	0.42
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD12	1	0.42
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD13	1	0.42
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD21	1	0.42
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD22	1	0.42
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD23	1	0.42
(1,87)	1:B:790:TRP:O	1:B:794:LYS:H	3	0.42
(1,173)	1:B:790:TRP:O	1:B:794:LYS:H	3	0.42
(1,1)	1:B:790:TRP:O	1:B:794:LYS:H	3	0.42
(2,984)	1:A:778:VAL:H	1:A:775:LEU:HA	10	0.41
(2,984)	1:A:778:VAL:H	1:A:775:LEU:HA	12	0.41
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD2	6	0.41
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD3	6	0.41
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB2	2	0.41
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB3	2	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB2	2	0.41
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB3	2	0.41
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB2	2	0.41
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB3	2	0.41
(2,854)	1:A:708:VAL:HG21	1:A:707:ARG:HD2	1	0.41
(2,854)	1:A:708:VAL:HG21	1:A:707:ARG:HD3	1	0.41
(2,854)	1:A:708:VAL:HG22	1:A:707:ARG:HD2	1	0.41
(2,854)	1:A:708:VAL:HG22	1:A:707:ARG:HD3	1	0.41
(2,854)	1:A:708:VAL:HG23	1:A:707:ARG:HD2	1	0.41
(2,854)	1:A:708:VAL:HG23	1:A:707:ARG:HD3	1	0.41
(2,826)	1:A:705:VAL:HG11	1:A:702:LEU:HA	1	0.41
(2,826)	1:A:705:VAL:HG12	1:A:702:LEU:HA	1	0.41
(2,826)	1:A:705:VAL:HG13	1:A:702:LEU:HA	1	0.41
(2,826)	1:A:705:VAL:HG11	1:A:702:LEU:HA	7	0.41
(2,826)	1:A:705:VAL:HG12	1:A:702:LEU:HA	7	0.41
(2,826)	1:A:705:VAL:HG13	1:A:702:LEU:HA	7	0.41
(2,760)	1:A:693:ILE:HD11	1:A:694:GLY:HA2	1	0.41
(2,760)	1:A:693:ILE:HD11	1:A:694:GLY:HA3	1	0.41
(2,760)	1:A:693:ILE:HD12	1:A:694:GLY:HA2	1	0.41
(2,760)	1:A:693:ILE:HD12	1:A:694:GLY:HA3	1	0.41
(2,760)	1:A:693:ILE:HD13	1:A:694:GLY:HA2	1	0.41
(2,760)	1:A:693:ILE:HD13	1:A:694:GLY:HA3	1	0.41
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	7	0.41
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	7	0.41
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	7	0.41
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	7	0.41
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	7	0.41
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	7	0.41
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD11	10	0.41
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD12	10	0.41
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD13	10	0.41
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD21	10	0.41
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD22	10	0.41
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD23	10	0.41
(2,559)	1:B:778:VAL:H	1:B:775:LEU:HA	8	0.41
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE1	11	0.41
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE2	11	0.41
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE1	11	0.41
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE2	11	0.41
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE1	11	0.41
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE2	11	0.41
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE1	13	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE2	13	0.41
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE1	13	0.41
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE2	13	0.41
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE1	13	0.41
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE2	13	0.41
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB2	5	0.41
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB3	5	0.41
(2,472)	1:B:746:ILE:HG21	1:B:750:ASN:HD21	3	0.41
(2,472)	1:B:746:ILE:HG22	1:B:750:ASN:HD21	3	0.41
(2,472)	1:B:746:ILE:HG23	1:B:750:ASN:HD21	3	0.41
(2,432)	1:B:709:ARG:H	1:B:707:ARG:H	7	0.41
(2,432)	1:B:709:ARG:H	1:B:707:ARG:H	9	0.41
(2,432)	1:B:709:ARG:H	1:B:707:ARG:H	15	0.41
(2,401)	1:B:705:VAL:HG11	1:B:702:LEU:HA	10	0.41
(2,401)	1:B:705:VAL:HG12	1:B:702:LEU:HA	10	0.41
(2,401)	1:B:705:VAL:HG13	1:B:702:LEU:HA	10	0.41
(2,401)	1:B:705:VAL:HG11	1:B:702:LEU:HA	11	0.41
(2,401)	1:B:705:VAL:HG12	1:B:702:LEU:HA	11	0.41
(2,401)	1:B:705:VAL:HG13	1:B:702:LEU:HA	11	0.41
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD11	1	0.41
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD12	1	0.41
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD13	1	0.41
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG12	15	0.41
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG13	15	0.41
(2,180)	1:A:806:GLU:H	1:B:771:LEU:HG	15	0.41
(2,169)	1:B:797:TRP:HE1	1:B:848:ARG:HB2	14	0.41
(2,169)	1:B:797:TRP:HE1	1:B:848:ARG:HB3	14	0.41
(2,1409)	1:A:778:VAL:H	1:A:775:LEU:HA	10	0.41
(2,1409)	1:A:778:VAL:H	1:A:775:LEU:HA	12	0.41
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD2	6	0.41
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD3	6	0.41
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD1	13	0.41
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD2	13	0.41
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB2	2	0.41
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB3	2	0.41
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB2	2	0.41
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB3	2	0.41
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB2	2	0.41
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB3	2	0.41
(2,1279)	1:A:708:VAL:HG21	1:A:707:ARG:HD2	1	0.41
(2,1279)	1:A:708:VAL:HG21	1:A:707:ARG:HD3	1	0.41
(2,1279)	1:A:708:VAL:HG22	1:A:707:ARG:HD2	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1279)	1:A:708:VAL:HG22	1:A:707:ARG:HD3	1	0.41
(2,1279)	1:A:708:VAL:HG23	1:A:707:ARG:HD2	1	0.41
(2,1279)	1:A:708:VAL:HG23	1:A:707:ARG:HD3	1	0.41
(2,1251)	1:A:705:VAL:HG11	1:A:702:LEU:HA	1	0.41
(2,1251)	1:A:705:VAL:HG12	1:A:702:LEU:HA	1	0.41
(2,1251)	1:A:705:VAL:HG13	1:A:702:LEU:HA	1	0.41
(2,1251)	1:A:705:VAL:HG11	1:A:702:LEU:HA	7	0.41
(2,1251)	1:A:705:VAL:HG12	1:A:702:LEU:HA	7	0.41
(2,1251)	1:A:705:VAL:HG13	1:A:702:LEU:HA	7	0.41
(2,1185)	1:A:693:ILE:HD11	1:A:694:GLY:HA2	1	0.41
(2,1185)	1:A:693:ILE:HD11	1:A:694:GLY:HA3	1	0.41
(2,1185)	1:A:693:ILE:HD12	1:A:694:GLY:HA2	1	0.41
(2,1185)	1:A:693:ILE:HD12	1:A:694:GLY:HA3	1	0.41
(2,1185)	1:A:693:ILE:HD13	1:A:694:GLY:HA2	1	0.41
(2,1185)	1:A:693:ILE:HD13	1:A:694:GLY:HA3	1	0.41
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB2	2	0.41
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB3	2	0.41
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB2	2	0.41
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB3	2	0.41
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB2	2	0.41
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB3	2	0.41
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	7	0.41
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	7	0.41
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	7	0.41
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	7	0.41
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	7	0.41
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	7	0.41
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD11	10	0.41
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD12	10	0.41
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD13	10	0.41
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD21	10	0.41
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD22	10	0.41
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD23	10	0.41
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG21	8	0.41
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG22	8	0.41
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG23	8	0.41
(1,87)	1:B:790:TRP:O	1:B:794:LYS:H	2	0.41
(1,173)	1:B:790:TRP:O	1:B:794:LYS:H	2	0.41
(1,1)	1:B:790:TRP:O	1:B:794:LYS:H	2	0.41
(2,984)	1:A:778:VAL:H	1:A:775:LEU:HA	5	0.4
(2,961)	1:A:774:LEU:H	1:A:764:SER:HA	9	0.4
(2,961)	1:A:774:LEU:H	1:A:764:SER:HA	15	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,857)	1:A:709:ARG:H	1:A:707:ARG:H	5	0.4
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB2	3	0.4
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB3	3	0.4
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB2	3	0.4
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB3	3	0.4
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB2	3	0.4
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB3	3	0.4
(2,782)	1:A:698:VAL:HG11	1:A:699:PHE:HD1	13	0.4
(2,782)	1:A:698:VAL:HG11	1:A:699:PHE:HD2	13	0.4
(2,782)	1:A:698:VAL:HG12	1:A:699:PHE:HD1	13	0.4
(2,782)	1:A:698:VAL:HG12	1:A:699:PHE:HD2	13	0.4
(2,782)	1:A:698:VAL:HG13	1:A:699:PHE:HD1	13	0.4
(2,782)	1:A:698:VAL:HG13	1:A:699:PHE:HD2	13	0.4
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	3	0.4
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	3	0.4
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	3	0.4
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	3	0.4
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	3	0.4
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	3	0.4
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	6	0.4
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	6	0.4
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	6	0.4
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	6	0.4
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	6	0.4
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	6	0.4
(2,614)	1:B:793:LEU:H	1:B:790:TRP:HE3	4	0.4
(2,559)	1:B:778:VAL:H	1:B:775:LEU:HA	7	0.4
(2,5)	1:A:663:LEU:H	1:A:661:LEU:HB2	3	0.4
(2,5)	1:A:663:LEU:H	1:A:661:LEU:HB3	3	0.4
(2,420)	1:B:707:ARG:H	1:B:707:ARG:HG2	9	0.4
(2,420)	1:B:707:ARG:H	1:B:707:ARG:HG3	9	0.4
(2,401)	1:B:705:VAL:HG11	1:B:702:LEU:HA	5	0.4
(2,401)	1:B:705:VAL:HG12	1:B:702:LEU:HA	5	0.4
(2,401)	1:B:705:VAL:HG13	1:B:702:LEU:HA	5	0.4
(2,295)	1:B:682:ILE:HG21	1:B:685:PHE:HD1	13	0.4
(2,295)	1:B:682:ILE:HG21	1:B:685:PHE:HD2	13	0.4
(2,295)	1:B:682:ILE:HG22	1:B:685:PHE:HD1	13	0.4
(2,295)	1:B:682:ILE:HG22	1:B:685:PHE:HD2	13	0.4
(2,295)	1:B:682:ILE:HG23	1:B:685:PHE:HD1	13	0.4
(2,295)	1:B:682:ILE:HG23	1:B:685:PHE:HD2	13	0.4
(2,204)	1:A:827:ASP:H	1:A:820:ILE:HG12	6	0.4
(2,204)	1:A:827:ASP:H	1:A:820:ILE:HG13	6	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,203)	1:A:827:ASP:H	1:A:820:ILE:HG12	6	0.4
(2,203)	1:A:827:ASP:H	1:A:820:ILE:HG13	6	0.4
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG12	10	0.4
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG13	10	0.4
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD11	5	0.4
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD12	5	0.4
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD13	5	0.4
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD21	5	0.4
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD22	5	0.4
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD23	5	0.4
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD11	10	0.4
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD12	10	0.4
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD13	10	0.4
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD21	10	0.4
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD22	10	0.4
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD23	10	0.4
(2,1482)	1:A:852:GLU:H	1:A:848:ARG:HG2	8	0.4
(2,1482)	1:A:852:GLU:H	1:A:848:ARG:HG3	8	0.4
(2,1464)	1:A:793:LEU:H	1:A:790:TRP:HE3	9	0.4
(2,1464)	1:A:793:LEU:H	1:A:790:TRP:HE3	14	0.4
(2,1409)	1:A:778:VAL:H	1:A:775:LEU:HA	5	0.4
(2,1386)	1:A:774:LEU:H	1:A:764:SER:HA	9	0.4
(2,1386)	1:A:774:LEU:H	1:A:764:SER:HA	15	0.4
(2,1282)	1:A:709:ARG:H	1:A:707:ARG:H	5	0.4
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB2	3	0.4
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB3	3	0.4
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB2	3	0.4
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB3	3	0.4
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB2	3	0.4
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB3	3	0.4
(2,1207)	1:A:698:VAL:HG11	1:A:699:PHE:HD1	13	0.4
(2,1207)	1:A:698:VAL:HG11	1:A:699:PHE:HD2	13	0.4
(2,1207)	1:A:698:VAL:HG12	1:A:699:PHE:HD1	13	0.4
(2,1207)	1:A:698:VAL:HG12	1:A:699:PHE:HD2	13	0.4
(2,1207)	1:A:698:VAL:HG13	1:A:699:PHE:HD1	13	0.4
(2,1207)	1:A:698:VAL:HG13	1:A:699:PHE:HD2	13	0.4
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	3	0.4
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	3	0.4
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	3	0.4
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	3	0.4
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	3	0.4
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	3	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	6	0.4
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	6	0.4
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	6	0.4
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	6	0.4
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	6	0.4
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	6	0.4
(2,1057)	1:A:852:GLU:H	1:A:848:ARG:HG2	8	0.4
(2,1057)	1:A:852:GLU:H	1:A:848:ARG:HG3	8	0.4
(2,1039)	1:A:793:LEU:H	1:A:790:TRP:HE3	9	0.4
(2,1039)	1:A:793:LEU:H	1:A:790:TRP:HE3	14	0.4
(1,88)	1:B:790:TRP:O	1:B:794:LYS:N	7	0.4
(1,87)	1:B:790:TRP:O	1:B:794:LYS:H	6	0.4
(1,2)	1:B:790:TRP:O	1:B:794:LYS:N	7	0.4
(1,174)	1:B:790:TRP:O	1:B:794:LYS:N	7	0.4
(1,173)	1:B:790:TRP:O	1:B:794:LYS:H	6	0.4
(1,1)	1:B:790:TRP:O	1:B:794:LYS:H	6	0.4
(2,990)	1:A:779:THR:H	1:A:776:LEU:HA	5	0.39
(2,984)	1:A:778:VAL:H	1:A:775:LEU:HA	7	0.39
(2,965)	1:A:775:LEU:H	1:A:772:ARG:HA	11	0.39
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD2	13	0.39
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD3	13	0.39
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD2	13	0.39
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD3	13	0.39
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD2	14	0.39
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD3	14	0.39
(2,826)	1:A:705:VAL:HG11	1:A:702:LEU:HA	3	0.39
(2,826)	1:A:705:VAL:HG12	1:A:702:LEU:HA	3	0.39
(2,826)	1:A:705:VAL:HG13	1:A:702:LEU:HA	3	0.39
(2,826)	1:A:705:VAL:HG11	1:A:702:LEU:HA	15	0.39
(2,826)	1:A:705:VAL:HG12	1:A:702:LEU:HA	15	0.39
(2,826)	1:A:705:VAL:HG13	1:A:702:LEU:HA	15	0.39
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD2	12	0.39
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD3	12	0.39
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD2	12	0.39
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD3	12	0.39
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD2	12	0.39
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD3	12	0.39
(2,721)	1:A:682:ILE:HD11	1:A:681:TYR:H	14	0.39
(2,721)	1:A:682:ILE:HD12	1:A:681:TYR:H	14	0.39
(2,721)	1:A:682:ILE:HD13	1:A:681:TYR:H	14	0.39
(2,536)	1:B:774:LEU:H	1:B:764:SER:HA	11	0.39
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE1	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE2	5	0.39
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE1	5	0.39
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE2	5	0.39
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE1	5	0.39
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE2	5	0.39
(2,5)	1:A:663:LEU:H	1:A:661:LEU:HB2	2	0.39
(2,5)	1:A:663:LEU:H	1:A:661:LEU:HB3	2	0.39
(2,463)	1:B:746:ILE:H	1:B:742:ARG:HA	7	0.39
(2,390)	1:B:704:LEU:H	1:B:704:LEU:HB3	5	0.39
(2,222)	1:B:663:LEU:HD21	1:B:667:ALA:HB1	15	0.39
(2,222)	1:B:663:LEU:HD21	1:B:667:ALA:HB2	15	0.39
(2,222)	1:B:663:LEU:HD21	1:B:667:ALA:HB3	15	0.39
(2,222)	1:B:663:LEU:HD22	1:B:667:ALA:HB1	15	0.39
(2,222)	1:B:663:LEU:HD22	1:B:667:ALA:HB2	15	0.39
(2,222)	1:B:663:LEU:HD22	1:B:667:ALA:HB3	15	0.39
(2,222)	1:B:663:LEU:HD23	1:B:667:ALA:HB1	15	0.39
(2,222)	1:B:663:LEU:HD23	1:B:667:ALA:HB2	15	0.39
(2,222)	1:B:663:LEU:HD23	1:B:667:ALA:HB3	15	0.39
(2,213)	1:A:839:ALA:H	1:A:808:LYS:HZ1	9	0.39
(2,213)	1:A:839:ALA:H	1:A:808:LYS:HZ2	9	0.39
(2,213)	1:A:839:ALA:H	1:A:808:LYS:HZ3	9	0.39
(2,212)	1:A:839:ALA:H	1:A:808:LYS:HZ1	9	0.39
(2,212)	1:A:839:ALA:H	1:A:808:LYS:HZ2	9	0.39
(2,212)	1:A:839:ALA:H	1:A:808:LYS:HZ3	9	0.39
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG12	8	0.39
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG13	8	0.39
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG12	8	0.39
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG13	8	0.39
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG12	7	0.39
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG13	7	0.39
(2,1482)	1:A:852:GLU:H	1:A:848:ARG:HG2	3	0.39
(2,1482)	1:A:852:GLU:H	1:A:848:ARG:HG3	3	0.39
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG12	5	0.39
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG13	5	0.39
(2,1464)	1:A:793:LEU:H	1:A:790:TRP:HE3	1	0.39
(2,1464)	1:A:793:LEU:H	1:A:790:TRP:HE3	7	0.39
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD2	3	0.39
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD3	3	0.39
(2,1415)	1:A:779:THR:H	1:A:776:LEU:HA	5	0.39
(2,1409)	1:A:778:VAL:H	1:A:775:LEU:HA	7	0.39
(2,1390)	1:A:775:LEU:H	1:A:772:ARG:HA	11	0.39
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD2	13	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD3	13	0.39
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD1	15	0.39
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD2	15	0.39
(2,1251)	1:A:705:VAL:HG11	1:A:702:LEU:HA	3	0.39
(2,1251)	1:A:705:VAL:HG12	1:A:702:LEU:HA	3	0.39
(2,1251)	1:A:705:VAL:HG13	1:A:702:LEU:HA	3	0.39
(2,1251)	1:A:705:VAL:HG11	1:A:702:LEU:HA	15	0.39
(2,1251)	1:A:705:VAL:HG12	1:A:702:LEU:HA	15	0.39
(2,1251)	1:A:705:VAL:HG13	1:A:702:LEU:HA	15	0.39
(2,1146)	1:A:682:ILE:HD11	1:A:681:TYR:H	14	0.39
(2,1146)	1:A:682:ILE:HD12	1:A:681:TYR:H	14	0.39
(2,1146)	1:A:682:ILE:HD13	1:A:681:TYR:H	14	0.39
(2,1057)	1:A:852:GLU:H	1:A:848:ARG:HG2	3	0.39
(2,1057)	1:A:852:GLU:H	1:A:848:ARG:HG3	3	0.39
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD2	7	0.39
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD3	7	0.39
(2,1039)	1:A:793:LEU:H	1:A:790:TRP:HE3	1	0.39
(2,1039)	1:A:793:LEU:H	1:A:790:TRP:HE3	7	0.39
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD2	3	0.39
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD3	3	0.39
(2,990)	1:A:779:THR:H	1:A:776:LEU:HA	4	0.38
(2,984)	1:A:778:VAL:H	1:A:775:LEU:HA	8	0.38
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB2	12	0.38
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB3	12	0.38
(2,907)	1:A:749:VAL:H	1:A:746:ILE:HA	3	0.38
(2,864)	1:A:710:GLN:H	1:A:708:VAL:HA	9	0.38
(2,857)	1:A:709:ARG:H	1:A:707:ARG:H	12	0.38
(2,839)	1:A:707:ARG:H	1:A:704:LEU:HA	1	0.38
(2,826)	1:A:705:VAL:HG11	1:A:702:LEU:HA	10	0.38
(2,826)	1:A:705:VAL:HG12	1:A:702:LEU:HA	10	0.38
(2,826)	1:A:705:VAL:HG13	1:A:702:LEU:HA	10	0.38
(2,798)	1:A:701:VAL:HG21	1:A:698:VAL:HA	6	0.38
(2,798)	1:A:701:VAL:HG22	1:A:698:VAL:HA	6	0.38
(2,798)	1:A:701:VAL:HG23	1:A:698:VAL:HA	6	0.38
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD2	1	0.38
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD3	1	0.38
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD2	1	0.38
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD3	1	0.38
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD2	1	0.38
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD3	1	0.38
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	2	0.38
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	2	0.38
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	2	0.38
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	2	0.38
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	2	0.38
(2,721)	1:A:682:ILE:HD11	1:A:681:TYR:H	15	0.38
(2,721)	1:A:682:ILE:HD12	1:A:681:TYR:H	15	0.38
(2,721)	1:A:682:ILE:HD13	1:A:681:TYR:H	15	0.38
(2,626)	1:B:817:ALA:H	1:B:816:ASN:HB2	13	0.38
(2,626)	1:B:817:ALA:H	1:B:816:ASN:HB3	13	0.38
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD11	4	0.38
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD12	4	0.38
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD13	4	0.38
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD21	4	0.38
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD22	4	0.38
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD23	4	0.38
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD11	11	0.38
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD12	11	0.38
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD13	11	0.38
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD21	11	0.38
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD22	11	0.38
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD23	11	0.38
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD11	9	0.38
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD12	9	0.38
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD13	9	0.38
(2,614)	1:B:793:LEU:H	1:B:790:TRP:HE3	7	0.38
(2,614)	1:B:793:LEU:H	1:B:790:TRP:HE3	12	0.38
(2,565)	1:B:779:THR:H	1:B:776:LEU:HA	15	0.38
(2,540)	1:B:775:LEU:H	1:B:772:ARG:HA	9	0.38
(2,472)	1:B:746:ILE:HG21	1:B:750:ASN:HD21	6	0.38
(2,472)	1:B:746:ILE:HG22	1:B:750:ASN:HD21	6	0.38
(2,472)	1:B:746:ILE:HG23	1:B:750:ASN:HD21	6	0.38
(2,463)	1:B:746:ILE:H	1:B:742:ARG:HA	8	0.38
(2,463)	1:B:746:ILE:H	1:B:742:ARG:HA	15	0.38
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB2	3	0.38
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB3	3	0.38
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB2	3	0.38
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB3	3	0.38
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB2	3	0.38
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB3	3	0.38
(2,393)	1:B:704:LEU:HD11	1:B:707:ARG:HD2	9	0.38
(2,393)	1:B:704:LEU:HD11	1:B:707:ARG:HD3	9	0.38
(2,393)	1:B:704:LEU:HD12	1:B:707:ARG:HD2	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:B:704:LEU:HD12	1:B:707:ARG:HD3	9	0.38
(2,393)	1:B:704:LEU:HD13	1:B:707:ARG:HD2	9	0.38
(2,393)	1:B:704:LEU:HD13	1:B:707:ARG:HD3	9	0.38
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG12	5	0.38
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG13	5	0.38
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD2	6	0.38
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD3	6	0.38
(2,1415)	1:A:779:THR:H	1:A:776:LEU:HA	4	0.38
(2,1409)	1:A:778:VAL:H	1:A:775:LEU:HA	8	0.38
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB2	12	0.38
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB3	12	0.38
(2,1332)	1:A:749:VAL:H	1:A:746:ILE:HA	3	0.38
(2,1289)	1:A:710:GLN:H	1:A:708:VAL:HA	9	0.38
(2,1282)	1:A:709:ARG:H	1:A:707:ARG:H	12	0.38
(2,1264)	1:A:707:ARG:H	1:A:704:LEU:HA	1	0.38
(2,1251)	1:A:705:VAL:HG11	1:A:702:LEU:HA	10	0.38
(2,1251)	1:A:705:VAL:HG12	1:A:702:LEU:HA	10	0.38
(2,1251)	1:A:705:VAL:HG13	1:A:702:LEU:HA	10	0.38
(2,1223)	1:A:701:VAL:HG21	1:A:698:VAL:HA	6	0.38
(2,1223)	1:A:701:VAL:HG22	1:A:698:VAL:HA	6	0.38
(2,1223)	1:A:701:VAL:HG23	1:A:698:VAL:HA	6	0.38
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	2	0.38
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	2	0.38
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	2	0.38
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	2	0.38
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	2	0.38
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	2	0.38
(2,1146)	1:A:682:ILE:HD11	1:A:681:TYR:H	15	0.38
(2,1146)	1:A:682:ILE:HD12	1:A:681:TYR:H	15	0.38
(2,1146)	1:A:682:ILE:HD13	1:A:681:TYR:H	15	0.38
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD2	6	0.38
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD3	6	0.38
(1,87)	1:B:790:TRP:O	1:B:794:LYS:H	8	0.38
(1,173)	1:B:790:TRP:O	1:B:794:LYS:H	8	0.38
(1,1)	1:B:790:TRP:O	1:B:794:LYS:H	8	0.38
(2,950)	1:A:771:LEU:HD11	1:A:764:SER:HA	7	0.37
(2,950)	1:A:771:LEU:HD12	1:A:764:SER:HA	7	0.37
(2,950)	1:A:771:LEU:HD13	1:A:764:SER:HA	7	0.37
(2,948)	1:A:764:SER:H	1:A:771:LEU:HB2	7	0.37
(2,948)	1:A:764:SER:H	1:A:771:LEU:HB3	7	0.37
(2,857)	1:A:709:ARG:H	1:A:707:ARG:H	3	0.37
(2,853)	1:A:708:VAL:HG11	1:A:705:VAL:HA	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,853)	1:A:708:VAL:HG12	1:A:705:VAL:HA	6	0.37
(2,853)	1:A:708:VAL:HG13	1:A:705:VAL:HA	6	0.37
(2,826)	1:A:705:VAL:HG11	1:A:702:LEU:HA	14	0.37
(2,826)	1:A:705:VAL:HG12	1:A:702:LEU:HA	14	0.37
(2,826)	1:A:705:VAL:HG13	1:A:702:LEU:HA	14	0.37
(2,81)	1:A:708:VAL:HG21	1:B:714:PRO:HA	4	0.37
(2,81)	1:A:708:VAL:HG22	1:B:714:PRO:HA	4	0.37
(2,81)	1:A:708:VAL:HG23	1:B:714:PRO:HA	4	0.37
(2,764)	1:A:693:ILE:HG21	1:A:694:GLY:H	4	0.37
(2,764)	1:A:693:ILE:HG22	1:A:694:GLY:H	4	0.37
(2,764)	1:A:693:ILE:HG23	1:A:694:GLY:H	4	0.37
(2,721)	1:A:682:ILE:HD11	1:A:681:TYR:H	12	0.37
(2,721)	1:A:682:ILE:HD12	1:A:681:TYR:H	12	0.37
(2,721)	1:A:682:ILE:HD13	1:A:681:TYR:H	12	0.37
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	3	0.37
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	3	0.37
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	3	0.37
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	3	0.37
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	3	0.37
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	3	0.37
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB2	11	0.37
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB3	11	0.37
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB2	11	0.37
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB3	11	0.37
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB2	11	0.37
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB3	11	0.37
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE1	14	0.37
(2,638)	1:B:780:ARG:HH11	1:B:783:GLU:OE2	14	0.37
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE1	14	0.37
(2,638)	1:B:780:ARG:HH12	1:B:783:GLU:OE2	14	0.37
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE1	14	0.37
(2,638)	1:B:780:ARG:HH21	1:B:783:GLU:OE2	14	0.37
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE1	14	0.37
(2,638)	1:B:780:ARG:HH22	1:B:783:GLU:OE2	14	0.37
(2,614)	1:B:793:LEU:H	1:B:790:TRP:HE3	15	0.37
(2,581)	1:B:782:VAL:H	1:B:779:THR:HA	10	0.37
(2,565)	1:B:779:THR:H	1:B:776:LEU:HA	12	0.37
(2,540)	1:B:775:LEU:H	1:B:772:ARG:HA	12	0.37
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB2	9	0.37
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB3	9	0.37
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD2	6	0.37
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD3	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB2	13	0.37
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB3	13	0.37
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB2	13	0.37
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB3	13	0.37
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB2	13	0.37
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB3	13	0.37
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB2	14	0.37
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB3	14	0.37
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB2	14	0.37
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB3	14	0.37
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB2	14	0.37
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB3	14	0.37
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB2	1	0.37
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB3	1	0.37
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB2	1	0.37
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB3	1	0.37
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB2	1	0.37
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB3	1	0.37
(2,401)	1:B:705:VAL:HG11	1:B:702:LEU:HA	1	0.37
(2,401)	1:B:705:VAL:HG12	1:B:702:LEU:HA	1	0.37
(2,401)	1:B:705:VAL:HG13	1:B:702:LEU:HA	1	0.37
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD11	6	0.37
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD12	6	0.37
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD13	6	0.37
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG21	8	0.37
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG22	8	0.37
(2,27)	1:A:686:ILE:H	1:B:686:ILE:HG23	8	0.37
(2,228)	1:B:665:LYS:H	1:B:662:GLU:HA	9	0.37
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ1	6	0.37
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ2	6	0.37
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ3	6	0.37
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ1	10	0.37
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ2	10	0.37
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ3	10	0.37
(2,204)	1:A:827:ASP:H	1:A:820:ILE:HG12	5	0.37
(2,204)	1:A:827:ASP:H	1:A:820:ILE:HG13	5	0.37
(2,203)	1:A:827:ASP:H	1:A:820:ILE:HG12	5	0.37
(2,203)	1:A:827:ASP:H	1:A:820:ILE:HG13	5	0.37
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG12	6	0.37
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG13	6	0.37
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG12	6	0.37
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG13	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,180)	1:A:806:GLU:H	1:B:771:LEU:HG	8	0.37
(2,160)	1:B:794:LYS:H	1:B:848:ARG:HG2	12	0.37
(2,160)	1:B:794:LYS:H	1:B:848:ARG:HG3	12	0.37
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG12	12	0.37
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG13	12	0.37
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD2	1	0.37
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD3	1	0.37
(2,1375)	1:A:771:LEU:HD11	1:A:764:SER:HA	7	0.37
(2,1375)	1:A:771:LEU:HD12	1:A:764:SER:HA	7	0.37
(2,1375)	1:A:771:LEU:HD13	1:A:764:SER:HA	7	0.37
(2,1373)	1:A:764:SER:H	1:A:771:LEU:HB2	7	0.37
(2,1373)	1:A:764:SER:H	1:A:771:LEU:HB3	7	0.37
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD1	14	0.37
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD2	14	0.37
(2,1282)	1:A:709:ARG:H	1:A:707:ARG:H	3	0.37
(2,1278)	1:A:708:VAL:HG11	1:A:705:VAL:HA	6	0.37
(2,1278)	1:A:708:VAL:HG12	1:A:705:VAL:HA	6	0.37
(2,1278)	1:A:708:VAL:HG13	1:A:705:VAL:HA	6	0.37
(2,1251)	1:A:705:VAL:HG11	1:A:702:LEU:HA	14	0.37
(2,1251)	1:A:705:VAL:HG12	1:A:702:LEU:HA	14	0.37
(2,1251)	1:A:705:VAL:HG13	1:A:702:LEU:HA	14	0.37
(2,12)	1:A:666:TRP:HE1	1:B:666:TRP:HZ2	11	0.37
(2,1189)	1:A:693:ILE:HG21	1:A:694:GLY:H	4	0.37
(2,1189)	1:A:693:ILE:HG22	1:A:694:GLY:H	4	0.37
(2,1189)	1:A:693:ILE:HG23	1:A:694:GLY:H	4	0.37
(2,1146)	1:A:682:ILE:HD11	1:A:681:TYR:H	12	0.37
(2,1146)	1:A:682:ILE:HD12	1:A:681:TYR:H	12	0.37
(2,1146)	1:A:682:ILE:HD13	1:A:681:TYR:H	12	0.37
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	3	0.37
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	3	0.37
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	3	0.37
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	3	0.37
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	3	0.37
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	3	0.37
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD2	1	0.37
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD3	1	0.37
(1,88)	1:B:790:TRP:O	1:B:794:LYS:N	4	0.37
(1,88)	1:B:790:TRP:O	1:B:794:LYS:N	9	0.37
(1,2)	1:B:790:TRP:O	1:B:794:LYS:N	4	0.37
(1,2)	1:B:790:TRP:O	1:B:794:LYS:N	9	0.37
(1,174)	1:B:790:TRP:O	1:B:794:LYS:N	4	0.37
(1,174)	1:B:790:TRP:O	1:B:794:LYS:N	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,961)	1:A:774:LEU:H	1:A:764:SER:HA	2	0.36
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	1	0.36
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	1	0.36
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	1	0.36
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	1	0.36
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	1	0.36
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	1	0.36
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	5	0.36
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	5	0.36
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	5	0.36
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	5	0.36
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	5	0.36
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	5	0.36
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	10	0.36
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	10	0.36
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	10	0.36
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	10	0.36
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	10	0.36
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	10	0.36
(2,943)	1:A:763:LEU:HD11	1:A:759:ASP:HA	11	0.36
(2,943)	1:A:763:LEU:HD12	1:A:759:ASP:HA	11	0.36
(2,943)	1:A:763:LEU:HD13	1:A:759:ASP:HA	11	0.36
(2,907)	1:A:749:VAL:H	1:A:746:ILE:HA	7	0.36
(2,907)	1:A:749:VAL:H	1:A:746:ILE:HA	9	0.36
(2,907)	1:A:749:VAL:H	1:A:746:ILE:HA	10	0.36
(2,897)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	5	0.36
(2,897)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	5	0.36
(2,897)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	5	0.36
(2,888)	1:A:746:ILE:H	1:A:742:ARG:HA	2	0.36
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB2	8	0.36
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB3	8	0.36
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB2	8	0.36
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB3	8	0.36
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB2	8	0.36
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB3	8	0.36
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB2	9	0.36
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB3	9	0.36
(2,826)	1:A:705:VAL:HG11	1:A:702:LEU:HA	9	0.36
(2,826)	1:A:705:VAL:HG12	1:A:702:LEU:HA	9	0.36
(2,826)	1:A:705:VAL:HG13	1:A:702:LEU:HA	9	0.36
(2,81)	1:A:708:VAL:HG21	1:B:714:PRO:HA	6	0.36
(2,81)	1:A:708:VAL:HG22	1:B:714:PRO:HA	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,81)	1:A:708:VAL:HG23	1:B:714:PRO:HA	6	0.36
(2,758)	1:A:692:LEU:HD11	1:A:696:ARG:HH11	10	0.36
(2,758)	1:A:692:LEU:HD11	1:A:696:ARG:HH12	10	0.36
(2,758)	1:A:692:LEU:HD11	1:A:696:ARG:HH21	10	0.36
(2,758)	1:A:692:LEU:HD11	1:A:696:ARG:HH22	10	0.36
(2,758)	1:A:692:LEU:HD12	1:A:696:ARG:HH11	10	0.36
(2,758)	1:A:692:LEU:HD12	1:A:696:ARG:HH12	10	0.36
(2,758)	1:A:692:LEU:HD12	1:A:696:ARG:HH21	10	0.36
(2,758)	1:A:692:LEU:HD12	1:A:696:ARG:HH22	10	0.36
(2,758)	1:A:692:LEU:HD13	1:A:696:ARG:HH11	10	0.36
(2,758)	1:A:692:LEU:HD13	1:A:696:ARG:HH12	10	0.36
(2,758)	1:A:692:LEU:HD13	1:A:696:ARG:HH21	10	0.36
(2,758)	1:A:692:LEU:HD13	1:A:696:ARG:HH22	10	0.36
(2,752)	1:A:689:VAL:HG21	1:A:685:PHE:HE1	8	0.36
(2,752)	1:A:689:VAL:HG21	1:A:685:PHE:HE2	8	0.36
(2,752)	1:A:689:VAL:HG22	1:A:685:PHE:HE1	8	0.36
(2,752)	1:A:689:VAL:HG22	1:A:685:PHE:HE2	8	0.36
(2,752)	1:A:689:VAL:HG23	1:A:685:PHE:HE1	8	0.36
(2,752)	1:A:689:VAL:HG23	1:A:685:PHE:HE2	8	0.36
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	10	0.36
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	10	0.36
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	10	0.36
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	10	0.36
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	10	0.36
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	10	0.36
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	15	0.36
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	15	0.36
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	15	0.36
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	15	0.36
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	15	0.36
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	15	0.36
(2,703)	1:A:676:THR:HG21	1:A:670:TRP:HE1	5	0.36
(2,703)	1:A:676:THR:HG22	1:A:670:TRP:HE1	5	0.36
(2,703)	1:A:676:THR:HG23	1:A:670:TRP:HE1	5	0.36
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB2	7	0.36
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB3	7	0.36
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB2	7	0.36
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB3	7	0.36
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB2	7	0.36
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB3	7	0.36
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD11	14	0.36
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD12	14	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD13	14	0.36
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD21	14	0.36
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD22	14	0.36
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD23	14	0.36
(2,614)	1:B:793:LEU:H	1:B:790:TRP:HE3	9	0.36
(2,565)	1:B:779:THR:H	1:B:776:LEU:HA	8	0.36
(2,545)	1:B:775:LEU:HD11	1:B:772:ARG:HA	8	0.36
(2,545)	1:B:775:LEU:HD12	1:B:772:ARG:HA	8	0.36
(2,545)	1:B:775:LEU:HD13	1:B:772:ARG:HA	8	0.36
(2,540)	1:B:775:LEU:H	1:B:772:ARG:HA	13	0.36
(2,518)	1:B:763:LEU:HD11	1:B:759:ASP:HA	2	0.36
(2,518)	1:B:763:LEU:HD12	1:B:759:ASP:HA	2	0.36
(2,518)	1:B:763:LEU:HD13	1:B:759:ASP:HA	2	0.36
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB2	14	0.36
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB3	14	0.36
(2,472)	1:B:746:ILE:HG21	1:B:750:ASN:HD21	9	0.36
(2,472)	1:B:746:ILE:HG22	1:B:750:ASN:HD21	9	0.36
(2,472)	1:B:746:ILE:HG23	1:B:750:ASN:HD21	9	0.36
(2,432)	1:B:709:ARG:H	1:B:707:ARG:H	11	0.36
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD11	13	0.36
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD12	13	0.36
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD13	13	0.36
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD21	13	0.36
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD22	13	0.36
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD23	13	0.36
(2,401)	1:B:705:VAL:HG11	1:B:702:LEU:HA	3	0.36
(2,401)	1:B:705:VAL:HG12	1:B:702:LEU:HA	3	0.36
(2,401)	1:B:705:VAL:HG13	1:B:702:LEU:HA	3	0.36
(2,355)	1:B:698:VAL:HG11	1:B:695:LEU:HA	3	0.36
(2,355)	1:B:698:VAL:HG12	1:B:695:LEU:HA	3	0.36
(2,355)	1:B:698:VAL:HG13	1:B:695:LEU:HA	3	0.36
(2,355)	1:B:698:VAL:HG11	1:B:695:LEU:HA	15	0.36
(2,355)	1:B:698:VAL:HG12	1:B:695:LEU:HA	15	0.36
(2,355)	1:B:698:VAL:HG13	1:B:695:LEU:HA	15	0.36
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD11	3	0.36
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD12	3	0.36
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD13	3	0.36
(2,268)	1:B:672:TRP:H	1:B:673:PHE:H	6	0.36
(2,234)	1:B:666:TRP:H	1:B:663:LEU:HA	7	0.36
(2,187)	1:B:816:ASN:H	1:B:830:ILE:HD11	15	0.36
(2,187)	1:B:816:ASN:H	1:B:830:ILE:HD12	15	0.36
(2,187)	1:B:816:ASN:H	1:B:830:ILE:HD13	15	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,180)	1:A:806:GLU:H	1:B:771:LEU:HG	5	0.36
(2,1386)	1:A:774:LEU:H	1:A:764:SER:HA	2	0.36
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	1	0.36
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	1	0.36
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	1	0.36
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	1	0.36
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	1	0.36
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	1	0.36
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	5	0.36
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	5	0.36
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	5	0.36
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	5	0.36
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	5	0.36
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	5	0.36
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	10	0.36
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	10	0.36
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	10	0.36
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	10	0.36
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	10	0.36
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	10	0.36
(2,1368)	1:A:763:LEU:HD11	1:A:759:ASP:HA	11	0.36
(2,1368)	1:A:763:LEU:HD12	1:A:759:ASP:HA	11	0.36
(2,1368)	1:A:763:LEU:HD13	1:A:759:ASP:HA	11	0.36
(2,1332)	1:A:749:VAL:H	1:A:746:ILE:HA	7	0.36
(2,1332)	1:A:749:VAL:H	1:A:746:ILE:HA	9	0.36
(2,1332)	1:A:749:VAL:H	1:A:746:ILE:HA	10	0.36
(2,1322)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	5	0.36
(2,1322)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	5	0.36
(2,1322)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	5	0.36
(2,1313)	1:A:746:ILE:H	1:A:742:ARG:HA	2	0.36
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB2	8	0.36
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB3	8	0.36
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB2	8	0.36
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB3	8	0.36
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB2	8	0.36
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB3	8	0.36
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB2	9	0.36
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB3	9	0.36
(2,1251)	1:A:705:VAL:HG11	1:A:702:LEU:HA	9	0.36
(2,1251)	1:A:705:VAL:HG12	1:A:702:LEU:HA	9	0.36
(2,1251)	1:A:705:VAL:HG13	1:A:702:LEU:HA	9	0.36
(2,1183)	1:A:692:LEU:HD11	1:A:696:ARG:HH11	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1183)	1:A:692:LEU:HD11	1:A:696:ARG:HH12	10	0.36
(2,1183)	1:A:692:LEU:HD11	1:A:696:ARG:HH21	10	0.36
(2,1183)	1:A:692:LEU:HD11	1:A:696:ARG:HH22	10	0.36
(2,1183)	1:A:692:LEU:HD12	1:A:696:ARG:HH11	10	0.36
(2,1183)	1:A:692:LEU:HD12	1:A:696:ARG:HH12	10	0.36
(2,1183)	1:A:692:LEU:HD12	1:A:696:ARG:HH21	10	0.36
(2,1183)	1:A:692:LEU:HD12	1:A:696:ARG:HH22	10	0.36
(2,1183)	1:A:692:LEU:HD13	1:A:696:ARG:HH11	10	0.36
(2,1183)	1:A:692:LEU:HD13	1:A:696:ARG:HH12	10	0.36
(2,1183)	1:A:692:LEU:HD13	1:A:696:ARG:HH21	10	0.36
(2,1183)	1:A:692:LEU:HD13	1:A:696:ARG:HH22	10	0.36
(2,1177)	1:A:689:VAL:HG21	1:A:685:PHE:HE1	8	0.36
(2,1177)	1:A:689:VAL:HG21	1:A:685:PHE:HE2	8	0.36
(2,1177)	1:A:689:VAL:HG22	1:A:685:PHE:HE1	8	0.36
(2,1177)	1:A:689:VAL:HG22	1:A:685:PHE:HE2	8	0.36
(2,1177)	1:A:689:VAL:HG23	1:A:685:PHE:HE1	8	0.36
(2,1177)	1:A:689:VAL:HG23	1:A:685:PHE:HE2	8	0.36
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	10	0.36
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	10	0.36
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	10	0.36
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	10	0.36
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	10	0.36
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	10	0.36
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	15	0.36
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	15	0.36
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	15	0.36
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	15	0.36
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	15	0.36
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	15	0.36
(2,1128)	1:A:676:THR:HG21	1:A:670:TRP:HE1	5	0.36
(2,1128)	1:A:676:THR:HG22	1:A:670:TRP:HE1	5	0.36
(2,1128)	1:A:676:THR:HG23	1:A:670:TRP:HE1	5	0.36
(1,88)	1:B:790:TRP:O	1:B:794:LYS:N	2	0.36
(1,88)	1:B:790:TRP:O	1:B:794:LYS:N	10	0.36
(1,87)	1:B:790:TRP:O	1:B:794:LYS:H	12	0.36
(1,87)	1:B:790:TRP:O	1:B:794:LYS:H	13	0.36
(1,2)	1:B:790:TRP:O	1:B:794:LYS:N	2	0.36
(1,2)	1:B:790:TRP:O	1:B:794:LYS:N	10	0.36
(1,174)	1:B:790:TRP:O	1:B:794:LYS:N	2	0.36
(1,174)	1:B:790:TRP:O	1:B:794:LYS:N	10	0.36
(1,173)	1:B:790:TRP:O	1:B:794:LYS:H	12	0.36
(1,173)	1:B:790:TRP:O	1:B:794:LYS:H	13	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:B:790:TRP:O	1:B:794:LYS:H	12	0.36
(1,1)	1:B:790:TRP:O	1:B:794:LYS:H	13	0.36
(2,990)	1:A:779:THR:H	1:A:776:LEU:HA	1	0.35
(2,990)	1:A:779:THR:H	1:A:776:LEU:HA	2	0.35
(2,965)	1:A:775:LEU:H	1:A:772:ARG:HA	1	0.35
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	14	0.35
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	14	0.35
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	14	0.35
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	14	0.35
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	14	0.35
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	14	0.35
(2,907)	1:A:749:VAL:H	1:A:746:ILE:HA	13	0.35
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD2	1	0.35
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD3	1	0.35
(2,896)	1:A:746:ILE:HD11	1:A:743:ASP:HB2	7	0.35
(2,896)	1:A:746:ILE:HD11	1:A:743:ASP:HB3	7	0.35
(2,896)	1:A:746:ILE:HD12	1:A:743:ASP:HB2	7	0.35
(2,896)	1:A:746:ILE:HD12	1:A:743:ASP:HB3	7	0.35
(2,896)	1:A:746:ILE:HD13	1:A:743:ASP:HB2	7	0.35
(2,896)	1:A:746:ILE:HD13	1:A:743:ASP:HB3	7	0.35
(2,888)	1:A:746:ILE:H	1:A:742:ARG:HA	11	0.35
(2,869)	1:A:710:GLN:H	1:A:710:GLN:HB3	14	0.35
(2,857)	1:A:709:ARG:H	1:A:707:ARG:H	11	0.35
(2,757)	1:A:692:LEU:HD11	1:A:691:SER:HB2	13	0.35
(2,757)	1:A:692:LEU:HD11	1:A:691:SER:HB3	13	0.35
(2,757)	1:A:692:LEU:HD12	1:A:691:SER:HB2	13	0.35
(2,757)	1:A:692:LEU:HD12	1:A:691:SER:HB3	13	0.35
(2,757)	1:A:692:LEU:HD13	1:A:691:SER:HB2	13	0.35
(2,757)	1:A:692:LEU:HD13	1:A:691:SER:HB3	13	0.35
(2,670)	1:A:667:ALA:H	1:A:666:TRP:HD1	5	0.35
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB1	2	0.35
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB2	2	0.35
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB3	2	0.35
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB1	2	0.35
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB2	2	0.35
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB3	2	0.35
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB1	2	0.35
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB2	2	0.35
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB3	2	0.35
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB1	7	0.35
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB2	7	0.35
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB3	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB1	7	0.35
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB2	7	0.35
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB3	7	0.35
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB1	7	0.35
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB2	7	0.35
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB3	7	0.35
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB1	10	0.35
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB2	10	0.35
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB3	10	0.35
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB1	10	0.35
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB2	10	0.35
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB3	10	0.35
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB1	10	0.35
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB2	10	0.35
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB3	10	0.35
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG11	13	0.35
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG12	13	0.35
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG13	13	0.35
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG21	13	0.35
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG22	13	0.35
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG23	13	0.35
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD11	10	0.35
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD12	10	0.35
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD13	10	0.35
(2,620)	1:B:802:TYR:H	1:B:802:TYR:HB3	5	0.35
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD11	5	0.35
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD12	5	0.35
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD13	5	0.35
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE1	6	0.35
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE2	6	0.35
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE1	6	0.35
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE2	6	0.35
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE1	6	0.35
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE2	6	0.35
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE1	15	0.35
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE2	15	0.35
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE1	15	0.35
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE2	15	0.35
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE1	15	0.35
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE2	15	0.35
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA2	11	0.35
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA3	11	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA2	11	0.35
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA3	11	0.35
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA2	11	0.35
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA3	11	0.35
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD2	10	0.35
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD3	10	0.35
(2,472)	1:B:746:ILE:HG21	1:B:750:ASN:HD21	10	0.35
(2,472)	1:B:746:ILE:HG22	1:B:750:ASN:HD21	10	0.35
(2,472)	1:B:746:ILE:HG23	1:B:750:ASN:HD21	10	0.35
(2,471)	1:B:746:ILE:HD11	1:B:743:ASP:HB2	12	0.35
(2,471)	1:B:746:ILE:HD11	1:B:743:ASP:HB3	12	0.35
(2,471)	1:B:746:ILE:HD12	1:B:743:ASP:HB2	12	0.35
(2,471)	1:B:746:ILE:HD12	1:B:743:ASP:HB3	12	0.35
(2,471)	1:B:746:ILE:HD13	1:B:743:ASP:HB2	12	0.35
(2,471)	1:B:746:ILE:HD13	1:B:743:ASP:HB3	12	0.35
(2,432)	1:B:709:ARG:H	1:B:707:ARG:H	1	0.35
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB2	1	0.35
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB3	1	0.35
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB2	1	0.35
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB3	1	0.35
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB2	1	0.35
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB3	1	0.35
(2,420)	1:B:707:ARG:H	1:B:707:ARG:HG2	15	0.35
(2,420)	1:B:707:ARG:H	1:B:707:ARG:HG3	15	0.35
(2,241)	1:B:666:TRP:HE1	1:B:662:GLU:H	7	0.35
(2,234)	1:B:666:TRP:H	1:B:663:LEU:HA	2	0.35
(2,228)	1:B:665:LYS:H	1:B:662:GLU:HA	5	0.35
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD2	10	0.35
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD3	10	0.35
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG12	14	0.35
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG13	14	0.35
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG12	14	0.35
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG13	14	0.35
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB2	14	0.35
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB3	14	0.35
(2,165)	1:A:796:TRP:HE1	1:B:755:LEU:HD21	3	0.35
(2,165)	1:A:796:TRP:HE1	1:B:755:LEU:HD22	3	0.35
(2,165)	1:A:796:TRP:HE1	1:B:755:LEU:HD23	3	0.35
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG12	13	0.35
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG13	13	0.35
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG12	13	0.35
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG13	13	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG12	14	0.35
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG13	14	0.35
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	6	0.35
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	6	0.35
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	6	0.35
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	6	0.35
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	6	0.35
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	6	0.35
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	6	0.35
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	6	0.35
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD2	2	0.35
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD3	2	0.35
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG11	13	0.35
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG12	13	0.35
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG13	13	0.35
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG21	13	0.35
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG22	13	0.35
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG23	13	0.35
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	6	0.35
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	6	0.35
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	6	0.35
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	6	0.35
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	6	0.35
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	6	0.35
(2,1451)	1:A:785:LEU:H	1:A:782:VAL:HA	7	0.35
(2,1431)	1:A:782:VAL:H	1:A:779:THR:HA	15	0.35
(2,1415)	1:A:779:THR:H	1:A:776:LEU:HA	1	0.35
(2,1415)	1:A:779:THR:H	1:A:776:LEU:HA	2	0.35
(2,1390)	1:A:775:LEU:H	1:A:772:ARG:HA	1	0.35
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	14	0.35
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	14	0.35
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	14	0.35
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	14	0.35
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	14	0.35
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	14	0.35
(2,1332)	1:A:749:VAL:H	1:A:746:ILE:HA	13	0.35
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD2	1	0.35
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD3	1	0.35
(2,1321)	1:A:746:ILE:HD11	1:A:743:ASP:HB2	7	0.35
(2,1321)	1:A:746:ILE:HD11	1:A:743:ASP:HB3	7	0.35
(2,1321)	1:A:746:ILE:HD12	1:A:743:ASP:HB2	7	0.35
(2,1321)	1:A:746:ILE:HD12	1:A:743:ASP:HB3	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1321)	1:A:746:ILE:HD13	1:A:743:ASP:HB2	7	0.35
(2,1321)	1:A:746:ILE:HD13	1:A:743:ASP:HB3	7	0.35
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD1	10	0.35
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD2	10	0.35
(2,1313)	1:A:746:ILE:H	1:A:742:ARG:HA	11	0.35
(2,1294)	1:A:710:GLN:H	1:A:710:GLN:HB3	14	0.35
(2,1282)	1:A:709:ARG:H	1:A:707:ARG:H	11	0.35
(2,1182)	1:A:692:LEU:HD11	1:A:691:SER:HB2	13	0.35
(2,1182)	1:A:692:LEU:HD11	1:A:691:SER:HB3	13	0.35
(2,1182)	1:A:692:LEU:HD12	1:A:691:SER:HB2	13	0.35
(2,1182)	1:A:692:LEU:HD12	1:A:691:SER:HB3	13	0.35
(2,1182)	1:A:692:LEU:HD13	1:A:691:SER:HB2	13	0.35
(2,1182)	1:A:692:LEU:HD13	1:A:691:SER:HB3	13	0.35
(2,1095)	1:A:667:ALA:H	1:A:666:TRP:HD1	5	0.35
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	6	0.35
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	6	0.35
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	6	0.35
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	6	0.35
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	6	0.35
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	6	0.35
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	6	0.35
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	6	0.35
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD2	2	0.35
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD3	2	0.35
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG11	13	0.35
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG12	13	0.35
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG13	13	0.35
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG21	13	0.35
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG22	13	0.35
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG23	13	0.35
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	6	0.35
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	6	0.35
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	6	0.35
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	6	0.35
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	6	0.35
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	6	0.35
(2,1026)	1:A:785:LEU:H	1:A:782:VAL:HA	7	0.35
(2,1006)	1:A:782:VAL:H	1:A:779:THR:HA	15	0.35
(1,88)	1:B:790:TRP:O	1:B:794:LYS:N	3	0.35
(1,87)	1:B:790:TRP:O	1:B:794:LYS:H	11	0.35
(1,2)	1:B:790:TRP:O	1:B:794:LYS:N	3	0.35
(1,174)	1:B:790:TRP:O	1:B:794:LYS:N	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:B:790:TRP:O	1:B:794:LYS:H	11	0.35
(1,1)	1:B:790:TRP:O	1:B:794:LYS:H	11	0.35
(2,984)	1:A:778:VAL:H	1:A:775:LEU:HA	4	0.34
(2,896)	1:A:746:ILE:HD11	1:A:743:ASP:HB2	13	0.34
(2,896)	1:A:746:ILE:HD11	1:A:743:ASP:HB3	13	0.34
(2,896)	1:A:746:ILE:HD12	1:A:743:ASP:HB2	13	0.34
(2,896)	1:A:746:ILE:HD12	1:A:743:ASP:HB3	13	0.34
(2,896)	1:A:746:ILE:HD13	1:A:743:ASP:HB2	13	0.34
(2,896)	1:A:746:ILE:HD13	1:A:743:ASP:HB3	13	0.34
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB2	4	0.34
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB3	4	0.34
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB2	4	0.34
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB3	4	0.34
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB2	4	0.34
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB3	4	0.34
(2,854)	1:A:708:VAL:HG21	1:A:707:ARG:HD2	13	0.34
(2,854)	1:A:708:VAL:HG21	1:A:707:ARG:HD3	13	0.34
(2,854)	1:A:708:VAL:HG22	1:A:707:ARG:HD2	13	0.34
(2,854)	1:A:708:VAL:HG22	1:A:707:ARG:HD3	13	0.34
(2,854)	1:A:708:VAL:HG23	1:A:707:ARG:HD2	13	0.34
(2,854)	1:A:708:VAL:HG23	1:A:707:ARG:HD3	13	0.34
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD2	9	0.34
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD3	9	0.34
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD2	1	0.34
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD3	1	0.34
(2,839)	1:A:707:ARG:H	1:A:704:LEU:HA	12	0.34
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB2	1	0.34
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB3	1	0.34
(2,780)	1:A:698:VAL:HG11	1:A:695:LEU:HA	14	0.34
(2,780)	1:A:698:VAL:HG12	1:A:695:LEU:HA	14	0.34
(2,780)	1:A:698:VAL:HG13	1:A:695:LEU:HA	14	0.34
(2,752)	1:A:689:VAL:HG21	1:A:685:PHE:HE1	3	0.34
(2,752)	1:A:689:VAL:HG21	1:A:685:PHE:HE2	3	0.34
(2,752)	1:A:689:VAL:HG22	1:A:685:PHE:HE1	3	0.34
(2,752)	1:A:689:VAL:HG22	1:A:685:PHE:HE2	3	0.34
(2,752)	1:A:689:VAL:HG23	1:A:685:PHE:HE1	3	0.34
(2,752)	1:A:689:VAL:HG23	1:A:685:PHE:HE2	3	0.34
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB2	6	0.34
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB3	6	0.34
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB2	6	0.34
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB3	6	0.34
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB2	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB3	6	0.34
(2,711)	1:A:678:TRP:HE1	1:A:682:ILE:H	9	0.34
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD1	1	0.34
(2,637)	1:B:770:ARG:HH11	1:B:773:ASP:OD2	1	0.34
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD1	1	0.34
(2,637)	1:B:770:ARG:HH12	1:B:773:ASP:OD2	1	0.34
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD1	1	0.34
(2,637)	1:B:770:ARG:HH21	1:B:773:ASP:OD2	1	0.34
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD1	1	0.34
(2,637)	1:B:770:ARG:HH22	1:B:773:ASP:OD2	1	0.34
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD2	5	0.34
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD3	5	0.34
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG11	8	0.34
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG12	8	0.34
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG13	8	0.34
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG21	8	0.34
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG22	8	0.34
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG23	8	0.34
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD11	1	0.34
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD12	1	0.34
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD13	1	0.34
(2,581)	1:B:782:VAL:H	1:B:779:THR:HA	13	0.34
(2,565)	1:B:779:THR:H	1:B:776:LEU:HA	3	0.34
(2,540)	1:B:775:LEU:H	1:B:772:ARG:HA	5	0.34
(2,482)	1:B:749:VAL:H	1:B:746:ILE:HA	2	0.34
(2,482)	1:B:749:VAL:H	1:B:746:ILE:HA	11	0.34
(2,482)	1:B:749:VAL:H	1:B:746:ILE:HA	13	0.34
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD2	11	0.34
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD3	11	0.34
(2,428)	1:B:708:VAL:HG11	1:B:705:VAL:HA	7	0.34
(2,428)	1:B:708:VAL:HG12	1:B:705:VAL:HA	7	0.34
(2,428)	1:B:708:VAL:HG13	1:B:705:VAL:HA	7	0.34
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB2	10	0.34
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB3	10	0.34
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB2	10	0.34
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB3	10	0.34
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB2	10	0.34
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB3	10	0.34
(2,373)	1:B:701:VAL:HG21	1:B:698:VAL:HA	4	0.34
(2,373)	1:B:701:VAL:HG22	1:B:698:VAL:HA	4	0.34
(2,373)	1:B:701:VAL:HG23	1:B:698:VAL:HA	4	0.34
(2,294)	1:B:682:ILE:HG21	1:B:685:PHE:HB2	13	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,294)	1:B:682:ILE:HG21	1:B:685:PHE:HB3	13	0.34
(2,294)	1:B:682:ILE:HG22	1:B:685:PHE:HB2	13	0.34
(2,294)	1:B:682:ILE:HG22	1:B:685:PHE:HB3	13	0.34
(2,294)	1:B:682:ILE:HG23	1:B:685:PHE:HB2	13	0.34
(2,294)	1:B:682:ILE:HG23	1:B:685:PHE:HB3	13	0.34
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ1	13	0.34
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ2	13	0.34
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ3	13	0.34
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD2	2	0.34
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD3	2	0.34
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD2	5	0.34
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD3	5	0.34
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD2	13	0.34
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD3	13	0.34
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG12	2	0.34
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG13	2	0.34
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG12	2	0.34
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG13	2	0.34
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD11	4	0.34
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD12	4	0.34
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD13	4	0.34
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD21	4	0.34
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD22	4	0.34
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD23	4	0.34
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD11	3	0.34
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD12	3	0.34
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD13	3	0.34
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD21	3	0.34
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD22	3	0.34
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD23	3	0.34
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD11	6	0.34
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD12	6	0.34
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD13	6	0.34
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD21	6	0.34
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD22	6	0.34
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD23	6	0.34
(2,1409)	1:A:778:VAL:H	1:A:775:LEU:HA	4	0.34
(2,1321)	1:A:746:ILE:HD11	1:A:743:ASP:HB2	13	0.34
(2,1321)	1:A:746:ILE:HD11	1:A:743:ASP:HB3	13	0.34
(2,1321)	1:A:746:ILE:HD12	1:A:743:ASP:HB2	13	0.34
(2,1321)	1:A:746:ILE:HD12	1:A:743:ASP:HB3	13	0.34
(2,1321)	1:A:746:ILE:HD13	1:A:743:ASP:HB2	13	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1321)	1:A:746:ILE:HD13	1:A:743:ASP:HB3	13	0.34
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB2	4	0.34
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB3	4	0.34
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB2	4	0.34
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB3	4	0.34
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB2	4	0.34
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB3	4	0.34
(2,1279)	1:A:708:VAL:HG21	1:A:707:ARG:HD2	13	0.34
(2,1279)	1:A:708:VAL:HG21	1:A:707:ARG:HD3	13	0.34
(2,1279)	1:A:708:VAL:HG22	1:A:707:ARG:HD2	13	0.34
(2,1279)	1:A:708:VAL:HG22	1:A:707:ARG:HD3	13	0.34
(2,1279)	1:A:708:VAL:HG23	1:A:707:ARG:HD2	13	0.34
(2,1279)	1:A:708:VAL:HG23	1:A:707:ARG:HD3	13	0.34
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD2	9	0.34
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD3	9	0.34
(2,1264)	1:A:707:ARG:H	1:A:704:LEU:HA	12	0.34
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB2	1	0.34
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB3	1	0.34
(2,1205)	1:A:698:VAL:HG11	1:A:695:LEU:HA	14	0.34
(2,1205)	1:A:698:VAL:HG12	1:A:695:LEU:HA	14	0.34
(2,1205)	1:A:698:VAL:HG13	1:A:695:LEU:HA	14	0.34
(2,1177)	1:A:689:VAL:HG21	1:A:685:PHE:HE1	3	0.34
(2,1177)	1:A:689:VAL:HG21	1:A:685:PHE:HE2	3	0.34
(2,1177)	1:A:689:VAL:HG22	1:A:685:PHE:HE1	3	0.34
(2,1177)	1:A:689:VAL:HG22	1:A:685:PHE:HE2	3	0.34
(2,1177)	1:A:689:VAL:HG23	1:A:685:PHE:HE1	3	0.34
(2,1177)	1:A:689:VAL:HG23	1:A:685:PHE:HE2	3	0.34
(2,1136)	1:A:678:TRP:HE1	1:A:682:ILE:H	9	0.34
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG21	6	0.34
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG22	6	0.34
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG23	6	0.34
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD2	10	0.34
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD3	10	0.34
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD2	10	0.34
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD3	10	0.34
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD2	10	0.34
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD3	10	0.34
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD2	10	0.34
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD3	10	0.34
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD11	3	0.34
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD12	3	0.34
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD13	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD21	3	0.34
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD22	3	0.34
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD23	3	0.34
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD11	6	0.34
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD12	6	0.34
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD13	6	0.34
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD21	6	0.34
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD22	6	0.34
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD23	6	0.34
(2,102)	1:A:759:ASP:H	1:B:709:ARG:HD2	12	0.34
(2,102)	1:A:759:ASP:H	1:B:709:ARG:HD3	12	0.34
(1,23)	1:B:801:GLN:O	1:B:805:GLN:H	13	0.34
(1,195)	1:B:801:GLN:O	1:B:805:GLN:H	13	0.34
(1,109)	1:B:801:GLN:O	1:B:805:GLN:H	13	0.34
(2,990)	1:A:779:THR:H	1:A:776:LEU:HA	8	0.33
(2,961)	1:A:774:LEU:H	1:A:764:SER:HA	3	0.33
(2,961)	1:A:774:LEU:H	1:A:764:SER:HA	12	0.33
(2,947)	1:A:764:SER:H	1:A:761:ARG:HA	7	0.33
(2,907)	1:A:749:VAL:H	1:A:746:ILE:HA	2	0.33
(2,857)	1:A:709:ARG:H	1:A:707:ARG:H	2	0.33
(2,857)	1:A:709:ARG:H	1:A:707:ARG:H	8	0.33
(2,857)	1:A:709:ARG:H	1:A:707:ARG:H	15	0.33
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB2	7	0.33
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB3	7	0.33
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB2	7	0.33
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB3	7	0.33
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB2	7	0.33
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB3	7	0.33
(2,853)	1:A:708:VAL:HG11	1:A:705:VAL:HA	5	0.33
(2,853)	1:A:708:VAL:HG12	1:A:705:VAL:HA	5	0.33
(2,853)	1:A:708:VAL:HG13	1:A:705:VAL:HA	5	0.33
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD2	6	0.33
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD3	6	0.33
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	4	0.33
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	4	0.33
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	4	0.33
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	4	0.33
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	4	0.33
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	4	0.33
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	10	0.33
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	10	0.33
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	10	0.33
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	10	0.33
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	10	0.33
(2,804)	1:A:702:LEU:HD21	1:A:706:ASN:HB2	6	0.33
(2,804)	1:A:702:LEU:HD21	1:A:706:ASN:HB3	6	0.33
(2,804)	1:A:702:LEU:HD22	1:A:706:ASN:HB2	6	0.33
(2,804)	1:A:702:LEU:HD22	1:A:706:ASN:HB3	6	0.33
(2,804)	1:A:702:LEU:HD23	1:A:706:ASN:HB2	6	0.33
(2,804)	1:A:702:LEU:HD23	1:A:706:ASN:HB3	6	0.33
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD2	6	0.33
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD3	6	0.33
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD2	6	0.33
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD3	6	0.33
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD2	6	0.33
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD3	6	0.33
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD2	12	0.33
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD3	12	0.33
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD2	10	0.33
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD3	10	0.33
(2,540)	1:B:775:LEU:H	1:B:772:ARG:HA	2	0.33
(2,540)	1:B:775:LEU:H	1:B:772:ARG:HA	10	0.33
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE1	12	0.33
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE2	12	0.33
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE1	12	0.33
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE2	12	0.33
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE1	12	0.33
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE2	12	0.33
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA2	2	0.33
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA3	2	0.33
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA2	2	0.33
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA3	2	0.33
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA2	2	0.33
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA3	2	0.33
(2,491)	1:B:753:LEU:HD11	1:B:757:TRP:HB2	6	0.33
(2,491)	1:B:753:LEU:HD11	1:B:757:TRP:HB3	6	0.33
(2,491)	1:B:753:LEU:HD12	1:B:757:TRP:HB2	6	0.33
(2,491)	1:B:753:LEU:HD12	1:B:757:TRP:HB3	6	0.33
(2,491)	1:B:753:LEU:HD13	1:B:757:TRP:HB2	6	0.33
(2,491)	1:B:753:LEU:HD13	1:B:757:TRP:HB3	6	0.33
(2,482)	1:B:749:VAL:H	1:B:746:ILE:HA	9	0.33
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD2	7	0.33
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD3	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,439)	1:B:710:GLN:H	1:B:708:VAL:HA	13	0.33
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB2	6	0.33
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB3	6	0.33
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB2	6	0.33
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB3	6	0.33
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB2	6	0.33
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB3	6	0.33
(2,421)	1:B:707:ARG:H	1:B:707:ARG:HD2	10	0.33
(2,421)	1:B:707:ARG:H	1:B:707:ARG:HD3	10	0.33
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB2	11	0.33
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB3	11	0.33
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB2	11	0.33
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB3	11	0.33
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB2	11	0.33
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB3	11	0.33
(2,401)	1:B:705:VAL:HG11	1:B:702:LEU:HA	7	0.33
(2,401)	1:B:705:VAL:HG12	1:B:702:LEU:HA	7	0.33
(2,401)	1:B:705:VAL:HG13	1:B:702:LEU:HA	7	0.33
(2,401)	1:B:705:VAL:HG11	1:B:702:LEU:HA	8	0.33
(2,401)	1:B:705:VAL:HG12	1:B:702:LEU:HA	8	0.33
(2,401)	1:B:705:VAL:HG13	1:B:702:LEU:HA	8	0.33
(2,355)	1:B:698:VAL:HG11	1:B:695:LEU:HA	13	0.33
(2,355)	1:B:698:VAL:HG12	1:B:695:LEU:HA	13	0.33
(2,355)	1:B:698:VAL:HG13	1:B:695:LEU:HA	13	0.33
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD2	14	0.33
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD3	14	0.33
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD2	14	0.33
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD3	14	0.33
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD2	14	0.33
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD3	14	0.33
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG21	7	0.33
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG22	7	0.33
(2,32)	1:A:687:ILE:HG21	1:A:689:VAL:HG23	7	0.33
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG21	7	0.33
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG22	7	0.33
(2,32)	1:A:687:ILE:HG22	1:A:689:VAL:HG23	7	0.33
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG21	7	0.33
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG22	7	0.33
(2,32)	1:A:687:ILE:HG23	1:A:689:VAL:HG23	7	0.33
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ1	3	0.33
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ2	3	0.33
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ3	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,210)	1:A:839:ALA:H	1:A:808:LYS:HD2	15	0.33
(2,210)	1:A:839:ALA:H	1:A:808:LYS:HD3	15	0.33
(2,209)	1:A:839:ALA:H	1:A:808:LYS:HD2	15	0.33
(2,209)	1:A:839:ALA:H	1:A:808:LYS:HD3	15	0.33
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD11	4	0.33
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD12	4	0.33
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD13	4	0.33
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG12	11	0.33
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG13	11	0.33
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG12	11	0.33
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG13	11	0.33
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG12	3	0.33
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG13	3	0.33
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG12	14	0.33
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG13	14	0.33
(2,186)	1:A:808:LYS:H	1:A:838:ARG:HD2	15	0.33
(2,186)	1:A:808:LYS:H	1:A:838:ARG:HD3	15	0.33
(2,185)	1:A:808:LYS:H	1:A:838:ARG:HD2	15	0.33
(2,185)	1:A:808:LYS:H	1:A:838:ARG:HD3	15	0.33
(2,180)	1:A:806:GLU:H	1:B:771:LEU:HG	6	0.33
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB2	15	0.33
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB3	15	0.33
(2,1468)	1:A:797:TRP:H	1:A:796:TRP:HD1	3	0.33
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD11	10	0.33
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD12	10	0.33
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD13	10	0.33
(2,1415)	1:A:779:THR:H	1:A:776:LEU:HA	8	0.33
(2,1386)	1:A:774:LEU:H	1:A:764:SER:HA	3	0.33
(2,1386)	1:A:774:LEU:H	1:A:764:SER:HA	12	0.33
(2,1372)	1:A:764:SER:H	1:A:761:ARG:HA	7	0.33
(2,1332)	1:A:749:VAL:H	1:A:746:ILE:HA	2	0.33
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD1	4	0.33
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD2	4	0.33
(2,1282)	1:A:709:ARG:H	1:A:707:ARG:H	2	0.33
(2,1282)	1:A:709:ARG:H	1:A:707:ARG:H	8	0.33
(2,1282)	1:A:709:ARG:H	1:A:707:ARG:H	15	0.33
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB2	7	0.33
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB3	7	0.33
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB2	7	0.33
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB3	7	0.33
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB2	7	0.33
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB3	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1278)	1:A:708:VAL:HG11	1:A:705:VAL:HA	5	0.33
(2,1278)	1:A:708:VAL:HG12	1:A:705:VAL:HA	5	0.33
(2,1278)	1:A:708:VAL:HG13	1:A:705:VAL:HA	5	0.33
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD2	6	0.33
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD3	6	0.33
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	4	0.33
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	4	0.33
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	4	0.33
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	4	0.33
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	4	0.33
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	4	0.33
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	10	0.33
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	10	0.33
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	10	0.33
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	10	0.33
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	10	0.33
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	10	0.33
(2,1229)	1:A:702:LEU:HD21	1:A:706:ASN:HB2	6	0.33
(2,1229)	1:A:702:LEU:HD21	1:A:706:ASN:HB3	6	0.33
(2,1229)	1:A:702:LEU:HD22	1:A:706:ASN:HB2	6	0.33
(2,1229)	1:A:702:LEU:HD22	1:A:706:ASN:HB3	6	0.33
(2,1229)	1:A:702:LEU:HD23	1:A:706:ASN:HB2	6	0.33
(2,1229)	1:A:702:LEU:HD23	1:A:706:ASN:HB3	6	0.33
(2,1043)	1:A:797:TRP:H	1:A:796:TRP:HD1	3	0.33
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD11	10	0.33
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD12	10	0.33
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD13	10	0.33
(2,965)	1:A:775:LEU:H	1:A:772:ARG:HA	13	0.32
(2,952)	1:A:771:LEU:HD21	1:A:772:ARG:HH21	10	0.32
(2,952)	1:A:771:LEU:HD21	1:A:772:ARG:HH22	10	0.32
(2,952)	1:A:771:LEU:HD22	1:A:772:ARG:HH21	10	0.32
(2,952)	1:A:771:LEU:HD22	1:A:772:ARG:HH22	10	0.32
(2,952)	1:A:771:LEU:HD23	1:A:772:ARG:HH21	10	0.32
(2,952)	1:A:771:LEU:HD23	1:A:772:ARG:HH22	10	0.32
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	13	0.32
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	13	0.32
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	13	0.32
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	13	0.32
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	13	0.32
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	13	0.32
(2,943)	1:A:763:LEU:HD11	1:A:759:ASP:HA	9	0.32
(2,943)	1:A:763:LEU:HD12	1:A:759:ASP:HA	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,943)	1:A:763:LEU:HD13	1:A:759:ASP:HA	9	0.32
(2,907)	1:A:749:VAL:H	1:A:746:ILE:HA	12	0.32
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD2	9	0.32
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD3	9	0.32
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD2	15	0.32
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD3	15	0.32
(2,897)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	15	0.32
(2,897)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	15	0.32
(2,897)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	15	0.32
(2,888)	1:A:746:ILE:H	1:A:742:ARG:HA	9	0.32
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD2	6	0.32
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD3	6	0.32
(2,828)	1:A:705:VAL:HG11	1:A:709:ARG:HD2	10	0.32
(2,828)	1:A:705:VAL:HG11	1:A:709:ARG:HD3	10	0.32
(2,828)	1:A:705:VAL:HG12	1:A:709:ARG:HD2	10	0.32
(2,828)	1:A:705:VAL:HG12	1:A:709:ARG:HD3	10	0.32
(2,828)	1:A:705:VAL:HG13	1:A:709:ARG:HD2	10	0.32
(2,828)	1:A:705:VAL:HG13	1:A:709:ARG:HD3	10	0.32
(2,826)	1:A:705:VAL:HG11	1:A:702:LEU:HA	12	0.32
(2,826)	1:A:705:VAL:HG12	1:A:702:LEU:HA	12	0.32
(2,826)	1:A:705:VAL:HG13	1:A:702:LEU:HA	12	0.32
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	14	0.32
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	14	0.32
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	14	0.32
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	14	0.32
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	14	0.32
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	14	0.32
(2,752)	1:A:689:VAL:HG21	1:A:685:PHE:HE1	9	0.32
(2,752)	1:A:689:VAL:HG21	1:A:685:PHE:HE2	9	0.32
(2,752)	1:A:689:VAL:HG22	1:A:685:PHE:HE1	9	0.32
(2,752)	1:A:689:VAL:HG22	1:A:685:PHE:HE2	9	0.32
(2,752)	1:A:689:VAL:HG23	1:A:685:PHE:HE1	9	0.32
(2,752)	1:A:689:VAL:HG23	1:A:685:PHE:HE2	9	0.32
(2,748)	1:A:688:ILE:HD11	1:A:684:ILE:HD11	7	0.32
(2,748)	1:A:688:ILE:HD11	1:A:684:ILE:HD12	7	0.32
(2,748)	1:A:688:ILE:HD11	1:A:684:ILE:HD13	7	0.32
(2,748)	1:A:688:ILE:HD12	1:A:684:ILE:HD11	7	0.32
(2,748)	1:A:688:ILE:HD12	1:A:684:ILE:HD12	7	0.32
(2,748)	1:A:688:ILE:HD12	1:A:684:ILE:HD13	7	0.32
(2,748)	1:A:688:ILE:HD13	1:A:684:ILE:HD11	7	0.32
(2,748)	1:A:688:ILE:HD13	1:A:684:ILE:HD12	7	0.32
(2,748)	1:A:688:ILE:HD13	1:A:684:ILE:HD13	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	3	0.32
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	3	0.32
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	3	0.32
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	3	0.32
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	3	0.32
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	3	0.32
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB2	1	0.32
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB3	1	0.32
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB2	1	0.32
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB3	1	0.32
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB2	1	0.32
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB3	1	0.32
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB2	13	0.32
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB3	13	0.32
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB2	13	0.32
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB3	13	0.32
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB2	13	0.32
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB3	13	0.32
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB2	14	0.32
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB3	14	0.32
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB2	14	0.32
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB3	14	0.32
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB2	14	0.32
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB3	14	0.32
(2,718)	1:A:682:ILE:HG21	1:A:679:LEU:H	6	0.32
(2,718)	1:A:682:ILE:HG22	1:A:679:LEU:H	6	0.32
(2,718)	1:A:682:ILE:HG23	1:A:679:LEU:H	6	0.32
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD11	13	0.32
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD12	13	0.32
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD13	13	0.32
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD21	13	0.32
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD22	13	0.32
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD23	13	0.32
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD11	2	0.32
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD12	2	0.32
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD13	2	0.32
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD11	10	0.32
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD12	10	0.32
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD13	10	0.32
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD21	10	0.32
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD22	10	0.32
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD23	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,559)	1:B:778:VAL:H	1:B:775:LEU:HA	9	0.32
(2,432)	1:B:709:ARG:H	1:B:707:ARG:H	10	0.32
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB2	12	0.32
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB3	12	0.32
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB2	12	0.32
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB3	12	0.32
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB2	12	0.32
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB3	12	0.32
(2,393)	1:B:704:LEU:HD11	1:B:707:ARG:HD2	2	0.32
(2,393)	1:B:704:LEU:HD11	1:B:707:ARG:HD3	2	0.32
(2,393)	1:B:704:LEU:HD12	1:B:707:ARG:HD2	2	0.32
(2,393)	1:B:704:LEU:HD12	1:B:707:ARG:HD3	2	0.32
(2,393)	1:B:704:LEU:HD13	1:B:707:ARG:HD2	2	0.32
(2,393)	1:B:704:LEU:HD13	1:B:707:ARG:HD3	2	0.32
(2,355)	1:B:698:VAL:HG11	1:B:695:LEU:HA	7	0.32
(2,355)	1:B:698:VAL:HG12	1:B:695:LEU:HA	7	0.32
(2,355)	1:B:698:VAL:HG13	1:B:695:LEU:HA	7	0.32
(2,352)	1:B:697:ILE:HG21	1:B:694:GLY:HA2	4	0.32
(2,352)	1:B:697:ILE:HG21	1:B:694:GLY:HA3	4	0.32
(2,352)	1:B:697:ILE:HG22	1:B:694:GLY:HA2	4	0.32
(2,352)	1:B:697:ILE:HG22	1:B:694:GLY:HA3	4	0.32
(2,352)	1:B:697:ILE:HG23	1:B:694:GLY:HA2	4	0.32
(2,352)	1:B:697:ILE:HG23	1:B:694:GLY:HA3	4	0.32
(2,327)	1:B:689:VAL:HG21	1:B:685:PHE:HE1	13	0.32
(2,327)	1:B:689:VAL:HG21	1:B:685:PHE:HE2	13	0.32
(2,327)	1:B:689:VAL:HG22	1:B:685:PHE:HE1	13	0.32
(2,327)	1:B:689:VAL:HG22	1:B:685:PHE:HE2	13	0.32
(2,327)	1:B:689:VAL:HG23	1:B:685:PHE:HE1	13	0.32
(2,327)	1:B:689:VAL:HG23	1:B:685:PHE:HE2	13	0.32
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD11	15	0.32
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD12	15	0.32
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD13	15	0.32
(2,222)	1:B:663:LEU:HD21	1:B:667:ALA:HB1	9	0.32
(2,222)	1:B:663:LEU:HD21	1:B:667:ALA:HB2	9	0.32
(2,222)	1:B:663:LEU:HD21	1:B:667:ALA:HB3	9	0.32
(2,222)	1:B:663:LEU:HD22	1:B:667:ALA:HB1	9	0.32
(2,222)	1:B:663:LEU:HD22	1:B:667:ALA:HB2	9	0.32
(2,222)	1:B:663:LEU:HD22	1:B:667:ALA:HB3	9	0.32
(2,222)	1:B:663:LEU:HD23	1:B:667:ALA:HB1	9	0.32
(2,222)	1:B:663:LEU:HD23	1:B:667:ALA:HB2	9	0.32
(2,222)	1:B:663:LEU:HD23	1:B:667:ALA:HB3	9	0.32
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG12	15	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG13	15	0.32
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG12	2	0.32
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG13	2	0.32
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG12	2	0.32
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG13	2	0.32
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG12	2	0.32
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG13	2	0.32
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD2	4	0.32
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD3	4	0.32
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD2	11	0.32
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD3	11	0.32
(2,183)	1:A:806:GLU:H	1:B:772:ARG:HE	9	0.32
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG12	1	0.32
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG13	1	0.32
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG12	1	0.32
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG13	1	0.32
(2,1476)	1:A:817:ALA:H	1:A:816:ASN:HB2	1	0.32
(2,1476)	1:A:817:ALA:H	1:A:816:ASN:HB3	1	0.32
(2,1473)	1:A:803:TRP:HE1	1:A:799:LEU:HD11	7	0.32
(2,1473)	1:A:803:TRP:HE1	1:A:799:LEU:HD12	7	0.32
(2,1473)	1:A:803:TRP:HE1	1:A:799:LEU:HD13	7	0.32
(2,1473)	1:A:803:TRP:HE1	1:A:799:LEU:HD21	7	0.32
(2,1473)	1:A:803:TRP:HE1	1:A:799:LEU:HD22	7	0.32
(2,1473)	1:A:803:TRP:HE1	1:A:799:LEU:HD23	7	0.32
(2,1464)	1:A:793:LEU:H	1:A:790:TRP:HE3	4	0.32
(2,142)	1:A:781:ILE:H	1:B:746:ILE:HG12	15	0.32
(2,142)	1:A:781:ILE:H	1:B:746:ILE:HG13	15	0.32
(2,1390)	1:A:775:LEU:H	1:A:772:ARG:HA	13	0.32
(2,1377)	1:A:771:LEU:HD21	1:A:772:ARG:HH21	10	0.32
(2,1377)	1:A:771:LEU:HD21	1:A:772:ARG:HH22	10	0.32
(2,1377)	1:A:771:LEU:HD22	1:A:772:ARG:HH21	10	0.32
(2,1377)	1:A:771:LEU:HD22	1:A:772:ARG:HH22	10	0.32
(2,1377)	1:A:771:LEU:HD23	1:A:772:ARG:HH21	10	0.32
(2,1377)	1:A:771:LEU:HD23	1:A:772:ARG:HH22	10	0.32
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	13	0.32
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	13	0.32
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	13	0.32
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	13	0.32
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	13	0.32
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	13	0.32
(2,1368)	1:A:763:LEU:HD11	1:A:759:ASP:HA	9	0.32
(2,1368)	1:A:763:LEU:HD12	1:A:759:ASP:HA	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1368)	1:A:763:LEU:HD13	1:A:759:ASP:HA	9	0.32
(2,1332)	1:A:749:VAL:H	1:A:746:ILE:HA	12	0.32
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD2	9	0.32
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD3	9	0.32
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD2	15	0.32
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD3	15	0.32
(2,1322)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	15	0.32
(2,1322)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	15	0.32
(2,1322)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	15	0.32
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD1	8	0.32
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD2	8	0.32
(2,1313)	1:A:746:ILE:H	1:A:742:ARG:HA	9	0.32
(2,1253)	1:A:705:VAL:HG11	1:A:709:ARG:HD2	10	0.32
(2,1253)	1:A:705:VAL:HG11	1:A:709:ARG:HD3	10	0.32
(2,1253)	1:A:705:VAL:HG12	1:A:709:ARG:HD2	10	0.32
(2,1253)	1:A:705:VAL:HG12	1:A:709:ARG:HD3	10	0.32
(2,1253)	1:A:705:VAL:HG13	1:A:709:ARG:HD2	10	0.32
(2,1253)	1:A:705:VAL:HG13	1:A:709:ARG:HD3	10	0.32
(2,1251)	1:A:705:VAL:HG11	1:A:702:LEU:HA	12	0.32
(2,1251)	1:A:705:VAL:HG12	1:A:702:LEU:HA	12	0.32
(2,1251)	1:A:705:VAL:HG13	1:A:702:LEU:HA	12	0.32
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	14	0.32
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	14	0.32
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	14	0.32
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	14	0.32
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	14	0.32
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	14	0.32
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB2	8	0.32
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB3	8	0.32
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB2	8	0.32
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB3	8	0.32
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB2	8	0.32
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB3	8	0.32
(2,1177)	1:A:689:VAL:HG21	1:A:685:PHE:HE1	9	0.32
(2,1177)	1:A:689:VAL:HG21	1:A:685:PHE:HE2	9	0.32
(2,1177)	1:A:689:VAL:HG22	1:A:685:PHE:HE1	9	0.32
(2,1177)	1:A:689:VAL:HG22	1:A:685:PHE:HE2	9	0.32
(2,1177)	1:A:689:VAL:HG23	1:A:685:PHE:HE1	9	0.32
(2,1177)	1:A:689:VAL:HG23	1:A:685:PHE:HE2	9	0.32
(2,1173)	1:A:688:ILE:HD11	1:A:684:ILE:HD11	7	0.32
(2,1173)	1:A:688:ILE:HD11	1:A:684:ILE:HD12	7	0.32
(2,1173)	1:A:688:ILE:HD11	1:A:684:ILE:HD13	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1173)	1:A:688:ILE:HD12	1:A:684:ILE:HD11	7	0.32
(2,1173)	1:A:688:ILE:HD12	1:A:684:ILE:HD12	7	0.32
(2,1173)	1:A:688:ILE:HD12	1:A:684:ILE:HD13	7	0.32
(2,1173)	1:A:688:ILE:HD13	1:A:684:ILE:HD11	7	0.32
(2,1173)	1:A:688:ILE:HD13	1:A:684:ILE:HD12	7	0.32
(2,1173)	1:A:688:ILE:HD13	1:A:684:ILE:HD13	7	0.32
(2,117)	1:A:781:ILE:HD11	1:B:746:ILE:HG12	2	0.32
(2,117)	1:A:781:ILE:HD11	1:B:746:ILE:HG13	2	0.32
(2,117)	1:A:781:ILE:HD12	1:B:746:ILE:HG12	2	0.32
(2,117)	1:A:781:ILE:HD12	1:B:746:ILE:HG13	2	0.32
(2,117)	1:A:781:ILE:HD13	1:B:746:ILE:HG12	2	0.32
(2,117)	1:A:781:ILE:HD13	1:B:746:ILE:HG13	2	0.32
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	3	0.32
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	3	0.32
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	3	0.32
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	3	0.32
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	3	0.32
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	3	0.32
(2,1143)	1:A:682:ILE:HG21	1:A:679:LEU:H	6	0.32
(2,1143)	1:A:682:ILE:HG22	1:A:679:LEU:H	6	0.32
(2,1143)	1:A:682:ILE:HG23	1:A:679:LEU:H	6	0.32
(2,1051)	1:A:817:ALA:H	1:A:816:ASN:HB2	1	0.32
(2,1051)	1:A:817:ALA:H	1:A:816:ASN:HB3	1	0.32
(2,1048)	1:A:803:TRP:HE1	1:A:799:LEU:HD11	7	0.32
(2,1048)	1:A:803:TRP:HE1	1:A:799:LEU:HD12	7	0.32
(2,1048)	1:A:803:TRP:HE1	1:A:799:LEU:HD13	7	0.32
(2,1048)	1:A:803:TRP:HE1	1:A:799:LEU:HD21	7	0.32
(2,1048)	1:A:803:TRP:HE1	1:A:799:LEU:HD22	7	0.32
(2,1048)	1:A:803:TRP:HE1	1:A:799:LEU:HD23	7	0.32
(2,1039)	1:A:793:LEU:H	1:A:790:TRP:HE3	4	0.32
(1,88)	1:B:790:TRP:O	1:B:794:LYS:N	11	0.32
(1,87)	1:B:790:TRP:O	1:B:794:LYS:H	1	0.32
(1,87)	1:B:790:TRP:O	1:B:794:LYS:H	15	0.32
(1,2)	1:B:790:TRP:O	1:B:794:LYS:N	11	0.32
(1,174)	1:B:790:TRP:O	1:B:794:LYS:N	11	0.32
(1,173)	1:B:790:TRP:O	1:B:794:LYS:H	1	0.32
(1,173)	1:B:790:TRP:O	1:B:794:LYS:H	15	0.32
(1,1)	1:B:790:TRP:O	1:B:794:LYS:H	1	0.32
(1,1)	1:B:790:TRP:O	1:B:794:LYS:H	15	0.32
(2,990)	1:A:779:THR:H	1:A:776:LEU:HA	6	0.31
(2,984)	1:A:778:VAL:H	1:A:775:LEU:HA	13	0.31
(2,970)	1:A:775:LEU:HD11	1:A:772:ARG:HA	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,970)	1:A:775:LEU:HD12	1:A:772:ARG:HA	6	0.31
(2,970)	1:A:775:LEU:HD13	1:A:772:ARG:HA	6	0.31
(2,965)	1:A:775:LEU:H	1:A:772:ARG:HA	2	0.31
(2,965)	1:A:775:LEU:H	1:A:772:ARG:HA	5	0.31
(2,948)	1:A:764:SER:H	1:A:771:LEU:HB2	5	0.31
(2,948)	1:A:764:SER:H	1:A:771:LEU:HB3	5	0.31
(2,943)	1:A:763:LEU:HD11	1:A:759:ASP:HA	5	0.31
(2,943)	1:A:763:LEU:HD12	1:A:759:ASP:HA	5	0.31
(2,943)	1:A:763:LEU:HD13	1:A:759:ASP:HA	5	0.31
(2,939)	1:A:760:LEU:HD11	1:A:756:ILE:HG12	13	0.31
(2,939)	1:A:760:LEU:HD11	1:A:756:ILE:HG13	13	0.31
(2,939)	1:A:760:LEU:HD12	1:A:756:ILE:HG12	13	0.31
(2,939)	1:A:760:LEU:HD12	1:A:756:ILE:HG13	13	0.31
(2,939)	1:A:760:LEU:HD13	1:A:756:ILE:HG12	13	0.31
(2,939)	1:A:760:LEU:HD13	1:A:756:ILE:HG13	13	0.31
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD2	12	0.31
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD3	12	0.31
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD2	3	0.31
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD3	3	0.31
(2,845)	1:A:707:ARG:H	1:A:707:ARG:HG2	14	0.31
(2,845)	1:A:707:ARG:H	1:A:707:ARG:HG3	14	0.31
(2,839)	1:A:707:ARG:H	1:A:704:LEU:HA	4	0.31
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	11	0.31
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	11	0.31
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	11	0.31
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	11	0.31
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	11	0.31
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	11	0.31
(2,815)	1:A:704:LEU:H	1:A:704:LEU:HB3	11	0.31
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD2	11	0.31
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD3	11	0.31
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD2	11	0.31
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD3	11	0.31
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD2	11	0.31
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD3	11	0.31
(2,755)	1:A:692:LEU:HD11	1:A:689:VAL:HA	8	0.31
(2,755)	1:A:692:LEU:HD12	1:A:689:VAL:HA	8	0.31
(2,755)	1:A:692:LEU:HD13	1:A:689:VAL:HA	8	0.31
(2,721)	1:A:682:ILE:HD11	1:A:681:TYR:H	7	0.31
(2,721)	1:A:682:ILE:HD12	1:A:681:TYR:H	7	0.31
(2,721)	1:A:682:ILE:HD13	1:A:681:TYR:H	7	0.31
(2,559)	1:B:778:VAL:H	1:B:775:LEU:HA	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,559)	1:B:778:VAL:H	1:B:775:LEU:HA	5	0.31
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA2	9	0.31
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA3	9	0.31
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA2	9	0.31
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA3	9	0.31
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA2	9	0.31
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA3	9	0.31
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD2	12	0.31
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD3	12	0.31
(2,439)	1:B:710:GLN:H	1:B:708:VAL:HA	6	0.31
(2,432)	1:B:709:ARG:H	1:B:707:ARG:H	5	0.31
(2,428)	1:B:708:VAL:HG11	1:B:705:VAL:HA	13	0.31
(2,428)	1:B:708:VAL:HG12	1:B:705:VAL:HA	13	0.31
(2,428)	1:B:708:VAL:HG13	1:B:705:VAL:HA	13	0.31
(2,428)	1:B:708:VAL:HG11	1:B:705:VAL:HA	14	0.31
(2,428)	1:B:708:VAL:HG12	1:B:705:VAL:HA	14	0.31
(2,428)	1:B:708:VAL:HG13	1:B:705:VAL:HA	14	0.31
(2,401)	1:B:705:VAL:HG11	1:B:702:LEU:HA	12	0.31
(2,401)	1:B:705:VAL:HG12	1:B:702:LEU:HA	12	0.31
(2,401)	1:B:705:VAL:HG13	1:B:702:LEU:HA	12	0.31
(2,390)	1:B:704:LEU:H	1:B:704:LEU:HB3	6	0.31
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD11	5	0.31
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD12	5	0.31
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD13	5	0.31
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD11	6	0.31
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD12	6	0.31
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD13	6	0.31
(2,242)	1:B:667:ALA:H	1:B:664:ASP:HA	2	0.31
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG12	8	0.31
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG13	8	0.31
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG2	2	0.31
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG3	2	0.31
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG2	8	0.31
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG3	8	0.31
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD2	15	0.31
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD3	15	0.31
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB2	1	0.31
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB3	1	0.31
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	7	0.31
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	7	0.31
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	7	0.31
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1470)	1:A:802:TYR:H	1:A:802:TYR:HB3	3	0.31
(2,1415)	1:A:779:THR:H	1:A:776:LEU:HA	6	0.31
(2,1409)	1:A:778:VAL:H	1:A:775:LEU:HA	13	0.31
(2,1395)	1:A:775:LEU:HD11	1:A:772:ARG:HA	6	0.31
(2,1395)	1:A:775:LEU:HD12	1:A:772:ARG:HA	6	0.31
(2,1395)	1:A:775:LEU:HD13	1:A:772:ARG:HA	6	0.31
(2,1390)	1:A:775:LEU:H	1:A:772:ARG:HA	2	0.31
(2,1390)	1:A:775:LEU:H	1:A:772:ARG:HA	5	0.31
(2,1373)	1:A:764:SER:H	1:A:771:LEU:HB2	5	0.31
(2,1373)	1:A:764:SER:H	1:A:771:LEU:HB3	5	0.31
(2,1368)	1:A:763:LEU:HD11	1:A:759:ASP:HA	5	0.31
(2,1368)	1:A:763:LEU:HD12	1:A:759:ASP:HA	5	0.31
(2,1368)	1:A:763:LEU:HD13	1:A:759:ASP:HA	5	0.31
(2,1364)	1:A:760:LEU:HD11	1:A:756:ILE:HG12	13	0.31
(2,1364)	1:A:760:LEU:HD11	1:A:756:ILE:HG13	13	0.31
(2,1364)	1:A:760:LEU:HD12	1:A:756:ILE:HG12	13	0.31
(2,1364)	1:A:760:LEU:HD12	1:A:756:ILE:HG13	13	0.31
(2,1364)	1:A:760:LEU:HD13	1:A:756:ILE:HG12	13	0.31
(2,1364)	1:A:760:LEU:HD13	1:A:756:ILE:HG13	13	0.31
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD2	12	0.31
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD3	12	0.31
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD2	3	0.31
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD3	3	0.31
(2,1270)	1:A:707:ARG:H	1:A:707:ARG:HG2	14	0.31
(2,1270)	1:A:707:ARG:H	1:A:707:ARG:HG3	14	0.31
(2,1264)	1:A:707:ARG:H	1:A:704:LEU:HA	4	0.31
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	11	0.31
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	11	0.31
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	11	0.31
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	11	0.31
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	11	0.31
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	11	0.31
(2,1240)	1:A:704:LEU:H	1:A:704:LEU:HB3	11	0.31
(2,1180)	1:A:692:LEU:HD11	1:A:689:VAL:HA	8	0.31
(2,1180)	1:A:692:LEU:HD12	1:A:689:VAL:HA	8	0.31
(2,1180)	1:A:692:LEU:HD13	1:A:689:VAL:HA	8	0.31
(2,1146)	1:A:682:ILE:HD11	1:A:681:TYR:H	7	0.31
(2,1146)	1:A:682:ILE:HD12	1:A:681:TYR:H	7	0.31
(2,1146)	1:A:682:ILE:HD13	1:A:681:TYR:H	7	0.31
(2,1045)	1:A:802:TYR:H	1:A:802:TYR:HB3	3	0.31
(1,88)	1:B:790:TRP:O	1:B:794:LYS:N	13	0.31
(1,87)	1:B:790:TRP:O	1:B:794:LYS:H	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:B:790:TRP:O	1:B:794:LYS:N	13	0.31
(1,174)	1:B:790:TRP:O	1:B:794:LYS:N	13	0.31
(1,173)	1:B:790:TRP:O	1:B:794:LYS:H	5	0.31
(1,1)	1:B:790:TRP:O	1:B:794:LYS:H	5	0.31
(2,983)	1:A:777:ILE:HG21	1:A:780:ARG:HD2	6	0.3
(2,983)	1:A:777:ILE:HG21	1:A:780:ARG:HD3	6	0.3
(2,983)	1:A:777:ILE:HG22	1:A:780:ARG:HD2	6	0.3
(2,983)	1:A:777:ILE:HG22	1:A:780:ARG:HD3	6	0.3
(2,983)	1:A:777:ILE:HG23	1:A:780:ARG:HD2	6	0.3
(2,983)	1:A:777:ILE:HG23	1:A:780:ARG:HD3	6	0.3
(2,965)	1:A:775:LEU:H	1:A:772:ARG:HA	10	0.3
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	8	0.3
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	8	0.3
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	8	0.3
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	8	0.3
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	8	0.3
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	8	0.3
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD2	2	0.3
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD3	2	0.3
(2,90)	1:B:713:SER:H	1:A:708:VAL:HG21	1	0.3
(2,90)	1:B:713:SER:H	1:A:708:VAL:HG22	1	0.3
(2,90)	1:B:713:SER:H	1:A:708:VAL:HG23	1	0.3
(2,90)	1:B:713:SER:H	1:A:708:VAL:HG21	7	0.3
(2,90)	1:B:713:SER:H	1:A:708:VAL:HG22	7	0.3
(2,90)	1:B:713:SER:H	1:A:708:VAL:HG23	7	0.3
(2,857)	1:A:709:ARG:H	1:A:707:ARG:H	7	0.3
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD2	11	0.3
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD3	11	0.3
(2,839)	1:A:707:ARG:H	1:A:704:LEU:HA	7	0.3
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	1	0.3
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	1	0.3
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	1	0.3
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	1	0.3
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	1	0.3
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	1	0.3
(2,826)	1:A:705:VAL:HG11	1:A:702:LEU:HA	5	0.3
(2,826)	1:A:705:VAL:HG12	1:A:702:LEU:HA	5	0.3
(2,826)	1:A:705:VAL:HG13	1:A:702:LEU:HA	5	0.3
(2,797)	1:A:701:VAL:HG11	1:A:698:VAL:HA	15	0.3
(2,797)	1:A:701:VAL:HG12	1:A:698:VAL:HA	15	0.3
(2,797)	1:A:701:VAL:HG13	1:A:698:VAL:HA	15	0.3
(2,794)	1:A:701:VAL:H	1:A:698:VAL:HA	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,758)	1:A:692:LEU:HD11	1:A:696:ARG:HH11	8	0.3
(2,758)	1:A:692:LEU:HD11	1:A:696:ARG:HH12	8	0.3
(2,758)	1:A:692:LEU:HD11	1:A:696:ARG:HH21	8	0.3
(2,758)	1:A:692:LEU:HD11	1:A:696:ARG:HH22	8	0.3
(2,758)	1:A:692:LEU:HD12	1:A:696:ARG:HH11	8	0.3
(2,758)	1:A:692:LEU:HD12	1:A:696:ARG:HH12	8	0.3
(2,758)	1:A:692:LEU:HD12	1:A:696:ARG:HH21	8	0.3
(2,758)	1:A:692:LEU:HD12	1:A:696:ARG:HH22	8	0.3
(2,758)	1:A:692:LEU:HD13	1:A:696:ARG:HH11	8	0.3
(2,758)	1:A:692:LEU:HD13	1:A:696:ARG:HH12	8	0.3
(2,758)	1:A:692:LEU:HD13	1:A:696:ARG:HH21	8	0.3
(2,758)	1:A:692:LEU:HD13	1:A:696:ARG:HH22	8	0.3
(2,757)	1:A:692:LEU:HD11	1:A:691:SER:HB2	10	0.3
(2,757)	1:A:692:LEU:HD11	1:A:691:SER:HB3	10	0.3
(2,757)	1:A:692:LEU:HD12	1:A:691:SER:HB2	10	0.3
(2,757)	1:A:692:LEU:HD12	1:A:691:SER:HB3	10	0.3
(2,757)	1:A:692:LEU:HD13	1:A:691:SER:HB2	10	0.3
(2,757)	1:A:692:LEU:HD13	1:A:691:SER:HB3	10	0.3
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB2	4	0.3
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB3	4	0.3
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB2	4	0.3
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB3	4	0.3
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB2	4	0.3
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB3	4	0.3
(2,719)	1:A:682:ILE:HG21	1:A:685:PHE:HB2	9	0.3
(2,719)	1:A:682:ILE:HG21	1:A:685:PHE:HB3	9	0.3
(2,719)	1:A:682:ILE:HG22	1:A:685:PHE:HB2	9	0.3
(2,719)	1:A:682:ILE:HG22	1:A:685:PHE:HB3	9	0.3
(2,719)	1:A:682:ILE:HG23	1:A:685:PHE:HB2	9	0.3
(2,719)	1:A:682:ILE:HG23	1:A:685:PHE:HB3	9	0.3
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD11	9	0.3
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD12	9	0.3
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD13	9	0.3
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD11	9	0.3
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD12	9	0.3
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD13	9	0.3
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD21	9	0.3
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD22	9	0.3
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD23	9	0.3
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD11	7	0.3
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD12	7	0.3
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD13	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD21	7	0.3
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD22	7	0.3
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD23	7	0.3
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD11	8	0.3
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD12	8	0.3
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD13	8	0.3
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD21	8	0.3
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD22	8	0.3
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD23	8	0.3
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD1	14	0.3
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD2	14	0.3
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD1	14	0.3
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD2	14	0.3
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD1	14	0.3
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD2	14	0.3
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD2	12	0.3
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD3	12	0.3
(2,586)	1:B:782:VAL:HG21	1:B:779:THR:HA	6	0.3
(2,586)	1:B:782:VAL:HG22	1:B:779:THR:HA	6	0.3
(2,586)	1:B:782:VAL:HG23	1:B:779:THR:HA	6	0.3
(2,581)	1:B:782:VAL:H	1:B:779:THR:HA	6	0.3
(2,565)	1:B:779:THR:H	1:B:776:LEU:HA	9	0.3
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE1	1	0.3
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE2	1	0.3
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE1	1	0.3
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE2	1	0.3
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE1	1	0.3
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE2	1	0.3
(2,473)	1:B:746:ILE:HG21	1:B:750:ASN:HD22	3	0.3
(2,473)	1:B:746:ILE:HG22	1:B:750:ASN:HD22	3	0.3
(2,473)	1:B:746:ILE:HG23	1:B:750:ASN:HD22	3	0.3
(2,472)	1:B:746:ILE:HG21	1:B:750:ASN:HD21	8	0.3
(2,472)	1:B:746:ILE:HG22	1:B:750:ASN:HD21	8	0.3
(2,472)	1:B:746:ILE:HG23	1:B:750:ASN:HD21	8	0.3
(2,463)	1:B:746:ILE:H	1:B:742:ARG:HA	9	0.3
(2,439)	1:B:710:GLN:H	1:B:708:VAL:HA	12	0.3
(2,438)	1:B:709:ARG:HE	1:B:709:ARG:H	11	0.3
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB2	7	0.3
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB3	7	0.3
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB2	7	0.3
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB3	7	0.3
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB2	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB3	7	0.3
(2,369)	1:B:701:VAL:H	1:B:698:VAL:HA	10	0.3
(2,369)	1:B:701:VAL:H	1:B:698:VAL:HA	12	0.3
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD2	4	0.3
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD3	4	0.3
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD2	4	0.3
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD3	4	0.3
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD2	4	0.3
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD3	4	0.3
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD2	11	0.3
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD3	11	0.3
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD2	11	0.3
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD3	11	0.3
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD2	11	0.3
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD3	11	0.3
(2,296)	1:B:682:ILE:HD11	1:B:681:TYR:H	14	0.3
(2,296)	1:B:682:ILE:HD12	1:B:681:TYR:H	14	0.3
(2,296)	1:B:682:ILE:HD13	1:B:681:TYR:H	14	0.3
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ1	14	0.3
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ2	14	0.3
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ3	14	0.3
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD2	4	0.3
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD3	4	0.3
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD2	3	0.3
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD3	3	0.3
(2,183)	1:A:806:GLU:H	1:B:772:ARG:HE	4	0.3
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG12	5	0.3
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG13	5	0.3
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG12	8	0.3
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG13	8	0.3
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG12	5	0.3
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG13	5	0.3
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG12	8	0.3
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG13	8	0.3
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG12	12	0.3
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG13	12	0.3
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD11	4	0.3
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD12	4	0.3
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD13	4	0.3
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD21	4	0.3
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD22	4	0.3
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD23	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,142)	1:A:781:ILE:H	1:B:746:ILE:HG12	1	0.3
(2,142)	1:A:781:ILE:H	1:B:746:ILE:HG13	1	0.3
(2,1408)	1:A:777:ILE:HG21	1:A:780:ARG:HD2	6	0.3
(2,1408)	1:A:777:ILE:HG21	1:A:780:ARG:HD3	6	0.3
(2,1408)	1:A:777:ILE:HG22	1:A:780:ARG:HD2	6	0.3
(2,1408)	1:A:777:ILE:HG22	1:A:780:ARG:HD3	6	0.3
(2,1408)	1:A:777:ILE:HG23	1:A:780:ARG:HD2	6	0.3
(2,1408)	1:A:777:ILE:HG23	1:A:780:ARG:HD3	6	0.3
(2,1390)	1:A:775:LEU:H	1:A:772:ARG:HA	10	0.3
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	8	0.3
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	8	0.3
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	8	0.3
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	8	0.3
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	8	0.3
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	8	0.3
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD2	2	0.3
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD3	2	0.3
(2,1282)	1:A:709:ARG:H	1:A:707:ARG:H	7	0.3
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD2	11	0.3
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD3	11	0.3
(2,1264)	1:A:707:ARG:H	1:A:704:LEU:HA	7	0.3
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	1	0.3
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	1	0.3
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	1	0.3
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	1	0.3
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	1	0.3
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	1	0.3
(2,1251)	1:A:705:VAL:HG11	1:A:702:LEU:HA	5	0.3
(2,1251)	1:A:705:VAL:HG12	1:A:702:LEU:HA	5	0.3
(2,1251)	1:A:705:VAL:HG13	1:A:702:LEU:HA	5	0.3
(2,1222)	1:A:701:VAL:HG11	1:A:698:VAL:HA	15	0.3
(2,1222)	1:A:701:VAL:HG12	1:A:698:VAL:HA	15	0.3
(2,1222)	1:A:701:VAL:HG13	1:A:698:VAL:HA	15	0.3
(2,1219)	1:A:701:VAL:H	1:A:698:VAL:HA	3	0.3
(2,1183)	1:A:692:LEU:HD11	1:A:696:ARG:HH11	8	0.3
(2,1183)	1:A:692:LEU:HD11	1:A:696:ARG:HH12	8	0.3
(2,1183)	1:A:692:LEU:HD11	1:A:696:ARG:HH21	8	0.3
(2,1183)	1:A:692:LEU:HD11	1:A:696:ARG:HH22	8	0.3
(2,1183)	1:A:692:LEU:HD12	1:A:696:ARG:HH11	8	0.3
(2,1183)	1:A:692:LEU:HD12	1:A:696:ARG:HH12	8	0.3
(2,1183)	1:A:692:LEU:HD12	1:A:696:ARG:HH21	8	0.3
(2,1183)	1:A:692:LEU:HD12	1:A:696:ARG:HH22	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1183)	1:A:692:LEU:HD13	1:A:696:ARG:HH11	8	0.3
(2,1183)	1:A:692:LEU:HD13	1:A:696:ARG:HH12	8	0.3
(2,1183)	1:A:692:LEU:HD13	1:A:696:ARG:HH21	8	0.3
(2,1183)	1:A:692:LEU:HD13	1:A:696:ARG:HH22	8	0.3
(2,1182)	1:A:692:LEU:HD11	1:A:691:SER:HB2	10	0.3
(2,1182)	1:A:692:LEU:HD11	1:A:691:SER:HB3	10	0.3
(2,1182)	1:A:692:LEU:HD12	1:A:691:SER:HB2	10	0.3
(2,1182)	1:A:692:LEU:HD12	1:A:691:SER:HB3	10	0.3
(2,1182)	1:A:692:LEU:HD13	1:A:691:SER:HB2	10	0.3
(2,1182)	1:A:692:LEU:HD13	1:A:691:SER:HB3	10	0.3
(2,1144)	1:A:682:ILE:HG21	1:A:685:PHE:HB2	9	0.3
(2,1144)	1:A:682:ILE:HG21	1:A:685:PHE:HB3	9	0.3
(2,1144)	1:A:682:ILE:HG22	1:A:685:PHE:HB2	9	0.3
(2,1144)	1:A:682:ILE:HG22	1:A:685:PHE:HB3	9	0.3
(2,1144)	1:A:682:ILE:HG23	1:A:685:PHE:HB2	9	0.3
(2,1144)	1:A:682:ILE:HG23	1:A:685:PHE:HB3	9	0.3
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD11	9	0.3
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD12	9	0.3
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD13	9	0.3
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD11	4	0.3
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD12	4	0.3
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD13	4	0.3
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD21	4	0.3
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD22	4	0.3
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD23	4	0.3
(1,91)	1:B:792:ALA:O	1:B:796:TRP:H	11	0.3
(1,88)	1:B:790:TRP:O	1:B:794:LYS:N	6	0.3
(1,5)	1:B:792:ALA:O	1:B:796:TRP:H	11	0.3
(1,2)	1:B:790:TRP:O	1:B:794:LYS:N	6	0.3
(1,177)	1:B:792:ALA:O	1:B:796:TRP:H	11	0.3
(1,174)	1:B:790:TRP:O	1:B:794:LYS:N	6	0.3
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	5	0.29
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	5	0.29
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	5	0.29
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	5	0.29
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	5	0.29
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	5	0.29
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB2	3	0.29
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB3	3	0.29
(2,907)	1:A:749:VAL:H	1:A:746:ILE:HA	8	0.29
(2,907)	1:A:749:VAL:H	1:A:746:ILE:HA	14	0.29
(2,90)	1:B:713:SER:H	1:A:708:VAL:HG21	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,90)	1:B:713:SER:H	1:A:708:VAL:HG22	3	0.29
(2,90)	1:B:713:SER:H	1:A:708:VAL:HG23	3	0.29
(2,897)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	14	0.29
(2,897)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	14	0.29
(2,897)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	14	0.29
(2,815)	1:A:704:LEU:H	1:A:704:LEU:HB3	9	0.29
(2,697)	1:A:674:ASP:H	1:A:677:ASN:H	1	0.29
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD11	7	0.29
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD12	7	0.29
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD13	7	0.29
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD21	7	0.29
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD22	7	0.29
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD23	7	0.29
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB1	14	0.29
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB2	14	0.29
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB3	14	0.29
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB1	14	0.29
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB2	14	0.29
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB3	14	0.29
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB1	14	0.29
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB2	14	0.29
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB3	14	0.29
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG11	10	0.29
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG12	10	0.29
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG13	10	0.29
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG21	10	0.29
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG22	10	0.29
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG23	10	0.29
(2,586)	1:B:782:VAL:HG21	1:B:779:THR:HA	13	0.29
(2,586)	1:B:782:VAL:HG22	1:B:779:THR:HA	13	0.29
(2,586)	1:B:782:VAL:HG23	1:B:779:THR:HA	13	0.29
(2,575)	1:B:781:ILE:H	1:B:778:VAL:HA	5	0.29
(2,558)	1:B:777:ILE:HG21	1:B:780:ARG:HD2	12	0.29
(2,558)	1:B:777:ILE:HG21	1:B:780:ARG:HD3	12	0.29
(2,558)	1:B:777:ILE:HG22	1:B:780:ARG:HD2	12	0.29
(2,558)	1:B:777:ILE:HG22	1:B:780:ARG:HD3	12	0.29
(2,558)	1:B:777:ILE:HG23	1:B:780:ARG:HD2	12	0.29
(2,558)	1:B:777:ILE:HG23	1:B:780:ARG:HD3	12	0.29
(2,421)	1:B:707:ARG:H	1:B:707:ARG:HD2	14	0.29
(2,421)	1:B:707:ARG:H	1:B:707:ARG:HD3	14	0.29
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB2	2	0.29
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB3	2	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB2	9	0.29
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB3	9	0.29
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB2	5	0.29
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB3	5	0.29
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB2	5	0.29
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB3	5	0.29
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB2	5	0.29
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB3	5	0.29
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ1	2	0.29
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ2	2	0.29
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ3	2	0.29
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD2	3	0.29
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD3	3	0.29
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD2	14	0.29
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD3	14	0.29
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG12	9	0.29
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG13	9	0.29
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	6	0.29
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	6	0.29
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	6	0.29
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	6	0.29
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG2	4	0.29
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG3	4	0.29
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD11	12	0.29
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD12	12	0.29
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD13	12	0.29
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD2	14	0.29
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD3	14	0.29
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	5	0.29
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	5	0.29
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	5	0.29
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	5	0.29
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	5	0.29
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	5	0.29
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB2	3	0.29
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB3	3	0.29
(2,1332)	1:A:749:VAL:H	1:A:746:ILE:HA	8	0.29
(2,1332)	1:A:749:VAL:H	1:A:746:ILE:HA	14	0.29
(2,1322)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	14	0.29
(2,1322)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	14	0.29
(2,1322)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	14	0.29
(2,1240)	1:A:704:LEU:H	1:A:704:LEU:HB3	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB2	14	0.29
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB3	14	0.29
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB2	14	0.29
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB3	14	0.29
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB2	14	0.29
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB3	14	0.29
(2,1122)	1:A:674:ASP:H	1:A:677:ASN:H	1	0.29
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD11	7	0.29
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD12	7	0.29
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD13	7	0.29
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD21	7	0.29
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD22	7	0.29
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD23	7	0.29
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG2	4	0.29
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG3	4	0.29
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD11	12	0.29
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD12	12	0.29
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD13	12	0.29
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD2	14	0.29
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD3	14	0.29
(2,99)	1:A:758:ASP:H	1:B:715:LEU:HD21	10	0.28
(2,99)	1:A:758:ASP:H	1:B:715:LEU:HD22	10	0.28
(2,99)	1:A:758:ASP:H	1:B:715:LEU:HD23	10	0.28
(2,984)	1:A:778:VAL:H	1:A:775:LEU:HA	9	0.28
(2,965)	1:A:775:LEU:H	1:A:772:ARG:HA	8	0.28
(2,965)	1:A:775:LEU:H	1:A:772:ARG:HA	9	0.28
(2,952)	1:A:771:LEU:HD21	1:A:772:ARG:HH21	8	0.28
(2,952)	1:A:771:LEU:HD21	1:A:772:ARG:HH22	8	0.28
(2,952)	1:A:771:LEU:HD22	1:A:772:ARG:HH21	8	0.28
(2,952)	1:A:771:LEU:HD22	1:A:772:ARG:HH22	8	0.28
(2,952)	1:A:771:LEU:HD23	1:A:772:ARG:HH21	8	0.28
(2,952)	1:A:771:LEU:HD23	1:A:772:ARG:HH22	8	0.28
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	4	0.28
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	4	0.28
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	4	0.28
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	4	0.28
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	4	0.28
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	4	0.28
(2,941)	1:A:760:LEU:HD21	1:A:768:TYR:HE1	11	0.28
(2,941)	1:A:760:LEU:HD21	1:A:768:TYR:HE2	11	0.28
(2,941)	1:A:760:LEU:HD22	1:A:768:TYR:HE1	11	0.28
(2,941)	1:A:760:LEU:HD22	1:A:768:TYR:HE2	11	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,941)	1:A:760:LEU:HD23	1:A:768:TYR:HE1	11	0.28
(2,941)	1:A:760:LEU:HD23	1:A:768:TYR:HE2	11	0.28
(2,939)	1:A:760:LEU:HD11	1:A:756:ILE:HG12	5	0.28
(2,939)	1:A:760:LEU:HD11	1:A:756:ILE:HG13	5	0.28
(2,939)	1:A:760:LEU:HD12	1:A:756:ILE:HG12	5	0.28
(2,939)	1:A:760:LEU:HD12	1:A:756:ILE:HG13	5	0.28
(2,939)	1:A:760:LEU:HD13	1:A:756:ILE:HG12	5	0.28
(2,939)	1:A:760:LEU:HD13	1:A:756:ILE:HG13	5	0.28
(2,916)	1:A:753:LEU:HD11	1:A:757:TRP:HB2	9	0.28
(2,916)	1:A:753:LEU:HD11	1:A:757:TRP:HB3	9	0.28
(2,916)	1:A:753:LEU:HD12	1:A:757:TRP:HB2	9	0.28
(2,916)	1:A:753:LEU:HD12	1:A:757:TRP:HB3	9	0.28
(2,916)	1:A:753:LEU:HD13	1:A:757:TRP:HB2	9	0.28
(2,916)	1:A:753:LEU:HD13	1:A:757:TRP:HB3	9	0.28
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD2	14	0.28
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD3	14	0.28
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB2	12	0.28
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB3	12	0.28
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD2	11	0.28
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD3	11	0.28
(2,781)	1:A:698:VAL:HG11	1:A:695:LEU:HG	3	0.28
(2,781)	1:A:698:VAL:HG12	1:A:695:LEU:HG	3	0.28
(2,781)	1:A:698:VAL:HG13	1:A:695:LEU:HG	3	0.28
(2,751)	1:A:689:VAL:HG21	1:A:685:PHE:HD1	9	0.28
(2,751)	1:A:689:VAL:HG21	1:A:685:PHE:HD2	9	0.28
(2,751)	1:A:689:VAL:HG22	1:A:685:PHE:HD1	9	0.28
(2,751)	1:A:689:VAL:HG22	1:A:685:PHE:HD2	9	0.28
(2,751)	1:A:689:VAL:HG23	1:A:685:PHE:HD1	9	0.28
(2,751)	1:A:689:VAL:HG23	1:A:685:PHE:HD2	9	0.28
(2,744)	1:A:686:ILE:HD11	1:A:685:PHE:HD1	9	0.28
(2,744)	1:A:686:ILE:HD11	1:A:685:PHE:HD2	9	0.28
(2,744)	1:A:686:ILE:HD12	1:A:685:PHE:HD1	9	0.28
(2,744)	1:A:686:ILE:HD12	1:A:685:PHE:HD2	9	0.28
(2,744)	1:A:686:ILE:HD13	1:A:685:PHE:HD1	9	0.28
(2,744)	1:A:686:ILE:HD13	1:A:685:PHE:HD2	9	0.28
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	9	0.28
(2,720)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	9	0.28
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	9	0.28
(2,720)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	9	0.28
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	9	0.28
(2,720)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	9	0.28
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD11	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD12	4	0.28
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD13	4	0.28
(2,630)	1:B:835:GLY:H	1:B:834:GLN:HE21	7	0.28
(2,630)	1:B:835:GLY:H	1:B:834:GLN:HE22	7	0.28
(2,629)	1:B:835:GLY:H	1:B:834:GLN:HG2	6	0.28
(2,629)	1:B:835:GLY:H	1:B:834:GLN:HG3	6	0.28
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD11	6	0.28
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD12	6	0.28
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD13	6	0.28
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD11	11	0.28
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD12	11	0.28
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD13	11	0.28
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB2	10	0.28
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB3	10	0.28
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB2	10	0.28
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB3	10	0.28
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB2	10	0.28
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB3	10	0.28
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB2	12	0.28
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB3	12	0.28
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB2	12	0.28
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB3	12	0.28
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB2	12	0.28
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB3	12	0.28
(2,575)	1:B:781:ILE:H	1:B:778:VAL:HA	1	0.28
(2,575)	1:B:781:ILE:H	1:B:778:VAL:HA	14	0.28
(2,522)	1:B:764:SER:H	1:B:761:ARG:HA	7	0.28
(2,482)	1:B:749:VAL:H	1:B:746:ILE:HA	10	0.28
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD2	1	0.28
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD3	1	0.28
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD2	2	0.28
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD3	2	0.28
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD2	14	0.28
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD3	14	0.28
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD2	15	0.28
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD3	15	0.28
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB2	7	0.28
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB3	7	0.28
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB2	7	0.28
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB3	7	0.28
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB2	7	0.28
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB3	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB2	12	0.28
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB3	12	0.28
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB2	12	0.28
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB3	12	0.28
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB2	12	0.28
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB3	12	0.28
(2,401)	1:B:705:VAL:HG11	1:B:702:LEU:HA	6	0.28
(2,401)	1:B:705:VAL:HG12	1:B:702:LEU:HA	6	0.28
(2,401)	1:B:705:VAL:HG13	1:B:702:LEU:HA	6	0.28
(2,369)	1:B:701:VAL:H	1:B:698:VAL:HA	14	0.28
(2,242)	1:B:667:ALA:H	1:B:664:ASP:HA	9	0.28
(2,241)	1:B:666:TRP:HE1	1:B:662:GLU:H	10	0.28
(2,225)	1:B:664:ASP:H	1:B:663:LEU:H	13	0.28
(2,219)	1:B:663:LEU:H	1:B:664:ASP:H	13	0.28
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ1	12	0.28
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ2	12	0.28
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ3	12	0.28
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD2	12	0.28
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD3	12	0.28
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG2	9	0.28
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG3	9	0.28
(2,183)	1:A:806:GLU:H	1:B:772:ARG:HE	11	0.28
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	10	0.28
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	10	0.28
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	10	0.28
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	10	0.28
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG12	7	0.28
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG13	7	0.28
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG12	7	0.28
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG13	7	0.28
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD2	13	0.28
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD3	13	0.28
(2,1476)	1:A:817:ALA:H	1:A:816:ASN:HB2	2	0.28
(2,1476)	1:A:817:ALA:H	1:A:816:ASN:HB3	2	0.28
(2,1465)	1:A:796:TRP:HE1	1:A:796:TRP:H	13	0.28
(2,1431)	1:A:782:VAL:H	1:A:779:THR:HA	1	0.28
(2,1431)	1:A:782:VAL:H	1:A:779:THR:HA	5	0.28
(2,1409)	1:A:778:VAL:H	1:A:775:LEU:HA	9	0.28
(2,1390)	1:A:775:LEU:H	1:A:772:ARG:HA	8	0.28
(2,1390)	1:A:775:LEU:H	1:A:772:ARG:HA	9	0.28
(2,1377)	1:A:771:LEU:HD21	1:A:772:ARG:HH21	8	0.28
(2,1377)	1:A:771:LEU:HD21	1:A:772:ARG:HH22	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1377)	1:A:771:LEU:HD22	1:A:772:ARG:HH21	8	0.28
(2,1377)	1:A:771:LEU:HD22	1:A:772:ARG:HH22	8	0.28
(2,1377)	1:A:771:LEU:HD23	1:A:772:ARG:HH21	8	0.28
(2,1377)	1:A:771:LEU:HD23	1:A:772:ARG:HH22	8	0.28
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	4	0.28
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	4	0.28
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	4	0.28
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	4	0.28
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	4	0.28
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	4	0.28
(2,1366)	1:A:760:LEU:HD21	1:A:768:TYR:HE1	11	0.28
(2,1366)	1:A:760:LEU:HD21	1:A:768:TYR:HE2	11	0.28
(2,1366)	1:A:760:LEU:HD22	1:A:768:TYR:HE1	11	0.28
(2,1366)	1:A:760:LEU:HD22	1:A:768:TYR:HE2	11	0.28
(2,1366)	1:A:760:LEU:HD23	1:A:768:TYR:HE1	11	0.28
(2,1366)	1:A:760:LEU:HD23	1:A:768:TYR:HE2	11	0.28
(2,1364)	1:A:760:LEU:HD11	1:A:756:ILE:HG12	5	0.28
(2,1364)	1:A:760:LEU:HD11	1:A:756:ILE:HG13	5	0.28
(2,1364)	1:A:760:LEU:HD12	1:A:756:ILE:HG12	5	0.28
(2,1364)	1:A:760:LEU:HD12	1:A:756:ILE:HG13	5	0.28
(2,1364)	1:A:760:LEU:HD13	1:A:756:ILE:HG12	5	0.28
(2,1364)	1:A:760:LEU:HD13	1:A:756:ILE:HG13	5	0.28
(2,1341)	1:A:753:LEU:HD11	1:A:757:TRP:HB2	9	0.28
(2,1341)	1:A:753:LEU:HD11	1:A:757:TRP:HB3	9	0.28
(2,1341)	1:A:753:LEU:HD12	1:A:757:TRP:HB2	9	0.28
(2,1341)	1:A:753:LEU:HD12	1:A:757:TRP:HB3	9	0.28
(2,1341)	1:A:753:LEU:HD13	1:A:757:TRP:HB2	9	0.28
(2,1341)	1:A:753:LEU:HD13	1:A:757:TRP:HB3	9	0.28
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD2	14	0.28
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD3	14	0.28
(2,1206)	1:A:698:VAL:HG11	1:A:695:LEU:HG	3	0.28
(2,1206)	1:A:698:VAL:HG12	1:A:695:LEU:HG	3	0.28
(2,1206)	1:A:698:VAL:HG13	1:A:695:LEU:HG	3	0.28
(2,1176)	1:A:689:VAL:HG21	1:A:685:PHE:HD1	9	0.28
(2,1176)	1:A:689:VAL:HG21	1:A:685:PHE:HD2	9	0.28
(2,1176)	1:A:689:VAL:HG22	1:A:685:PHE:HD1	9	0.28
(2,1176)	1:A:689:VAL:HG22	1:A:685:PHE:HD2	9	0.28
(2,1176)	1:A:689:VAL:HG23	1:A:685:PHE:HD1	9	0.28
(2,1176)	1:A:689:VAL:HG23	1:A:685:PHE:HD2	9	0.28
(2,1169)	1:A:686:ILE:HD11	1:A:685:PHE:HD1	9	0.28
(2,1169)	1:A:686:ILE:HD11	1:A:685:PHE:HD2	9	0.28
(2,1169)	1:A:686:ILE:HD12	1:A:685:PHE:HD1	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1169)	1:A:686:ILE:HD12	1:A:685:PHE:HD2	9	0.28
(2,1169)	1:A:686:ILE:HD13	1:A:685:PHE:HD1	9	0.28
(2,1169)	1:A:686:ILE:HD13	1:A:685:PHE:HD2	9	0.28
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD1	9	0.28
(2,1145)	1:A:682:ILE:HG21	1:A:685:PHE:HD2	9	0.28
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD1	9	0.28
(2,1145)	1:A:682:ILE:HG22	1:A:685:PHE:HD2	9	0.28
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD1	9	0.28
(2,1145)	1:A:682:ILE:HG23	1:A:685:PHE:HD2	9	0.28
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD11	4	0.28
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD12	4	0.28
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD13	4	0.28
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD2	13	0.28
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD3	13	0.28
(2,1051)	1:A:817:ALA:H	1:A:816:ASN:HB2	2	0.28
(2,1051)	1:A:817:ALA:H	1:A:816:ASN:HB3	2	0.28
(2,1040)	1:A:796:TRP:HE1	1:A:796:TRP:H	13	0.28
(2,1006)	1:A:782:VAL:H	1:A:779:THR:HA	1	0.28
(2,1006)	1:A:782:VAL:H	1:A:779:THR:HA	5	0.28
(1,88)	1:B:790:TRP:O	1:B:794:LYS:N	5	0.28
(1,88)	1:B:790:TRP:O	1:B:794:LYS:N	8	0.28
(1,88)	1:B:790:TRP:O	1:B:794:LYS:N	12	0.28
(1,2)	1:B:790:TRP:O	1:B:794:LYS:N	5	0.28
(1,2)	1:B:790:TRP:O	1:B:794:LYS:N	8	0.28
(1,2)	1:B:790:TRP:O	1:B:794:LYS:N	12	0.28
(1,191)	1:B:799:LEU:O	1:B:803:TRP:H	9	0.28
(1,19)	1:B:799:LEU:O	1:B:803:TRP:H	9	0.28
(1,174)	1:B:790:TRP:O	1:B:794:LYS:N	5	0.28
(1,174)	1:B:790:TRP:O	1:B:794:LYS:N	8	0.28
(1,174)	1:B:790:TRP:O	1:B:794:LYS:N	12	0.28
(1,105)	1:B:799:LEU:O	1:B:803:TRP:H	9	0.28
(2,983)	1:A:777:ILE:HG21	1:A:780:ARG:HD2	14	0.27
(2,983)	1:A:777:ILE:HG21	1:A:780:ARG:HD3	14	0.27
(2,983)	1:A:777:ILE:HG22	1:A:780:ARG:HD2	14	0.27
(2,983)	1:A:777:ILE:HG22	1:A:780:ARG:HD3	14	0.27
(2,983)	1:A:777:ILE:HG23	1:A:780:ARG:HD2	14	0.27
(2,983)	1:A:777:ILE:HG23	1:A:780:ARG:HD3	14	0.27
(2,940)	1:A:760:LEU:HD11	1:A:757:TRP:HA	6	0.27
(2,940)	1:A:760:LEU:HD12	1:A:757:TRP:HA	6	0.27
(2,940)	1:A:760:LEU:HD13	1:A:757:TRP:HA	6	0.27
(2,907)	1:A:749:VAL:H	1:A:746:ILE:HA	1	0.27
(2,897)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,897)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	11	0.27
(2,897)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	11	0.27
(2,882)	1:A:740:ARG:H	1:A:739:GLU:HA	3	0.27
(2,864)	1:A:710:GLN:H	1:A:708:VAL:HA	4	0.27
(2,857)	1:A:709:ARG:H	1:A:707:ARG:H	6	0.27
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD2	10	0.27
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD3	10	0.27
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB2	4	0.27
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB3	4	0.27
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB2	6	0.27
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB3	6	0.27
(2,815)	1:A:704:LEU:H	1:A:704:LEU:HB3	10	0.27
(2,797)	1:A:701:VAL:HG11	1:A:698:VAL:HA	8	0.27
(2,797)	1:A:701:VAL:HG12	1:A:698:VAL:HA	8	0.27
(2,797)	1:A:701:VAL:HG13	1:A:698:VAL:HA	8	0.27
(2,794)	1:A:701:VAL:H	1:A:698:VAL:HA	14	0.27
(2,722)	1:A:682:ILE:HD11	1:A:685:PHE:HB2	11	0.27
(2,722)	1:A:682:ILE:HD11	1:A:685:PHE:HB3	11	0.27
(2,722)	1:A:682:ILE:HD12	1:A:685:PHE:HB2	11	0.27
(2,722)	1:A:682:ILE:HD12	1:A:685:PHE:HB3	11	0.27
(2,722)	1:A:682:ILE:HD13	1:A:685:PHE:HB2	11	0.27
(2,722)	1:A:682:ILE:HD13	1:A:685:PHE:HB3	11	0.27
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB2	10	0.27
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB3	10	0.27
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB2	10	0.27
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB3	10	0.27
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB2	10	0.27
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB3	10	0.27
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG11	1	0.27
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG12	1	0.27
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG13	1	0.27
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG21	1	0.27
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG22	1	0.27
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG23	1	0.27
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB2	11	0.27
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB3	11	0.27
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB2	11	0.27
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB3	11	0.27
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB2	11	0.27
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB3	11	0.27
(2,608)	1:B:786:GLY:H	1:B:782:VAL:HA	1	0.27
(2,580)	1:B:781:ILE:HG21	1:B:778:VAL:HA	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,580)	1:B:781:ILE:HG22	1:B:778:VAL:HA	7	0.27
(2,580)	1:B:781:ILE:HG23	1:B:778:VAL:HA	7	0.27
(2,559)	1:B:778:VAL:H	1:B:775:LEU:HA	6	0.27
(2,558)	1:B:777:ILE:HG21	1:B:780:ARG:HD2	2	0.27
(2,558)	1:B:777:ILE:HG21	1:B:780:ARG:HD3	2	0.27
(2,558)	1:B:777:ILE:HG22	1:B:780:ARG:HD2	2	0.27
(2,558)	1:B:777:ILE:HG22	1:B:780:ARG:HD3	2	0.27
(2,558)	1:B:777:ILE:HG23	1:B:780:ARG:HD2	2	0.27
(2,558)	1:B:777:ILE:HG23	1:B:780:ARG:HD3	2	0.27
(2,479)	1:B:748:LEU:H	1:B:745:SER:HA	6	0.27
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD2	4	0.27
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD3	4	0.27
(2,472)	1:B:746:ILE:HG21	1:B:750:ASN:HD21	5	0.27
(2,472)	1:B:746:ILE:HG22	1:B:750:ASN:HD21	5	0.27
(2,472)	1:B:746:ILE:HG23	1:B:750:ASN:HD21	5	0.27
(2,463)	1:B:746:ILE:H	1:B:742:ARG:HA	1	0.27
(2,432)	1:B:709:ARG:H	1:B:707:ARG:H	4	0.27
(2,414)	1:B:707:ARG:H	1:B:704:LEU:HA	9	0.27
(2,373)	1:B:701:VAL:HG21	1:B:698:VAL:HA	5	0.27
(2,373)	1:B:701:VAL:HG22	1:B:698:VAL:HA	5	0.27
(2,373)	1:B:701:VAL:HG23	1:B:698:VAL:HA	5	0.27
(2,369)	1:B:701:VAL:H	1:B:698:VAL:HA	1	0.27
(2,351)	1:B:696:ARG:H	1:B:696:ARG:HE	5	0.27
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD11	10	0.27
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD12	10	0.27
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD13	10	0.27
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD11	10	0.27
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD12	10	0.27
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD13	10	0.27
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD11	10	0.27
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD12	10	0.27
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD13	10	0.27
(2,234)	1:B:666:TRP:H	1:B:663:LEU:HA	13	0.27
(2,214)	1:B:661:LEU:HD11	1:B:662:GLU:HG2	3	0.27
(2,214)	1:B:661:LEU:HD11	1:B:662:GLU:HG3	3	0.27
(2,214)	1:B:661:LEU:HD12	1:B:662:GLU:HG2	3	0.27
(2,214)	1:B:661:LEU:HD12	1:B:662:GLU:HG3	3	0.27
(2,214)	1:B:661:LEU:HD13	1:B:662:GLU:HG2	3	0.27
(2,214)	1:B:661:LEU:HD13	1:B:662:GLU:HG3	3	0.27
(2,214)	1:B:661:LEU:HD21	1:B:662:GLU:HG2	3	0.27
(2,214)	1:B:661:LEU:HD21	1:B:662:GLU:HG3	3	0.27
(2,214)	1:B:661:LEU:HD22	1:B:662:GLU:HG2	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,214)	1:B:661:LEU:HD22	1:B:662:GLU:HG3	3	0.27
(2,214)	1:B:661:LEU:HD23	1:B:662:GLU:HG2	3	0.27
(2,214)	1:B:661:LEU:HD23	1:B:662:GLU:HG3	3	0.27
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG12	1	0.27
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG13	1	0.27
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG12	5	0.27
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG13	5	0.27
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG12	1	0.27
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG13	1	0.27
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG12	5	0.27
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG13	5	0.27
(2,186)	1:A:808:LYS:H	1:A:838:ARG:HD2	13	0.27
(2,186)	1:A:808:LYS:H	1:A:838:ARG:HD3	13	0.27
(2,185)	1:A:808:LYS:H	1:A:838:ARG:HD2	13	0.27
(2,185)	1:A:808:LYS:H	1:A:838:ARG:HD3	13	0.27
(2,183)	1:A:806:GLU:H	1:B:772:ARG:HE	2	0.27
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG12	3	0.27
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG13	3	0.27
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG12	3	0.27
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG13	3	0.27
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD11	8	0.27
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD12	8	0.27
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD13	8	0.27
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD21	8	0.27
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD22	8	0.27
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD23	8	0.27
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	11	0.27
(2,1488)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	11	0.27
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	11	0.27
(2,1488)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	11	0.27
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	11	0.27
(2,1488)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	11	0.27
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	11	0.27
(2,1488)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	11	0.27
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG12	3	0.27
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG13	3	0.27
(2,1465)	1:A:796:TRP:HE1	1:A:796:TRP:H	4	0.27
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD2	10	0.27
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD3	10	0.27
(2,141)	1:B:771:LEU:H	1:A:806:GLU:HB2	10	0.27
(2,141)	1:B:771:LEU:H	1:A:806:GLU:HB3	10	0.27
(2,1408)	1:A:777:ILE:HG21	1:A:780:ARG:HD2	14	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1408)	1:A:777:ILE:HG21	1:A:780:ARG:HD3	14	0.27
(2,1408)	1:A:777:ILE:HG22	1:A:780:ARG:HD2	14	0.27
(2,1408)	1:A:777:ILE:HG22	1:A:780:ARG:HD3	14	0.27
(2,1408)	1:A:777:ILE:HG23	1:A:780:ARG:HD2	14	0.27
(2,1408)	1:A:777:ILE:HG23	1:A:780:ARG:HD3	14	0.27
(2,1365)	1:A:760:LEU:HD11	1:A:757:TRP:HA	6	0.27
(2,1365)	1:A:760:LEU:HD12	1:A:757:TRP:HA	6	0.27
(2,1365)	1:A:760:LEU:HD13	1:A:757:TRP:HA	6	0.27
(2,1332)	1:A:749:VAL:H	1:A:746:ILE:HA	1	0.27
(2,1322)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	11	0.27
(2,1322)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	11	0.27
(2,1322)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	11	0.27
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD1	5	0.27
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD2	5	0.27
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD1	9	0.27
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD2	9	0.27
(2,1307)	1:A:740:ARG:H	1:A:739:GLU:HA	3	0.27
(2,1289)	1:A:710:GLN:H	1:A:708:VAL:HA	4	0.27
(2,1282)	1:A:709:ARG:H	1:A:707:ARG:H	6	0.27
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD2	10	0.27
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD3	10	0.27
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB2	4	0.27
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB3	4	0.27
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB2	6	0.27
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB3	6	0.27
(2,1240)	1:A:704:LEU:H	1:A:704:LEU:HB3	10	0.27
(2,1222)	1:A:701:VAL:HG11	1:A:698:VAL:HA	8	0.27
(2,1222)	1:A:701:VAL:HG12	1:A:698:VAL:HA	8	0.27
(2,1222)	1:A:701:VAL:HG13	1:A:698:VAL:HA	8	0.27
(2,1219)	1:A:701:VAL:H	1:A:698:VAL:HA	14	0.27
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB2	10	0.27
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB3	10	0.27
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB2	10	0.27
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB3	10	0.27
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB2	10	0.27
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB3	10	0.27
(2,1147)	1:A:682:ILE:HD11	1:A:685:PHE:HB2	11	0.27
(2,1147)	1:A:682:ILE:HD11	1:A:685:PHE:HB3	11	0.27
(2,1147)	1:A:682:ILE:HD12	1:A:685:PHE:HB2	11	0.27
(2,1147)	1:A:682:ILE:HD12	1:A:685:PHE:HB3	11	0.27
(2,1147)	1:A:682:ILE:HD13	1:A:685:PHE:HB2	11	0.27
(2,1147)	1:A:682:ILE:HD13	1:A:685:PHE:HB3	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD2	6	0.27
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD3	6	0.27
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD2	6	0.27
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD3	6	0.27
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD2	6	0.27
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD3	6	0.27
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE1	11	0.27
(2,1063)	1:A:780:ARG:HH11	1:A:783:GLU:OE2	11	0.27
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE1	11	0.27
(2,1063)	1:A:780:ARG:HH12	1:A:783:GLU:OE2	11	0.27
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE1	11	0.27
(2,1063)	1:A:780:ARG:HH21	1:A:783:GLU:OE2	11	0.27
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE1	11	0.27
(2,1063)	1:A:780:ARG:HH22	1:A:783:GLU:OE2	11	0.27
(2,1040)	1:A:796:TRP:HE1	1:A:796:TRP:H	4	0.27
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD2	10	0.27
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD3	10	0.27
(1,88)	1:B:790:TRP:O	1:B:794:LYS:N	15	0.27
(1,2)	1:B:790:TRP:O	1:B:794:LYS:N	15	0.27
(1,174)	1:B:790:TRP:O	1:B:794:LYS:N	15	0.27
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	6	0.26
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	6	0.26
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	6	0.26
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	6	0.26
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	6	0.26
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	6	0.26
(2,798)	1:A:701:VAL:HG21	1:A:698:VAL:HA	2	0.26
(2,798)	1:A:701:VAL:HG22	1:A:698:VAL:HA	2	0.26
(2,798)	1:A:701:VAL:HG23	1:A:698:VAL:HA	2	0.26
(2,794)	1:A:701:VAL:H	1:A:698:VAL:HA	4	0.26
(2,794)	1:A:701:VAL:H	1:A:698:VAL:HA	10	0.26
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD2	14	0.26
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD3	14	0.26
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD2	14	0.26
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD3	14	0.26
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD2	14	0.26
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD3	14	0.26
(2,751)	1:A:689:VAL:HG21	1:A:685:PHE:HD1	8	0.26
(2,751)	1:A:689:VAL:HG21	1:A:685:PHE:HD2	8	0.26
(2,751)	1:A:689:VAL:HG22	1:A:685:PHE:HD1	8	0.26
(2,751)	1:A:689:VAL:HG22	1:A:685:PHE:HD2	8	0.26
(2,751)	1:A:689:VAL:HG23	1:A:685:PHE:HD1	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,751)	1:A:689:VAL:HG23	1:A:685:PHE:HD2	8	0.26
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	12	0.26
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	12	0.26
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	12	0.26
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	12	0.26
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	12	0.26
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	12	0.26
(2,721)	1:A:682:ILE:HD11	1:A:681:TYR:H	8	0.26
(2,721)	1:A:682:ILE:HD12	1:A:681:TYR:H	8	0.26
(2,721)	1:A:682:ILE:HD13	1:A:681:TYR:H	8	0.26
(2,719)	1:A:682:ILE:HG21	1:A:685:PHE:HB2	3	0.26
(2,719)	1:A:682:ILE:HG21	1:A:685:PHE:HB3	3	0.26
(2,719)	1:A:682:ILE:HG22	1:A:685:PHE:HB2	3	0.26
(2,719)	1:A:682:ILE:HG22	1:A:685:PHE:HB3	3	0.26
(2,719)	1:A:682:ILE:HG23	1:A:685:PHE:HB2	3	0.26
(2,719)	1:A:682:ILE:HG23	1:A:685:PHE:HB3	3	0.26
(2,701)	1:A:676:THR:HG21	1:A:666:TRP:HZ3	5	0.26
(2,701)	1:A:676:THR:HG22	1:A:666:TRP:HZ3	5	0.26
(2,701)	1:A:676:THR:HG23	1:A:666:TRP:HZ3	5	0.26
(2,653)	1:A:665:LYS:H	1:A:662:GLU:HA	14	0.26
(2,653)	1:A:665:LYS:H	1:A:662:GLU:HA	15	0.26
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD11	1	0.26
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD12	1	0.26
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD13	1	0.26
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD21	1	0.26
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD22	1	0.26
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD23	1	0.26
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB2	2	0.26
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB3	2	0.26
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB2	2	0.26
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB3	2	0.26
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB2	2	0.26
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB3	2	0.26
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB2	15	0.26
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB3	15	0.26
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB2	15	0.26
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB3	15	0.26
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB2	15	0.26
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB3	15	0.26
(2,618)	1:B:797:TRP:H	1:B:796:TRP:HD1	11	0.26
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD11	10	0.26
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD12	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD13	10	0.26
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD1	5	0.26
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD2	5	0.26
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD1	5	0.26
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD2	5	0.26
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD1	5	0.26
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD2	5	0.26
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD1	12	0.26
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD2	12	0.26
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD1	12	0.26
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD2	12	0.26
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD1	12	0.26
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD2	12	0.26
(2,565)	1:B:779:THR:H	1:B:776:LEU:HA	7	0.26
(2,565)	1:B:779:THR:H	1:B:776:LEU:HA	13	0.26
(2,559)	1:B:778:VAL:H	1:B:775:LEU:HA	12	0.26
(2,545)	1:B:775:LEU:HD11	1:B:772:ARG:HA	15	0.26
(2,545)	1:B:775:LEU:HD12	1:B:772:ARG:HA	15	0.26
(2,545)	1:B:775:LEU:HD13	1:B:772:ARG:HA	15	0.26
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH21	5	0.26
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH22	5	0.26
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH21	5	0.26
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH22	5	0.26
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH21	5	0.26
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH22	5	0.26
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH21	8	0.26
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH22	8	0.26
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH21	8	0.26
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH22	8	0.26
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH21	8	0.26
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH22	8	0.26
(2,518)	1:B:763:LEU:HD11	1:B:759:ASP:HA	6	0.26
(2,518)	1:B:763:LEU:HD12	1:B:759:ASP:HA	6	0.26
(2,518)	1:B:763:LEU:HD13	1:B:759:ASP:HA	6	0.26
(2,482)	1:B:749:VAL:H	1:B:746:ILE:HA	12	0.26
(2,482)	1:B:749:VAL:H	1:B:746:ILE:HA	15	0.26
(2,472)	1:B:746:ILE:HG21	1:B:750:ASN:HD21	11	0.26
(2,472)	1:B:746:ILE:HG22	1:B:750:ASN:HD21	11	0.26
(2,472)	1:B:746:ILE:HG23	1:B:750:ASN:HD21	11	0.26
(2,472)	1:B:746:ILE:HG21	1:B:750:ASN:HD21	13	0.26
(2,472)	1:B:746:ILE:HG22	1:B:750:ASN:HD21	13	0.26
(2,472)	1:B:746:ILE:HG23	1:B:750:ASN:HD21	13	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB2	9	0.26
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB3	9	0.26
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB2	9	0.26
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB3	9	0.26
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB2	9	0.26
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB3	9	0.26
(2,414)	1:B:707:ARG:H	1:B:704:LEU:HA	11	0.26
(2,393)	1:B:704:LEU:HD11	1:B:707:ARG:HD2	12	0.26
(2,393)	1:B:704:LEU:HD11	1:B:707:ARG:HD3	12	0.26
(2,393)	1:B:704:LEU:HD12	1:B:707:ARG:HD2	12	0.26
(2,393)	1:B:704:LEU:HD12	1:B:707:ARG:HD3	12	0.26
(2,393)	1:B:704:LEU:HD13	1:B:707:ARG:HD2	12	0.26
(2,393)	1:B:704:LEU:HD13	1:B:707:ARG:HD3	12	0.26
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB2	2	0.26
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB3	2	0.26
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB2	2	0.26
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB3	2	0.26
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB2	2	0.26
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB3	2	0.26
(2,296)	1:B:682:ILE:HD11	1:B:681:TYR:H	3	0.26
(2,296)	1:B:682:ILE:HD12	1:B:681:TYR:H	3	0.26
(2,296)	1:B:682:ILE:HD13	1:B:681:TYR:H	3	0.26
(2,234)	1:B:666:TRP:H	1:B:663:LEU:HA	10	0.26
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD11	13	0.26
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD12	13	0.26
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD13	13	0.26
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD11	13	0.26
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD12	13	0.26
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD13	13	0.26
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG12	4	0.26
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG13	4	0.26
(2,192)	1:A:816:ASN:H	1:A:831:GLU:HG2	11	0.26
(2,192)	1:A:816:ASN:H	1:A:831:GLU:HG3	11	0.26
(2,191)	1:A:816:ASN:H	1:A:831:GLU:HG2	11	0.26
(2,191)	1:A:816:ASN:H	1:A:831:GLU:HG3	11	0.26
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG2	5	0.26
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG3	5	0.26
(2,183)	1:A:806:GLU:H	1:B:772:ARG:HE	12	0.26
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG2	6	0.26
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG3	6	0.26
(2,1465)	1:A:796:TRP:HE1	1:A:796:TRP:H	7	0.26
(2,1465)	1:A:796:TRP:HE1	1:A:796:TRP:H	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1465)	1:A:796:TRP:HE1	1:A:796:TRP:H	15	0.26
(2,1457)	1:A:785:LEU:HD21	1:A:782:VAL:HA	6	0.26
(2,1457)	1:A:785:LEU:HD22	1:A:782:VAL:HA	6	0.26
(2,1457)	1:A:785:LEU:HD23	1:A:782:VAL:HA	6	0.26
(2,1431)	1:A:782:VAL:H	1:A:779:THR:HA	6	0.26
(2,1431)	1:A:782:VAL:H	1:A:779:THR:HA	11	0.26
(2,1430)	1:A:781:ILE:HG21	1:A:778:VAL:HA	11	0.26
(2,1430)	1:A:781:ILE:HG22	1:A:778:VAL:HA	11	0.26
(2,1430)	1:A:781:ILE:HG23	1:A:778:VAL:HA	11	0.26
(2,1425)	1:A:781:ILE:H	1:A:778:VAL:HA	3	0.26
(2,141)	1:B:771:LEU:H	1:A:806:GLU:HB2	12	0.26
(2,141)	1:B:771:LEU:H	1:A:806:GLU:HB3	12	0.26
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	6	0.26
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	6	0.26
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	6	0.26
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	6	0.26
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	6	0.26
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	6	0.26
(2,1223)	1:A:701:VAL:HG21	1:A:698:VAL:HA	2	0.26
(2,1223)	1:A:701:VAL:HG22	1:A:698:VAL:HA	2	0.26
(2,1223)	1:A:701:VAL:HG23	1:A:698:VAL:HA	2	0.26
(2,1219)	1:A:701:VAL:H	1:A:698:VAL:HA	4	0.26
(2,1219)	1:A:701:VAL:H	1:A:698:VAL:HA	10	0.26
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB2	12	0.26
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB3	12	0.26
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB2	12	0.26
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB3	12	0.26
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB2	12	0.26
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB3	12	0.26
(2,1176)	1:A:689:VAL:HG21	1:A:685:PHE:HD1	8	0.26
(2,1176)	1:A:689:VAL:HG21	1:A:685:PHE:HD2	8	0.26
(2,1176)	1:A:689:VAL:HG22	1:A:685:PHE:HD1	8	0.26
(2,1176)	1:A:689:VAL:HG22	1:A:685:PHE:HD2	8	0.26
(2,1176)	1:A:689:VAL:HG23	1:A:685:PHE:HD1	8	0.26
(2,1176)	1:A:689:VAL:HG23	1:A:685:PHE:HD2	8	0.26
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	12	0.26
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	12	0.26
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	12	0.26
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	12	0.26
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	12	0.26
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	12	0.26
(2,1146)	1:A:682:ILE:HD11	1:A:681:TYR:H	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1146)	1:A:682:ILE:HD12	1:A:681:TYR:H	8	0.26
(2,1146)	1:A:682:ILE:HD13	1:A:681:TYR:H	8	0.26
(2,1144)	1:A:682:ILE:HG21	1:A:685:PHE:HB2	3	0.26
(2,1144)	1:A:682:ILE:HG21	1:A:685:PHE:HB3	3	0.26
(2,1144)	1:A:682:ILE:HG22	1:A:685:PHE:HB2	3	0.26
(2,1144)	1:A:682:ILE:HG22	1:A:685:PHE:HB3	3	0.26
(2,1144)	1:A:682:ILE:HG23	1:A:685:PHE:HB2	3	0.26
(2,1144)	1:A:682:ILE:HG23	1:A:685:PHE:HB3	3	0.26
(2,1126)	1:A:676:THR:HG21	1:A:666:TRP:HZ3	5	0.26
(2,1126)	1:A:676:THR:HG22	1:A:666:TRP:HZ3	5	0.26
(2,1126)	1:A:676:THR:HG23	1:A:666:TRP:HZ3	5	0.26
(2,1078)	1:A:665:LYS:H	1:A:662:GLU:HA	14	0.26
(2,1078)	1:A:665:LYS:H	1:A:662:GLU:HA	15	0.26
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG2	6	0.26
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG3	6	0.26
(2,1040)	1:A:796:TRP:HE1	1:A:796:TRP:H	7	0.26
(2,1040)	1:A:796:TRP:HE1	1:A:796:TRP:H	9	0.26
(2,1040)	1:A:796:TRP:HE1	1:A:796:TRP:H	15	0.26
(2,1032)	1:A:785:LEU:HD21	1:A:782:VAL:HA	6	0.26
(2,1032)	1:A:785:LEU:HD22	1:A:782:VAL:HA	6	0.26
(2,1032)	1:A:785:LEU:HD23	1:A:782:VAL:HA	6	0.26
(2,1006)	1:A:782:VAL:H	1:A:779:THR:HA	6	0.26
(2,1006)	1:A:782:VAL:H	1:A:779:THR:HA	11	0.26
(2,1005)	1:A:781:ILE:HG21	1:A:778:VAL:HA	11	0.26
(2,1005)	1:A:781:ILE:HG22	1:A:778:VAL:HA	11	0.26
(2,1005)	1:A:781:ILE:HG23	1:A:778:VAL:HA	11	0.26
(2,1000)	1:A:781:ILE:H	1:A:778:VAL:HA	3	0.26
(1,95)	1:B:794:LYS:O	1:B:798:ASN:H	10	0.26
(1,92)	1:B:792:ALA:O	1:B:796:TRP:N	11	0.26
(1,9)	1:B:794:LYS:O	1:B:798:ASN:H	10	0.26
(1,6)	1:B:792:ALA:O	1:B:796:TRP:N	11	0.26
(1,181)	1:B:794:LYS:O	1:B:798:ASN:H	10	0.26
(1,178)	1:B:792:ALA:O	1:B:796:TRP:N	11	0.26
(2,990)	1:A:779:THR:H	1:A:776:LEU:HA	13	0.25
(2,989)	1:A:778:VAL:HG21	1:A:775:LEU:HA	7	0.25
(2,989)	1:A:778:VAL:HG22	1:A:775:LEU:HA	7	0.25
(2,989)	1:A:778:VAL:HG23	1:A:775:LEU:HA	7	0.25
(2,965)	1:A:775:LEU:H	1:A:772:ARG:HA	6	0.25
(2,956)	1:A:773:ASP:H	1:A:770:ARG:HD2	6	0.25
(2,956)	1:A:773:ASP:H	1:A:770:ARG:HD3	6	0.25
(2,951)	1:A:771:LEU:HD11	1:A:768:TYR:HE1	4	0.25
(2,951)	1:A:771:LEU:HD11	1:A:768:TYR:HE2	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,951)	1:A:771:LEU:HD12	1:A:768:TYR:HE1	4	0.25
(2,951)	1:A:771:LEU:HD12	1:A:768:TYR:HE2	4	0.25
(2,951)	1:A:771:LEU:HD13	1:A:768:TYR:HE1	4	0.25
(2,951)	1:A:771:LEU:HD13	1:A:768:TYR:HE2	4	0.25
(2,947)	1:A:764:SER:H	1:A:761:ARG:HA	1	0.25
(2,940)	1:A:760:LEU:HD11	1:A:757:TRP:HA	9	0.25
(2,940)	1:A:760:LEU:HD12	1:A:757:TRP:HA	9	0.25
(2,940)	1:A:760:LEU:HD13	1:A:757:TRP:HA	9	0.25
(2,940)	1:A:760:LEU:HD11	1:A:757:TRP:HA	14	0.25
(2,940)	1:A:760:LEU:HD12	1:A:757:TRP:HA	14	0.25
(2,940)	1:A:760:LEU:HD13	1:A:757:TRP:HA	14	0.25
(2,898)	1:A:746:ILE:HG21	1:A:750:ASN:HD22	4	0.25
(2,898)	1:A:746:ILE:HG22	1:A:750:ASN:HD22	4	0.25
(2,898)	1:A:746:ILE:HG23	1:A:750:ASN:HD22	4	0.25
(2,864)	1:A:710:GLN:H	1:A:708:VAL:HA	2	0.25
(2,839)	1:A:707:ARG:H	1:A:704:LEU:HA	2	0.25
(2,711)	1:A:678:TRP:HE1	1:A:682:ILE:H	4	0.25
(2,632)	1:B:852:GLU:H	1:B:848:ARG:HG2	12	0.25
(2,632)	1:B:852:GLU:H	1:B:848:ARG:HG3	12	0.25
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD2	10	0.25
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD3	10	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD11	5	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD12	5	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD13	5	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD21	5	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD22	5	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD23	5	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD11	6	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD12	6	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD13	6	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD21	6	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD22	6	0.25
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD23	6	0.25
(2,601)	1:B:785:LEU:H	1:B:782:VAL:HA	7	0.25
(2,581)	1:B:782:VAL:H	1:B:779:THR:HA	1	0.25
(2,565)	1:B:779:THR:H	1:B:776:LEU:HA	5	0.25
(2,559)	1:B:778:VAL:H	1:B:775:LEU:HA	11	0.25
(2,558)	1:B:777:ILE:HG21	1:B:780:ARG:HD2	10	0.25
(2,558)	1:B:777:ILE:HG21	1:B:780:ARG:HD3	10	0.25
(2,558)	1:B:777:ILE:HG22	1:B:780:ARG:HD2	10	0.25
(2,558)	1:B:777:ILE:HG22	1:B:780:ARG:HD3	10	0.25
(2,558)	1:B:777:ILE:HG23	1:B:780:ARG:HD2	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,558)	1:B:777:ILE:HG23	1:B:780:ARG:HD3	10	0.25
(2,540)	1:B:775:LEU:H	1:B:772:ARG:HA	4	0.25
(2,540)	1:B:775:LEU:H	1:B:772:ARG:HA	14	0.25
(2,522)	1:B:764:SER:H	1:B:761:ARG:HA	15	0.25
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB2	1	0.25
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB3	1	0.25
(2,482)	1:B:749:VAL:H	1:B:746:ILE:HA	6	0.25
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD2	8	0.25
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD3	8	0.25
(2,472)	1:B:746:ILE:HG21	1:B:750:ASN:HD21	2	0.25
(2,472)	1:B:746:ILE:HG22	1:B:750:ASN:HD21	2	0.25
(2,472)	1:B:746:ILE:HG23	1:B:750:ASN:HD21	2	0.25
(2,470)	1:B:746:ILE:HD11	1:B:743:ASP:HA	5	0.25
(2,470)	1:B:746:ILE:HD12	1:B:743:ASP:HA	5	0.25
(2,470)	1:B:746:ILE:HD13	1:B:743:ASP:HA	5	0.25
(2,438)	1:B:709:ARG:HE	1:B:709:ARG:H	13	0.25
(2,428)	1:B:708:VAL:HG11	1:B:705:VAL:HA	15	0.25
(2,428)	1:B:708:VAL:HG12	1:B:705:VAL:HA	15	0.25
(2,428)	1:B:708:VAL:HG13	1:B:705:VAL:HA	15	0.25
(2,421)	1:B:707:ARG:H	1:B:707:ARG:HD2	2	0.25
(2,421)	1:B:707:ARG:H	1:B:707:ARG:HD3	2	0.25
(2,401)	1:B:705:VAL:HG11	1:B:702:LEU:HA	9	0.25
(2,401)	1:B:705:VAL:HG12	1:B:702:LEU:HA	9	0.25
(2,401)	1:B:705:VAL:HG13	1:B:702:LEU:HA	9	0.25
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD2	10	0.25
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD3	10	0.25
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD2	10	0.25
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD3	10	0.25
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD2	10	0.25
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD3	10	0.25
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD11	3	0.25
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD12	3	0.25
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD13	3	0.25
(2,224)	1:B:664:ASP:H	1:B:663:LEU:HA	11	0.25
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ1	1	0.25
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ2	1	0.25
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ3	1	0.25
(2,183)	1:A:806:GLU:H	1:B:772:ARG:HE	10	0.25
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG2	5	0.25
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG3	5	0.25
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	9	0.25
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	9	0.25
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	9	0.25
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	9	0.25
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	9	0.25
(2,1449)	1:A:784:LEU:HD11	1:A:787:ARG:HD2	7	0.25
(2,1449)	1:A:784:LEU:HD11	1:A:787:ARG:HD3	7	0.25
(2,1449)	1:A:784:LEU:HD12	1:A:787:ARG:HD2	7	0.25
(2,1449)	1:A:784:LEU:HD12	1:A:787:ARG:HD3	7	0.25
(2,1449)	1:A:784:LEU:HD13	1:A:787:ARG:HD2	7	0.25
(2,1449)	1:A:784:LEU:HD13	1:A:787:ARG:HD3	7	0.25
(2,1431)	1:A:782:VAL:H	1:A:779:THR:HA	13	0.25
(2,1430)	1:A:781:ILE:HG21	1:A:778:VAL:HA	6	0.25
(2,1430)	1:A:781:ILE:HG22	1:A:778:VAL:HA	6	0.25
(2,1430)	1:A:781:ILE:HG23	1:A:778:VAL:HA	6	0.25
(2,1415)	1:A:779:THR:H	1:A:776:LEU:HA	13	0.25
(2,1414)	1:A:778:VAL:HG21	1:A:775:LEU:HA	7	0.25
(2,1414)	1:A:778:VAL:HG22	1:A:775:LEU:HA	7	0.25
(2,1414)	1:A:778:VAL:HG23	1:A:775:LEU:HA	7	0.25
(2,1390)	1:A:775:LEU:H	1:A:772:ARG:HA	6	0.25
(2,1381)	1:A:773:ASP:H	1:A:770:ARG:HD2	6	0.25
(2,1381)	1:A:773:ASP:H	1:A:770:ARG:HD3	6	0.25
(2,1376)	1:A:771:LEU:HD11	1:A:768:TYR:HE1	4	0.25
(2,1376)	1:A:771:LEU:HD11	1:A:768:TYR:HE2	4	0.25
(2,1376)	1:A:771:LEU:HD12	1:A:768:TYR:HE1	4	0.25
(2,1376)	1:A:771:LEU:HD12	1:A:768:TYR:HE2	4	0.25
(2,1376)	1:A:771:LEU:HD13	1:A:768:TYR:HE1	4	0.25
(2,1376)	1:A:771:LEU:HD13	1:A:768:TYR:HE2	4	0.25
(2,1372)	1:A:764:SER:H	1:A:761:ARG:HA	1	0.25
(2,1365)	1:A:760:LEU:HD11	1:A:757:TRP:HA	9	0.25
(2,1365)	1:A:760:LEU:HD12	1:A:757:TRP:HA	9	0.25
(2,1365)	1:A:760:LEU:HD13	1:A:757:TRP:HA	9	0.25
(2,1365)	1:A:760:LEU:HD11	1:A:757:TRP:HA	14	0.25
(2,1365)	1:A:760:LEU:HD12	1:A:757:TRP:HA	14	0.25
(2,1365)	1:A:760:LEU:HD13	1:A:757:TRP:HA	14	0.25
(2,1323)	1:A:746:ILE:HG21	1:A:750:ASN:HD22	4	0.25
(2,1323)	1:A:746:ILE:HG22	1:A:750:ASN:HD22	4	0.25
(2,1323)	1:A:746:ILE:HG23	1:A:750:ASN:HD22	4	0.25
(2,1289)	1:A:710:GLN:H	1:A:708:VAL:HA	2	0.25
(2,1264)	1:A:707:ARG:H	1:A:704:LEU:HA	2	0.25
(2,126)	1:A:785:LEU:HD21	1:B:749:VAL:HB	12	0.25
(2,126)	1:A:785:LEU:HD22	1:B:749:VAL:HB	12	0.25
(2,126)	1:A:785:LEU:HD23	1:B:749:VAL:HB	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1136)	1:A:678:TRP:HE1	1:A:682:ILE:H	4	0.25
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG2	5	0.25
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG3	5	0.25
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	9	0.25
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	9	0.25
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	9	0.25
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	9	0.25
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	9	0.25
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	9	0.25
(2,1024)	1:A:784:LEU:HD11	1:A:787:ARG:HD2	7	0.25
(2,1024)	1:A:784:LEU:HD11	1:A:787:ARG:HD3	7	0.25
(2,1024)	1:A:784:LEU:HD12	1:A:787:ARG:HD2	7	0.25
(2,1024)	1:A:784:LEU:HD12	1:A:787:ARG:HD3	7	0.25
(2,1024)	1:A:784:LEU:HD13	1:A:787:ARG:HD2	7	0.25
(2,1024)	1:A:784:LEU:HD13	1:A:787:ARG:HD3	7	0.25
(2,1006)	1:A:782:VAL:H	1:A:779:THR:HA	13	0.25
(2,1005)	1:A:781:ILE:HG21	1:A:778:VAL:HA	6	0.25
(2,1005)	1:A:781:ILE:HG22	1:A:778:VAL:HA	6	0.25
(2,1005)	1:A:781:ILE:HG23	1:A:778:VAL:HA	6	0.25
(1,88)	1:B:790:TRP:O	1:B:794:LYS:N	1	0.25
(1,55)	1:B:827:ASP:O	1:B:831:GLU:H	6	0.25
(1,227)	1:B:827:ASP:O	1:B:831:GLU:H	6	0.25
(1,2)	1:B:790:TRP:O	1:B:794:LYS:N	1	0.25
(1,174)	1:B:790:TRP:O	1:B:794:LYS:N	1	0.25
(1,141)	1:B:827:ASP:O	1:B:831:GLU:H	6	0.25
(2,984)	1:A:778:VAL:H	1:A:775:LEU:HA	3	0.24
(2,940)	1:A:760:LEU:HD11	1:A:757:TRP:HA	11	0.24
(2,940)	1:A:760:LEU:HD12	1:A:757:TRP:HA	11	0.24
(2,940)	1:A:760:LEU:HD13	1:A:757:TRP:HA	11	0.24
(2,916)	1:A:753:LEU:HD11	1:A:757:TRP:HB2	6	0.24
(2,916)	1:A:753:LEU:HD11	1:A:757:TRP:HB3	6	0.24
(2,916)	1:A:753:LEU:HD12	1:A:757:TRP:HB2	6	0.24
(2,916)	1:A:753:LEU:HD12	1:A:757:TRP:HB3	6	0.24
(2,916)	1:A:753:LEU:HD13	1:A:757:TRP:HB2	6	0.24
(2,916)	1:A:753:LEU:HD13	1:A:757:TRP:HB3	6	0.24
(2,907)	1:A:749:VAL:H	1:A:746:ILE:HA	11	0.24
(2,857)	1:A:709:ARG:H	1:A:707:ARG:H	10	0.24
(2,853)	1:A:708:VAL:HG11	1:A:705:VAL:HA	11	0.24
(2,853)	1:A:708:VAL:HG12	1:A:705:VAL:HA	11	0.24
(2,853)	1:A:708:VAL:HG13	1:A:705:VAL:HA	11	0.24
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD2	2	0.24
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD3	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	3	0.24
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	3	0.24
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	3	0.24
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	3	0.24
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	3	0.24
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	3	0.24
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	6	0.24
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	6	0.24
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	6	0.24
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	6	0.24
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	6	0.24
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	6	0.24
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	7	0.24
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	7	0.24
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	7	0.24
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	7	0.24
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	7	0.24
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	7	0.24
(2,670)	1:A:667:ALA:H	1:A:666:TRP:HD1	8	0.24
(2,670)	1:A:667:ALA:H	1:A:666:TRP:HD1	10	0.24
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB1	15	0.24
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB2	15	0.24
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB3	15	0.24
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB1	15	0.24
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB2	15	0.24
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB3	15	0.24
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB1	15	0.24
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB2	15	0.24
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB3	15	0.24
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD11	8	0.24
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD12	8	0.24
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD13	8	0.24
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB2	8	0.24
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB3	8	0.24
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB2	3	0.24
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB3	3	0.24
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB2	3	0.24
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB3	3	0.24
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB2	3	0.24
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB3	3	0.24
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD11	9	0.24
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD12	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD13	9	0.24
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD21	9	0.24
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD22	9	0.24
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD23	9	0.24
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD1	7	0.24
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD2	7	0.24
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD1	7	0.24
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD2	7	0.24
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD1	7	0.24
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD2	7	0.24
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD2	3	0.24
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD3	3	0.24
(2,565)	1:B:779:THR:H	1:B:776:LEU:HA	1	0.24
(2,531)	1:B:773:ASP:H	1:B:770:ARG:HD2	12	0.24
(2,531)	1:B:773:ASP:H	1:B:770:ARG:HD3	12	0.24
(2,522)	1:B:764:SER:H	1:B:761:ARG:HA	14	0.24
(2,52)	1:B:696:ARG:H	1:A:693:ILE:HD11	8	0.24
(2,52)	1:B:696:ARG:H	1:A:693:ILE:HD12	8	0.24
(2,52)	1:B:696:ARG:H	1:A:693:ILE:HD13	8	0.24
(2,482)	1:B:749:VAL:H	1:B:746:ILE:HA	8	0.24
(2,472)	1:B:746:ILE:HG21	1:B:750:ASN:HD21	14	0.24
(2,472)	1:B:746:ILE:HG22	1:B:750:ASN:HD21	14	0.24
(2,472)	1:B:746:ILE:HG23	1:B:750:ASN:HD21	14	0.24
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB2	5	0.24
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB3	5	0.24
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB2	5	0.24
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB3	5	0.24
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB2	5	0.24
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB3	5	0.24
(2,369)	1:B:701:VAL:H	1:B:698:VAL:HA	8	0.24
(2,357)	1:B:698:VAL:HG11	1:B:699:PHE:HD1	11	0.24
(2,357)	1:B:698:VAL:HG11	1:B:699:PHE:HD2	11	0.24
(2,357)	1:B:698:VAL:HG12	1:B:699:PHE:HD1	11	0.24
(2,357)	1:B:698:VAL:HG12	1:B:699:PHE:HD2	11	0.24
(2,357)	1:B:698:VAL:HG13	1:B:699:PHE:HD1	11	0.24
(2,357)	1:B:698:VAL:HG13	1:B:699:PHE:HD2	11	0.24
(2,355)	1:B:698:VAL:HG11	1:B:695:LEU:HA	8	0.24
(2,355)	1:B:698:VAL:HG12	1:B:695:LEU:HA	8	0.24
(2,355)	1:B:698:VAL:HG13	1:B:695:LEU:HA	8	0.24
(2,355)	1:B:698:VAL:HG11	1:B:695:LEU:HA	10	0.24
(2,355)	1:B:698:VAL:HG12	1:B:695:LEU:HA	10	0.24
(2,355)	1:B:698:VAL:HG13	1:B:695:LEU:HA	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD11	4	0.24
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD12	4	0.24
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD13	4	0.24
(2,272)	1:B:674:ASP:H	1:B:677:ASN:H	8	0.24
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD11	12	0.24
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD12	12	0.24
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD13	12	0.24
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD11	12	0.24
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD12	12	0.24
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD13	12	0.24
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD2	10	0.24
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD3	10	0.24
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB2	10	0.24
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB3	10	0.24
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	2	0.24
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	2	0.24
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	2	0.24
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	2	0.24
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG2	11	0.24
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG3	11	0.24
(2,1477)	1:A:819:ALA:H	1:A:820:ILE:HD11	5	0.24
(2,1477)	1:A:819:ALA:H	1:A:820:ILE:HD12	5	0.24
(2,1477)	1:A:819:ALA:H	1:A:820:ILE:HD13	5	0.24
(2,1465)	1:A:796:TRP:HE1	1:A:796:TRP:H	14	0.24
(2,1464)	1:A:793:LEU:H	1:A:790:TRP:HE3	13	0.24
(2,1430)	1:A:781:ILE:HG21	1:A:778:VAL:HA	2	0.24
(2,1430)	1:A:781:ILE:HG22	1:A:778:VAL:HA	2	0.24
(2,1430)	1:A:781:ILE:HG23	1:A:778:VAL:HA	2	0.24
(2,1430)	1:A:781:ILE:HG21	1:A:778:VAL:HA	8	0.24
(2,1430)	1:A:781:ILE:HG22	1:A:778:VAL:HA	8	0.24
(2,1430)	1:A:781:ILE:HG23	1:A:778:VAL:HA	8	0.24
(2,1430)	1:A:781:ILE:HG21	1:A:778:VAL:HA	10	0.24
(2,1430)	1:A:781:ILE:HG22	1:A:778:VAL:HA	10	0.24
(2,1430)	1:A:781:ILE:HG23	1:A:778:VAL:HA	10	0.24
(2,1409)	1:A:778:VAL:H	1:A:775:LEU:HA	3	0.24
(2,1365)	1:A:760:LEU:HD11	1:A:757:TRP:HA	11	0.24
(2,1365)	1:A:760:LEU:HD12	1:A:757:TRP:HA	11	0.24
(2,1365)	1:A:760:LEU:HD13	1:A:757:TRP:HA	11	0.24
(2,1341)	1:A:753:LEU:HD11	1:A:757:TRP:HB2	6	0.24
(2,1341)	1:A:753:LEU:HD11	1:A:757:TRP:HB3	6	0.24
(2,1341)	1:A:753:LEU:HD12	1:A:757:TRP:HB2	6	0.24
(2,1341)	1:A:753:LEU:HD12	1:A:757:TRP:HB3	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1341)	1:A:753:LEU:HD13	1:A:757:TRP:HB2	6	0.24
(2,1341)	1:A:753:LEU:HD13	1:A:757:TRP:HB3	6	0.24
(2,1332)	1:A:749:VAL:H	1:A:746:ILE:HA	11	0.24
(2,1282)	1:A:709:ARG:H	1:A:707:ARG:H	10	0.24
(2,1278)	1:A:708:VAL:HG11	1:A:705:VAL:HA	11	0.24
(2,1278)	1:A:708:VAL:HG12	1:A:705:VAL:HA	11	0.24
(2,1278)	1:A:708:VAL:HG13	1:A:705:VAL:HA	11	0.24
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD2	2	0.24
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD3	2	0.24
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	3	0.24
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	3	0.24
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	3	0.24
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	3	0.24
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	3	0.24
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	3	0.24
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	6	0.24
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	6	0.24
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	6	0.24
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	6	0.24
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	6	0.24
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	6	0.24
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	7	0.24
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	7	0.24
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	7	0.24
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	7	0.24
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	7	0.24
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	7	0.24
(2,1095)	1:A:667:ALA:H	1:A:666:TRP:HD1	8	0.24
(2,1095)	1:A:667:ALA:H	1:A:666:TRP:HD1	10	0.24
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG2	11	0.24
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG3	11	0.24
(2,1052)	1:A:819:ALA:H	1:A:820:ILE:HD11	5	0.24
(2,1052)	1:A:819:ALA:H	1:A:820:ILE:HD12	5	0.24
(2,1052)	1:A:819:ALA:H	1:A:820:ILE:HD13	5	0.24
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD2	4	0.24
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD3	4	0.24
(2,1040)	1:A:796:TRP:HE1	1:A:796:TRP:H	14	0.24
(2,1039)	1:A:793:LEU:H	1:A:790:TRP:HE3	13	0.24
(2,1005)	1:A:781:ILE:HG21	1:A:778:VAL:HA	2	0.24
(2,1005)	1:A:781:ILE:HG22	1:A:778:VAL:HA	2	0.24
(2,1005)	1:A:781:ILE:HG23	1:A:778:VAL:HA	2	0.24
(2,1005)	1:A:781:ILE:HG21	1:A:778:VAL:HA	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1005)	1:A:781:ILE:HG22	1:A:778:VAL:HA	8	0.24
(2,1005)	1:A:781:ILE:HG23	1:A:778:VAL:HA	8	0.24
(2,1005)	1:A:781:ILE:HG21	1:A:778:VAL:HA	10	0.24
(2,1005)	1:A:781:ILE:HG22	1:A:778:VAL:HA	10	0.24
(2,1005)	1:A:781:ILE:HG23	1:A:778:VAL:HA	10	0.24
(1,95)	1:B:794:LYS:O	1:B:798:ASN:H	13	0.24
(1,9)	1:B:794:LYS:O	1:B:798:ASN:H	13	0.24
(1,23)	1:B:801:GLN:O	1:B:805:GLN:H	4	0.24
(1,195)	1:B:801:GLN:O	1:B:805:GLN:H	4	0.24
(1,181)	1:B:794:LYS:O	1:B:798:ASN:H	13	0.24
(1,109)	1:B:801:GLN:O	1:B:805:GLN:H	4	0.24
(2,990)	1:A:779:THR:H	1:A:776:LEU:HA	7	0.23
(2,989)	1:A:778:VAL:HG21	1:A:775:LEU:HA	10	0.23
(2,989)	1:A:778:VAL:HG22	1:A:775:LEU:HA	10	0.23
(2,989)	1:A:778:VAL:HG23	1:A:775:LEU:HA	10	0.23
(2,982)	1:A:777:ILE:HD11	1:A:774:LEU:HA	11	0.23
(2,982)	1:A:777:ILE:HD12	1:A:774:LEU:HA	11	0.23
(2,982)	1:A:777:ILE:HD13	1:A:774:LEU:HA	11	0.23
(2,952)	1:A:771:LEU:HD21	1:A:772:ARG:HH21	12	0.23
(2,952)	1:A:771:LEU:HD21	1:A:772:ARG:HH22	12	0.23
(2,952)	1:A:771:LEU:HD22	1:A:772:ARG:HH21	12	0.23
(2,952)	1:A:771:LEU:HD22	1:A:772:ARG:HH22	12	0.23
(2,952)	1:A:771:LEU:HD23	1:A:772:ARG:HH21	12	0.23
(2,952)	1:A:771:LEU:HD23	1:A:772:ARG:HH22	12	0.23
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	2	0.23
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	2	0.23
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	2	0.23
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	2	0.23
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	2	0.23
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	2	0.23
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	11	0.23
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	11	0.23
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	11	0.23
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	11	0.23
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	11	0.23
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	11	0.23
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB2	8	0.23
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB3	8	0.23
(2,863)	1:A:709:ARG:HE	1:A:709:ARG:H	14	0.23
(2,857)	1:A:709:ARG:H	1:A:707:ARG:H	13	0.23
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB2	10	0.23
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB3	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB2	10	0.23
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB3	10	0.23
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB2	10	0.23
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB3	10	0.23
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB2	15	0.23
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB3	15	0.23
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB2	15	0.23
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB3	15	0.23
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB2	15	0.23
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB3	15	0.23
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD2	8	0.23
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD3	8	0.23
(2,839)	1:A:707:ARG:H	1:A:704:LEU:HA	14	0.23
(2,794)	1:A:701:VAL:H	1:A:698:VAL:HA	1	0.23
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD2	10	0.23
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD3	10	0.23
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD2	10	0.23
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD3	10	0.23
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD2	10	0.23
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD3	10	0.23
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD2	13	0.23
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD3	13	0.23
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD2	13	0.23
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD3	13	0.23
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD2	13	0.23
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD3	13	0.23
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	1	0.23
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	1	0.23
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	1	0.23
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	1	0.23
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	1	0.23
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	1	0.23
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	14	0.23
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	14	0.23
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	14	0.23
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	14	0.23
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	14	0.23
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	14	0.23
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD11	12	0.23
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD12	12	0.23
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD13	12	0.23
(2,670)	1:A:667:ALA:H	1:A:666:TRP:HD1	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,670)	1:A:667:ALA:H	1:A:666:TRP:HD1	15	0.23
(2,649)	1:A:664:ASP:H	1:A:663:LEU:HA	9	0.23
(2,565)	1:B:779:THR:H	1:B:776:LEU:HA	14	0.23
(2,540)	1:B:775:LEU:H	1:B:772:ARG:HA	8	0.23
(2,536)	1:B:774:LEU:H	1:B:764:SER:HA	3	0.23
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD11	11	0.23
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD12	11	0.23
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD13	11	0.23
(2,519)	1:B:763:LEU:HD11	1:B:764:SER:HG	7	0.23
(2,519)	1:B:763:LEU:HD12	1:B:764:SER:HG	7	0.23
(2,519)	1:B:763:LEU:HD13	1:B:764:SER:HG	7	0.23
(2,515)	1:B:760:LEU:HD11	1:B:757:TRP:HA	4	0.23
(2,515)	1:B:760:LEU:HD12	1:B:757:TRP:HA	4	0.23
(2,515)	1:B:760:LEU:HD13	1:B:757:TRP:HA	4	0.23
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA2	10	0.23
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA3	10	0.23
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA2	10	0.23
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA3	10	0.23
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA2	10	0.23
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA3	10	0.23
(2,482)	1:B:749:VAL:H	1:B:746:ILE:HA	4	0.23
(2,437)	1:B:709:ARG:HE	1:B:705:VAL:HG11	13	0.23
(2,437)	1:B:709:ARG:HE	1:B:705:VAL:HG12	13	0.23
(2,437)	1:B:709:ARG:HE	1:B:705:VAL:HG13	13	0.23
(2,404)	1:B:705:VAL:HG21	1:B:701:VAL:HA	12	0.23
(2,404)	1:B:705:VAL:HG22	1:B:701:VAL:HA	12	0.23
(2,404)	1:B:705:VAL:HG23	1:B:701:VAL:HA	12	0.23
(2,390)	1:B:704:LEU:H	1:B:704:LEU:HB3	2	0.23
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB2	14	0.23
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB3	14	0.23
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB2	14	0.23
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB3	14	0.23
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB2	14	0.23
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB3	14	0.23
(2,369)	1:B:701:VAL:H	1:B:698:VAL:HA	7	0.23
(2,369)	1:B:701:VAL:H	1:B:698:VAL:HA	9	0.23
(2,369)	1:B:701:VAL:H	1:B:698:VAL:HA	15	0.23
(2,305)	1:B:684:ILE:HG21	1:B:685:PHE:HD1	12	0.23
(2,305)	1:B:684:ILE:HG21	1:B:685:PHE:HD2	12	0.23
(2,305)	1:B:684:ILE:HG22	1:B:685:PHE:HD1	12	0.23
(2,305)	1:B:684:ILE:HG22	1:B:685:PHE:HD2	12	0.23
(2,305)	1:B:684:ILE:HG23	1:B:685:PHE:HD1	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,305)	1:B:684:ILE:HG23	1:B:685:PHE:HD2	12	0.23
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB2	1	0.23
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB3	1	0.23
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB2	1	0.23
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB3	1	0.23
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB2	1	0.23
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB3	1	0.23
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD11	1	0.23
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD12	1	0.23
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD13	1	0.23
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD21	1	0.23
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD22	1	0.23
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD23	1	0.23
(2,242)	1:B:667:ALA:H	1:B:664:ASP:HA	10	0.23
(2,242)	1:B:667:ALA:H	1:B:664:ASP:HA	15	0.23
(2,241)	1:B:666:TRP:HE1	1:B:662:GLU:H	9	0.23
(2,224)	1:B:664:ASP:H	1:B:663:LEU:HA	8	0.23
(2,213)	1:A:839:ALA:H	1:A:808:LYS:HZ1	15	0.23
(2,213)	1:A:839:ALA:H	1:A:808:LYS:HZ2	15	0.23
(2,213)	1:A:839:ALA:H	1:A:808:LYS:HZ3	15	0.23
(2,212)	1:A:839:ALA:H	1:A:808:LYS:HZ1	15	0.23
(2,212)	1:A:839:ALA:H	1:A:808:LYS:HZ2	15	0.23
(2,212)	1:A:839:ALA:H	1:A:808:LYS:HZ3	15	0.23
(2,177)	1:A:803:TRP:HE1	1:B:764:SER:HG	8	0.23
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	4	0.23
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	4	0.23
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	4	0.23
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	4	0.23
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG12	10	0.23
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG13	10	0.23
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG12	11	0.23
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG13	11	0.23
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG12	10	0.23
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG13	10	0.23
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG12	11	0.23
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG13	11	0.23
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG12	7	0.23
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG13	7	0.23
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD2	4	0.23
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD3	4	0.23
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	10	0.23
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	10	0.23
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	10	0.23
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	10	0.23
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	10	0.23
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG12	2	0.23
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG13	2	0.23
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG12	10	0.23
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG13	10	0.23
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD2	5	0.23
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD3	5	0.23
(2,1415)	1:A:779:THR:H	1:A:776:LEU:HA	7	0.23
(2,1414)	1:A:778:VAL:HG21	1:A:775:LEU:HA	10	0.23
(2,1414)	1:A:778:VAL:HG22	1:A:775:LEU:HA	10	0.23
(2,1414)	1:A:778:VAL:HG23	1:A:775:LEU:HA	10	0.23
(2,1407)	1:A:777:ILE:HD11	1:A:774:LEU:HA	11	0.23
(2,1407)	1:A:777:ILE:HD12	1:A:774:LEU:HA	11	0.23
(2,1407)	1:A:777:ILE:HD13	1:A:774:LEU:HA	11	0.23
(2,1377)	1:A:771:LEU:HD21	1:A:772:ARG:HH21	12	0.23
(2,1377)	1:A:771:LEU:HD21	1:A:772:ARG:HH22	12	0.23
(2,1377)	1:A:771:LEU:HD22	1:A:772:ARG:HH21	12	0.23
(2,1377)	1:A:771:LEU:HD22	1:A:772:ARG:HH22	12	0.23
(2,1377)	1:A:771:LEU:HD23	1:A:772:ARG:HH21	12	0.23
(2,1377)	1:A:771:LEU:HD23	1:A:772:ARG:HH22	12	0.23
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	2	0.23
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	2	0.23
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	2	0.23
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	2	0.23
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	2	0.23
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	2	0.23
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	11	0.23
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	11	0.23
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	11	0.23
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	11	0.23
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	11	0.23
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	11	0.23
(2,1288)	1:A:709:ARG:HE	1:A:709:ARG:H	14	0.23
(2,1282)	1:A:709:ARG:H	1:A:707:ARG:H	13	0.23
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB2	10	0.23
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB3	10	0.23
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB2	10	0.23
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB3	10	0.23
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB2	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB3	10	0.23
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB2	15	0.23
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB3	15	0.23
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB2	15	0.23
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB3	15	0.23
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB2	15	0.23
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB3	15	0.23
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD2	8	0.23
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD3	8	0.23
(2,1264)	1:A:707:ARG:H	1:A:704:LEU:HA	14	0.23
(2,1219)	1:A:701:VAL:H	1:A:698:VAL:HA	1	0.23
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	1	0.23
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	1	0.23
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	1	0.23
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	1	0.23
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	1	0.23
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	1	0.23
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	14	0.23
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	14	0.23
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	14	0.23
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	14	0.23
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	14	0.23
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	14	0.23
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD11	12	0.23
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD12	12	0.23
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD13	12	0.23
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG21	10	0.23
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG22	10	0.23
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG23	10	0.23
(2,1095)	1:A:667:ALA:H	1:A:666:TRP:HD1	7	0.23
(2,1095)	1:A:667:ALA:H	1:A:666:TRP:HD1	15	0.23
(2,1074)	1:A:664:ASP:H	1:A:663:LEU:HA	9	0.23
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD2	4	0.23
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD3	4	0.23
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	10	0.23
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	10	0.23
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	10	0.23
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	10	0.23
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	10	0.23
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	10	0.23
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD2	5	0.23
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD3	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:B:799:LEU:O	1:B:803:TRP:N	9	0.23
(1,192)	1:B:799:LEU:O	1:B:803:TRP:N	9	0.23
(1,191)	1:B:799:LEU:O	1:B:803:TRP:H	4	0.23
(1,19)	1:B:799:LEU:O	1:B:803:TRP:H	4	0.23
(1,106)	1:B:799:LEU:O	1:B:803:TRP:N	9	0.23
(1,105)	1:B:799:LEU:O	1:B:803:TRP:H	4	0.23
(2,990)	1:A:779:THR:H	1:A:776:LEU:HA	9	0.22
(2,982)	1:A:777:ILE:HD11	1:A:774:LEU:HA	3	0.22
(2,982)	1:A:777:ILE:HD12	1:A:774:LEU:HA	3	0.22
(2,982)	1:A:777:ILE:HD13	1:A:774:LEU:HA	3	0.22
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB2	7	0.22
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB3	7	0.22
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB2	8	0.22
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB3	8	0.22
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB2	10	0.22
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB3	10	0.22
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	8	0.22
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	8	0.22
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	8	0.22
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	8	0.22
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	8	0.22
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	8	0.22
(2,864)	1:A:710:GLN:H	1:A:708:VAL:HA	15	0.22
(2,854)	1:A:708:VAL:HG21	1:A:707:ARG:HD2	15	0.22
(2,854)	1:A:708:VAL:HG21	1:A:707:ARG:HD3	15	0.22
(2,854)	1:A:708:VAL:HG22	1:A:707:ARG:HD2	15	0.22
(2,854)	1:A:708:VAL:HG22	1:A:707:ARG:HD3	15	0.22
(2,854)	1:A:708:VAL:HG23	1:A:707:ARG:HD2	15	0.22
(2,854)	1:A:708:VAL:HG23	1:A:707:ARG:HD3	15	0.22
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD11	13	0.22
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD12	13	0.22
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD13	13	0.22
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD21	13	0.22
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD22	13	0.22
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD23	13	0.22
(2,839)	1:A:707:ARG:H	1:A:704:LEU:HA	13	0.22
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB2	10	0.22
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB3	10	0.22
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	5	0.22
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	5	0.22
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	5	0.22
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	5	0.22
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	5	0.22
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	15	0.22
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	15	0.22
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	15	0.22
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	15	0.22
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	15	0.22
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	15	0.22
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	8	0.22
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	8	0.22
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	8	0.22
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	8	0.22
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	8	0.22
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	8	0.22
(2,765)	1:A:693:ILE:HG21	1:A:696:ARG:HG2	6	0.22
(2,765)	1:A:693:ILE:HG21	1:A:696:ARG:HG3	6	0.22
(2,765)	1:A:693:ILE:HG22	1:A:696:ARG:HG2	6	0.22
(2,765)	1:A:693:ILE:HG22	1:A:696:ARG:HG3	6	0.22
(2,765)	1:A:693:ILE:HG23	1:A:696:ARG:HG2	6	0.22
(2,765)	1:A:693:ILE:HG23	1:A:696:ARG:HG3	6	0.22
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	1	0.22
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	1	0.22
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	1	0.22
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	1	0.22
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	1	0.22
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	1	0.22
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	9	0.22
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	9	0.22
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	9	0.22
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	9	0.22
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	9	0.22
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	9	0.22
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	11	0.22
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	11	0.22
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	11	0.22
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	11	0.22
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	11	0.22
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	11	0.22
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD11	13	0.22
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD12	13	0.22
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD13	13	0.22
(2,670)	1:A:667:ALA:H	1:A:666:TRP:HD1	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,670)	1:A:667:ALA:H	1:A:666:TRP:HD1	11	0.22
(2,654)	1:A:665:LYS:H	1:A:664:ASP:HA	8	0.22
(2,650)	1:A:664:ASP:H	1:A:663:LEU:H	15	0.22
(2,649)	1:A:664:ASP:H	1:A:663:LEU:HA	3	0.22
(2,649)	1:A:664:ASP:H	1:A:663:LEU:HA	11	0.22
(2,644)	1:A:663:LEU:H	1:A:664:ASP:H	15	0.22
(2,63)	1:A:700:ALA:HB1	1:B:702:LEU:HB2	4	0.22
(2,63)	1:A:700:ALA:HB1	1:B:702:LEU:HB3	4	0.22
(2,63)	1:A:700:ALA:HB2	1:B:702:LEU:HB2	4	0.22
(2,63)	1:A:700:ALA:HB2	1:B:702:LEU:HB3	4	0.22
(2,63)	1:A:700:ALA:HB3	1:B:702:LEU:HB2	4	0.22
(2,63)	1:A:700:ALA:HB3	1:B:702:LEU:HB3	4	0.22
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB2	4	0.22
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB3	4	0.22
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB2	4	0.22
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB3	4	0.22
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB2	4	0.22
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB3	4	0.22
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB2	9	0.22
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB3	9	0.22
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB2	9	0.22
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB3	9	0.22
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB2	9	0.22
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB3	9	0.22
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD21	3	0.22
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD22	3	0.22
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD23	3	0.22
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD21	4	0.22
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD22	4	0.22
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD23	4	0.22
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD11	4	0.22
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD12	4	0.22
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD13	4	0.22
(2,601)	1:B:785:LEU:H	1:B:782:VAL:HA	5	0.22
(2,581)	1:B:782:VAL:H	1:B:779:THR:HA	2	0.22
(2,581)	1:B:782:VAL:H	1:B:779:THR:HA	14	0.22
(2,575)	1:B:781:ILE:H	1:B:778:VAL:HA	11	0.22
(2,565)	1:B:779:THR:H	1:B:776:LEU:HA	4	0.22
(2,564)	1:B:778:VAL:HG21	1:B:775:LEU:HA	11	0.22
(2,564)	1:B:778:VAL:HG22	1:B:775:LEU:HA	11	0.22
(2,564)	1:B:778:VAL:HG23	1:B:775:LEU:HA	11	0.22
(2,559)	1:B:778:VAL:H	1:B:775:LEU:HA	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,559)	1:B:778:VAL:H	1:B:775:LEU:HA	15	0.22
(2,546)	1:B:776:LEU:H	1:B:773:ASP:HA	1	0.22
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA2	6	0.22
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA3	6	0.22
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA2	6	0.22
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA3	6	0.22
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA2	6	0.22
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA3	6	0.22
(2,444)	1:B:710:GLN:H	1:B:710:GLN:HB3	9	0.22
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB2	4	0.22
(2,430)	1:B:708:VAL:HG21	1:B:745:SER:HB3	4	0.22
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB2	4	0.22
(2,430)	1:B:708:VAL:HG22	1:B:745:SER:HB3	4	0.22
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB2	4	0.22
(2,430)	1:B:708:VAL:HG23	1:B:745:SER:HB3	4	0.22
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB2	7	0.22
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB3	7	0.22
(2,405)	1:B:705:VAL:HG21	1:B:702:LEU:HG	1	0.22
(2,405)	1:B:705:VAL:HG22	1:B:702:LEU:HG	1	0.22
(2,405)	1:B:705:VAL:HG23	1:B:702:LEU:HG	1	0.22
(2,401)	1:B:705:VAL:HG11	1:B:702:LEU:HA	4	0.22
(2,401)	1:B:705:VAL:HG12	1:B:702:LEU:HA	4	0.22
(2,401)	1:B:705:VAL:HG13	1:B:702:LEU:HA	4	0.22
(2,401)	1:B:705:VAL:HG11	1:B:702:LEU:HA	13	0.22
(2,401)	1:B:705:VAL:HG12	1:B:702:LEU:HA	13	0.22
(2,401)	1:B:705:VAL:HG13	1:B:702:LEU:HA	13	0.22
(2,369)	1:B:701:VAL:H	1:B:698:VAL:HA	3	0.22
(2,369)	1:B:701:VAL:H	1:B:698:VAL:HA	13	0.22
(2,367)	1:B:700:ALA:HB1	1:B:697:ILE:HA	5	0.22
(2,367)	1:B:700:ALA:HB2	1:B:697:ILE:HA	5	0.22
(2,367)	1:B:700:ALA:HB3	1:B:697:ILE:HA	5	0.22
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD11	5	0.22
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD12	5	0.22
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD13	5	0.22
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD11	5	0.22
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD12	5	0.22
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD13	5	0.22
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD11	5	0.22
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD12	5	0.22
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD13	5	0.22
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD11	14	0.22
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD12	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD13	14	0.22
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD11	14	0.22
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD12	14	0.22
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD13	14	0.22
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD11	14	0.22
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD12	14	0.22
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD13	14	0.22
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD11	9	0.22
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD12	9	0.22
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD13	9	0.22
(2,289)	1:B:680:TRP:HE1	1:B:683:ARG:HH21	10	0.22
(2,289)	1:B:680:TRP:HE1	1:B:683:ARG:HH22	10	0.22
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD11	4	0.22
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD12	4	0.22
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD13	4	0.22
(2,245)	1:B:667:ALA:H	1:B:666:TRP:HD1	14	0.22
(2,241)	1:B:666:TRP:HE1	1:B:662:GLU:H	2	0.22
(2,229)	1:B:665:LYS:H	1:B:664:ASP:HA	11	0.22
(2,224)	1:B:664:ASP:H	1:B:663:LEU:HA	3	0.22
(2,224)	1:B:664:ASP:H	1:B:663:LEU:HA	6	0.22
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD2	9	0.22
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD3	9	0.22
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG12	11	0.22
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG13	11	0.22
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD11	4	0.22
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD12	4	0.22
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD13	4	0.22
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD11	9	0.22
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD12	9	0.22
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD13	9	0.22
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD11	4	0.22
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD12	4	0.22
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD13	4	0.22
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD11	9	0.22
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD12	9	0.22
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD13	9	0.22
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD11	3	0.22
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD12	3	0.22
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD13	3	0.22
(2,187)	1:B:816:ASN:H	1:B:830:ILE:HD11	2	0.22
(2,187)	1:B:816:ASN:H	1:B:830:ILE:HD12	2	0.22
(2,187)	1:B:816:ASN:H	1:B:830:ILE:HD13	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD2	6	0.22
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD3	6	0.22
(2,180)	1:A:806:GLU:H	1:B:771:LEU:HG	4	0.22
(2,180)	1:A:806:GLU:H	1:B:771:LEU:HG	9	0.22
(2,177)	1:A:803:TRP:HE1	1:B:764:SER:HG	15	0.22
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB2	9	0.22
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB3	9	0.22
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG12	3	0.22
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG13	3	0.22
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG12	10	0.22
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG13	10	0.22
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG12	13	0.22
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG13	13	0.22
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD2	9	0.22
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD3	9	0.22
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG2	1	0.22
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG3	1	0.22
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG2	15	0.22
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG3	15	0.22
(2,1430)	1:A:781:ILE:HG21	1:A:778:VAL:HA	1	0.22
(2,1430)	1:A:781:ILE:HG22	1:A:778:VAL:HA	1	0.22
(2,1430)	1:A:781:ILE:HG23	1:A:778:VAL:HA	1	0.22
(2,1425)	1:A:781:ILE:H	1:A:778:VAL:HA	11	0.22
(2,1415)	1:A:779:THR:H	1:A:776:LEU:HA	9	0.22
(2,1407)	1:A:777:ILE:HD11	1:A:774:LEU:HA	3	0.22
(2,1407)	1:A:777:ILE:HD12	1:A:774:LEU:HA	3	0.22
(2,1407)	1:A:777:ILE:HD13	1:A:774:LEU:HA	3	0.22
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB2	7	0.22
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB3	7	0.22
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB2	8	0.22
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB3	8	0.22
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB2	10	0.22
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB3	10	0.22
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	8	0.22
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	8	0.22
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	8	0.22
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	8	0.22
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	8	0.22
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	8	0.22
(2,1289)	1:A:710:GLN:H	1:A:708:VAL:HA	15	0.22
(2,1279)	1:A:708:VAL:HG21	1:A:707:ARG:HD2	15	0.22
(2,1279)	1:A:708:VAL:HG21	1:A:707:ARG:HD3	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1279)	1:A:708:VAL:HG22	1:A:707:ARG:HD2	15	0.22
(2,1279)	1:A:708:VAL:HG22	1:A:707:ARG:HD3	15	0.22
(2,1279)	1:A:708:VAL:HG23	1:A:707:ARG:HD2	15	0.22
(2,1279)	1:A:708:VAL:HG23	1:A:707:ARG:HD3	15	0.22
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD11	13	0.22
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD12	13	0.22
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD13	13	0.22
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD21	13	0.22
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD22	13	0.22
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD23	13	0.22
(2,1264)	1:A:707:ARG:H	1:A:704:LEU:HA	13	0.22
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB2	10	0.22
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB3	10	0.22
(2,126)	1:A:785:LEU:HD21	1:B:749:VAL:HB	10	0.22
(2,126)	1:A:785:LEU:HD22	1:B:749:VAL:HB	10	0.22
(2,126)	1:A:785:LEU:HD23	1:B:749:VAL:HB	10	0.22
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	5	0.22
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	5	0.22
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	5	0.22
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	5	0.22
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	5	0.22
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	5	0.22
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	15	0.22
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	15	0.22
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	15	0.22
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	15	0.22
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	15	0.22
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	15	0.22
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	8	0.22
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	8	0.22
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	8	0.22
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	8	0.22
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	8	0.22
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	8	0.22
(2,1190)	1:A:693:ILE:HG21	1:A:696:ARG:HG2	6	0.22
(2,1190)	1:A:693:ILE:HG21	1:A:696:ARG:HG3	6	0.22
(2,1190)	1:A:693:ILE:HG22	1:A:696:ARG:HG2	6	0.22
(2,1190)	1:A:693:ILE:HG22	1:A:696:ARG:HG3	6	0.22
(2,1190)	1:A:693:ILE:HG23	1:A:696:ARG:HG2	6	0.22
(2,1190)	1:A:693:ILE:HG23	1:A:696:ARG:HG3	6	0.22
(2,117)	1:A:781:ILE:HD11	1:B:746:ILE:HG12	3	0.22
(2,117)	1:A:781:ILE:HD11	1:B:746:ILE:HG13	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,117)	1:A:781:ILE:HD12	1:B:746:ILE:HG12	3	0.22
(2,117)	1:A:781:ILE:HD12	1:B:746:ILE:HG13	3	0.22
(2,117)	1:A:781:ILE:HD13	1:B:746:ILE:HG12	3	0.22
(2,117)	1:A:781:ILE:HD13	1:B:746:ILE:HG13	3	0.22
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	1	0.22
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	1	0.22
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	1	0.22
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	1	0.22
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	1	0.22
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	1	0.22
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	9	0.22
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	9	0.22
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	9	0.22
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	9	0.22
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	9	0.22
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	9	0.22
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	11	0.22
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	11	0.22
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	11	0.22
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	11	0.22
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	11	0.22
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	11	0.22
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD11	13	0.22
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD12	13	0.22
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD13	13	0.22
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG21	14	0.22
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG22	14	0.22
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG23	14	0.22
(2,1095)	1:A:667:ALA:H	1:A:666:TRP:HD1	9	0.22
(2,1095)	1:A:667:ALA:H	1:A:666:TRP:HD1	11	0.22
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD2	7	0.22
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD3	7	0.22
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD2	7	0.22
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD3	7	0.22
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD2	7	0.22
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD3	7	0.22
(2,1079)	1:A:665:LYS:H	1:A:664:ASP:HA	8	0.22
(2,1075)	1:A:664:ASP:H	1:A:663:LEU:H	15	0.22
(2,1074)	1:A:664:ASP:H	1:A:663:LEU:HA	3	0.22
(2,1074)	1:A:664:ASP:H	1:A:663:LEU:HA	11	0.22
(2,1069)	1:A:663:LEU:H	1:A:664:ASP:H	15	0.22
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD2	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD3	9	0.22
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG2	1	0.22
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG3	1	0.22
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG2	15	0.22
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG3	15	0.22
(2,1005)	1:A:781:ILE:HG21	1:A:778:VAL:HA	1	0.22
(2,1005)	1:A:781:ILE:HG22	1:A:778:VAL:HA	1	0.22
(2,1005)	1:A:781:ILE:HG23	1:A:778:VAL:HA	1	0.22
(2,1000)	1:A:781:ILE:H	1:A:778:VAL:HA	11	0.22
(1,95)	1:B:794:LYS:O	1:B:798:ASN:H	12	0.22
(1,9)	1:B:794:LYS:O	1:B:798:ASN:H	12	0.22
(1,23)	1:B:801:GLN:O	1:B:805:GLN:H	8	0.22
(1,23)	1:B:801:GLN:O	1:B:805:GLN:H	14	0.22
(1,23)	1:B:801:GLN:O	1:B:805:GLN:H	15	0.22
(1,195)	1:B:801:GLN:O	1:B:805:GLN:H	8	0.22
(1,195)	1:B:801:GLN:O	1:B:805:GLN:H	14	0.22
(1,195)	1:B:801:GLN:O	1:B:805:GLN:H	15	0.22
(1,181)	1:B:794:LYS:O	1:B:798:ASN:H	12	0.22
(1,109)	1:B:801:GLN:O	1:B:805:GLN:H	8	0.22
(1,109)	1:B:801:GLN:O	1:B:805:GLN:H	14	0.22
(1,109)	1:B:801:GLN:O	1:B:805:GLN:H	15	0.22
(2,990)	1:A:779:THR:H	1:A:776:LEU:HA	12	0.21
(2,983)	1:A:777:ILE:HG21	1:A:780:ARG:HD2	12	0.21
(2,983)	1:A:777:ILE:HG21	1:A:780:ARG:HD3	12	0.21
(2,983)	1:A:777:ILE:HG22	1:A:780:ARG:HD2	12	0.21
(2,983)	1:A:777:ILE:HG22	1:A:780:ARG:HD3	12	0.21
(2,983)	1:A:777:ILE:HG23	1:A:780:ARG:HD2	12	0.21
(2,983)	1:A:777:ILE:HG23	1:A:780:ARG:HD3	12	0.21
(2,982)	1:A:777:ILE:HD11	1:A:774:LEU:HA	12	0.21
(2,982)	1:A:777:ILE:HD12	1:A:774:LEU:HA	12	0.21
(2,982)	1:A:777:ILE:HD13	1:A:774:LEU:HA	12	0.21
(2,944)	1:A:763:LEU:HD11	1:A:764:SER:HG	1	0.21
(2,944)	1:A:763:LEU:HD12	1:A:764:SER:HG	1	0.21
(2,944)	1:A:763:LEU:HD13	1:A:764:SER:HG	1	0.21
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB2	6	0.21
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB3	6	0.21
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB2	11	0.21
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB3	11	0.21
(2,916)	1:A:753:LEU:HD11	1:A:757:TRP:HB2	14	0.21
(2,916)	1:A:753:LEU:HD11	1:A:757:TRP:HB3	14	0.21
(2,916)	1:A:753:LEU:HD12	1:A:757:TRP:HB2	14	0.21
(2,916)	1:A:753:LEU:HD12	1:A:757:TRP:HB3	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,916)	1:A:753:LEU:HD13	1:A:757:TRP:HB2	14	0.21
(2,916)	1:A:753:LEU:HD13	1:A:757:TRP:HB3	14	0.21
(2,907)	1:A:749:VAL:H	1:A:746:ILE:HA	5	0.21
(2,904)	1:A:748:LEU:H	1:A:745:SER:HA	13	0.21
(2,898)	1:A:746:ILE:HG21	1:A:750:ASN:HD22	15	0.21
(2,898)	1:A:746:ILE:HG22	1:A:750:ASN:HD22	15	0.21
(2,898)	1:A:746:ILE:HG23	1:A:750:ASN:HD22	15	0.21
(2,894)	1:A:746:ILE:HD11	1:A:742:ARG:HD2	6	0.21
(2,894)	1:A:746:ILE:HD11	1:A:742:ARG:HD3	6	0.21
(2,894)	1:A:746:ILE:HD12	1:A:742:ARG:HD2	6	0.21
(2,894)	1:A:746:ILE:HD12	1:A:742:ARG:HD3	6	0.21
(2,894)	1:A:746:ILE:HD13	1:A:742:ARG:HD2	6	0.21
(2,894)	1:A:746:ILE:HD13	1:A:742:ARG:HD3	6	0.21
(2,864)	1:A:710:GLN:H	1:A:708:VAL:HA	8	0.21
(2,864)	1:A:710:GLN:H	1:A:708:VAL:HA	12	0.21
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD2	15	0.21
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD3	15	0.21
(2,839)	1:A:707:ARG:H	1:A:704:LEU:HA	11	0.21
(2,821)	1:A:705:VAL:H	1:A:702:LEU:HA	8	0.21
(2,794)	1:A:701:VAL:H	1:A:698:VAL:HA	11	0.21
(2,781)	1:A:698:VAL:HG11	1:A:695:LEU:HG	4	0.21
(2,781)	1:A:698:VAL:HG12	1:A:695:LEU:HG	4	0.21
(2,781)	1:A:698:VAL:HG13	1:A:695:LEU:HG	4	0.21
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB1	4	0.21
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB2	4	0.21
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB3	4	0.21
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB1	4	0.21
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB2	4	0.21
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB3	4	0.21
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB1	4	0.21
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB2	4	0.21
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB3	4	0.21
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	10	0.21
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	10	0.21
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	10	0.21
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	10	0.21
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	10	0.21
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	10	0.21
(2,727)	1:A:684:ILE:HD11	1:A:681:TYR:HE1	2	0.21
(2,727)	1:A:684:ILE:HD11	1:A:681:TYR:HE2	2	0.21
(2,727)	1:A:684:ILE:HD12	1:A:681:TYR:HE1	2	0.21
(2,727)	1:A:684:ILE:HD12	1:A:681:TYR:HE2	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,727)	1:A:684:ILE:HD13	1:A:681:TYR:HE1	2	0.21
(2,727)	1:A:684:ILE:HD13	1:A:681:TYR:HE2	2	0.21
(2,721)	1:A:682:ILE:HD11	1:A:681:TYR:H	6	0.21
(2,721)	1:A:682:ILE:HD12	1:A:681:TYR:H	6	0.21
(2,721)	1:A:682:ILE:HD13	1:A:681:TYR:H	6	0.21
(2,705)	1:A:676:THR:HG21	1:A:681:TYR:HH	9	0.21
(2,705)	1:A:676:THR:HG22	1:A:681:TYR:HH	9	0.21
(2,705)	1:A:676:THR:HG23	1:A:681:TYR:HH	9	0.21
(2,702)	1:A:676:THR:HG21	1:A:669:LEU:HA	5	0.21
(2,702)	1:A:676:THR:HG22	1:A:669:LEU:HA	5	0.21
(2,702)	1:A:676:THR:HG23	1:A:669:LEU:HA	5	0.21
(2,701)	1:A:676:THR:HG21	1:A:666:TRP:HZ3	7	0.21
(2,701)	1:A:676:THR:HG22	1:A:666:TRP:HZ3	7	0.21
(2,701)	1:A:676:THR:HG23	1:A:666:TRP:HZ3	7	0.21
(2,697)	1:A:674:ASP:H	1:A:677:ASN:H	15	0.21
(2,688)	1:A:670:TRP:HE1	1:A:667:ALA:HB1	5	0.21
(2,688)	1:A:670:TRP:HE1	1:A:667:ALA:HB2	5	0.21
(2,688)	1:A:670:TRP:HE1	1:A:667:ALA:HB3	5	0.21
(2,654)	1:A:665:LYS:H	1:A:664:ASP:HA	4	0.21
(2,654)	1:A:665:LYS:H	1:A:664:ASP:HA	10	0.21
(2,654)	1:A:665:LYS:H	1:A:664:ASP:HA	15	0.21
(2,649)	1:A:664:ASP:H	1:A:663:LEU:HA	2	0.21
(2,649)	1:A:664:ASP:H	1:A:663:LEU:HA	5	0.21
(2,649)	1:A:664:ASP:H	1:A:663:LEU:HA	13	0.21
(2,639)	1:A:661:LEU:HD11	1:A:662:GLU:HG2	14	0.21
(2,639)	1:A:661:LEU:HD11	1:A:662:GLU:HG3	14	0.21
(2,639)	1:A:661:LEU:HD12	1:A:662:GLU:HG2	14	0.21
(2,639)	1:A:661:LEU:HD12	1:A:662:GLU:HG3	14	0.21
(2,639)	1:A:661:LEU:HD13	1:A:662:GLU:HG2	14	0.21
(2,639)	1:A:661:LEU:HD13	1:A:662:GLU:HG3	14	0.21
(2,639)	1:A:661:LEU:HD21	1:A:662:GLU:HG2	14	0.21
(2,639)	1:A:661:LEU:HD21	1:A:662:GLU:HG3	14	0.21
(2,639)	1:A:661:LEU:HD22	1:A:662:GLU:HG2	14	0.21
(2,639)	1:A:661:LEU:HD22	1:A:662:GLU:HG3	14	0.21
(2,639)	1:A:661:LEU:HD23	1:A:662:GLU:HG2	14	0.21
(2,639)	1:A:661:LEU:HD23	1:A:662:GLU:HG3	14	0.21
(2,626)	1:B:817:ALA:H	1:B:816:ASN:HB2	12	0.21
(2,626)	1:B:817:ALA:H	1:B:816:ASN:HB3	12	0.21
(2,618)	1:B:797:TRP:H	1:B:796:TRP:HD1	5	0.21
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD21	1	0.21
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD22	1	0.21
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD23	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD11	2	0.21
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD12	2	0.21
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD13	2	0.21
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD21	2	0.21
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD22	2	0.21
(2,613)	1:B:790:TRP:HE1	1:B:793:LEU:HD23	2	0.21
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD2	1	0.21
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD3	1	0.21
(2,587)	1:B:783:GLU:H	1:B:780:ARG:HA	6	0.21
(2,565)	1:B:779:THR:H	1:B:776:LEU:HA	6	0.21
(2,557)	1:B:777:ILE:HD11	1:B:774:LEU:HA	6	0.21
(2,557)	1:B:777:ILE:HD12	1:B:774:LEU:HA	6	0.21
(2,557)	1:B:777:ILE:HD13	1:B:774:LEU:HA	6	0.21
(2,540)	1:B:775:LEU:H	1:B:772:ARG:HA	11	0.21
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH21	4	0.21
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH22	4	0.21
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH21	4	0.21
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH22	4	0.21
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH21	4	0.21
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH22	4	0.21
(2,506)	1:B:755:LEU:H	1:B:756:ILE:H	4	0.21
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA2	13	0.21
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA3	13	0.21
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA2	13	0.21
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA3	13	0.21
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA2	13	0.21
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA3	13	0.21
(2,479)	1:B:748:LEU:H	1:B:745:SER:HA	3	0.21
(2,473)	1:B:746:ILE:HG21	1:B:750:ASN:HD22	6	0.21
(2,473)	1:B:746:ILE:HG22	1:B:750:ASN:HD22	6	0.21
(2,473)	1:B:746:ILE:HG23	1:B:750:ASN:HD22	6	0.21
(2,463)	1:B:746:ILE:H	1:B:742:ARG:HA	4	0.21
(2,432)	1:B:709:ARG:H	1:B:707:ARG:H	8	0.21
(2,428)	1:B:708:VAL:HG11	1:B:705:VAL:HA	5	0.21
(2,428)	1:B:708:VAL:HG12	1:B:705:VAL:HA	5	0.21
(2,428)	1:B:708:VAL:HG13	1:B:705:VAL:HA	5	0.21
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD11	2	0.21
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD12	2	0.21
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD13	2	0.21
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD21	2	0.21
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD22	2	0.21
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD23	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:B:704:LEU:HD11	1:B:707:ARG:HD2	14	0.21
(2,393)	1:B:704:LEU:HD11	1:B:707:ARG:HD3	14	0.21
(2,393)	1:B:704:LEU:HD12	1:B:707:ARG:HD2	14	0.21
(2,393)	1:B:704:LEU:HD12	1:B:707:ARG:HD3	14	0.21
(2,393)	1:B:704:LEU:HD13	1:B:707:ARG:HD2	14	0.21
(2,393)	1:B:704:LEU:HD13	1:B:707:ARG:HD3	14	0.21
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB2	3	0.21
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB3	3	0.21
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB2	3	0.21
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB3	3	0.21
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB2	3	0.21
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB3	3	0.21
(2,37)	1:B:692:LEU:HD21	1:A:694:GLY:H	10	0.21
(2,37)	1:B:692:LEU:HD22	1:A:694:GLY:H	10	0.21
(2,37)	1:B:692:LEU:HD23	1:A:694:GLY:H	10	0.21
(2,369)	1:B:701:VAL:H	1:B:698:VAL:HA	2	0.21
(2,356)	1:B:698:VAL:HG11	1:B:695:LEU:HG	11	0.21
(2,356)	1:B:698:VAL:HG12	1:B:695:LEU:HG	11	0.21
(2,356)	1:B:698:VAL:HG13	1:B:695:LEU:HG	11	0.21
(2,354)	1:B:697:ILE:HG21	1:B:700:ALA:HB1	6	0.21
(2,354)	1:B:697:ILE:HG21	1:B:700:ALA:HB2	6	0.21
(2,354)	1:B:697:ILE:HG21	1:B:700:ALA:HB3	6	0.21
(2,354)	1:B:697:ILE:HG22	1:B:700:ALA:HB1	6	0.21
(2,354)	1:B:697:ILE:HG22	1:B:700:ALA:HB2	6	0.21
(2,354)	1:B:697:ILE:HG22	1:B:700:ALA:HB3	6	0.21
(2,354)	1:B:697:ILE:HG23	1:B:700:ALA:HB1	6	0.21
(2,354)	1:B:697:ILE:HG23	1:B:700:ALA:HB2	6	0.21
(2,354)	1:B:697:ILE:HG23	1:B:700:ALA:HB3	6	0.21
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD11	8	0.21
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD12	8	0.21
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD13	8	0.21
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD11	8	0.21
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD12	8	0.21
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD13	8	0.21
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD11	8	0.21
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD12	8	0.21
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD13	8	0.21
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD11	5	0.21
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD12	5	0.21
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD13	5	0.21
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD21	5	0.21
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD22	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD23	5	0.21
(2,242)	1:B:667:ALA:H	1:B:664:ASP:HA	1	0.21
(2,229)	1:B:665:LYS:H	1:B:664:ASP:HA	2	0.21
(2,229)	1:B:665:LYS:H	1:B:664:ASP:HA	6	0.21
(2,229)	1:B:665:LYS:H	1:B:664:ASP:HA	13	0.21
(2,224)	1:B:664:ASP:H	1:B:663:LEU:HA	4	0.21
(2,224)	1:B:664:ASP:H	1:B:663:LEU:HA	12	0.21
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG2	4	0.21
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG3	4	0.21
(2,189)	1:A:816:ASN:H	1:A:830:ILE:HD11	11	0.21
(2,189)	1:A:816:ASN:H	1:A:830:ILE:HD12	11	0.21
(2,189)	1:A:816:ASN:H	1:A:830:ILE:HD13	11	0.21
(2,188)	1:A:816:ASN:H	1:A:830:ILE:HD11	11	0.21
(2,188)	1:A:816:ASN:H	1:A:830:ILE:HD12	11	0.21
(2,188)	1:A:816:ASN:H	1:A:830:ILE:HD13	11	0.21
(2,186)	1:A:808:LYS:H	1:A:838:ARG:HD2	9	0.21
(2,186)	1:A:808:LYS:H	1:A:838:ARG:HD3	9	0.21
(2,185)	1:A:808:LYS:H	1:A:838:ARG:HD2	9	0.21
(2,185)	1:A:808:LYS:H	1:A:838:ARG:HD3	9	0.21
(2,183)	1:A:806:GLU:H	1:B:772:ARG:HE	1	0.21
(2,183)	1:A:806:GLU:H	1:B:772:ARG:HE	14	0.21
(2,162)	1:A:794:LYS:H	1:A:848:ARG:HG2	13	0.21
(2,162)	1:A:794:LYS:H	1:A:848:ARG:HG3	13	0.21
(2,161)	1:A:794:LYS:H	1:A:848:ARG:HG2	13	0.21
(2,161)	1:A:794:LYS:H	1:A:848:ARG:HG3	13	0.21
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE21	1	0.21
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE22	1	0.21
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE21	3	0.21
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE22	3	0.21
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE21	7	0.21
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE22	7	0.21
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE21	13	0.21
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE22	13	0.21
(2,1475)	1:A:806:GLU:H	1:A:803:TRP:HB2	1	0.21
(2,1475)	1:A:806:GLU:H	1:A:803:TRP:HB3	1	0.21
(2,1475)	1:A:806:GLU:H	1:A:803:TRP:HB2	9	0.21
(2,1475)	1:A:806:GLU:H	1:A:803:TRP:HB3	9	0.21
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	1	0.21
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	1	0.21
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	1	0.21
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	1	0.21
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	1	0.21
(2,1469)	1:A:797:TRP:HE1	1:A:793:LEU:HD11	4	0.21
(2,1469)	1:A:797:TRP:HE1	1:A:793:LEU:HD12	4	0.21
(2,1469)	1:A:797:TRP:HE1	1:A:793:LEU:HD13	4	0.21
(2,1469)	1:A:797:TRP:HE1	1:A:793:LEU:HD21	4	0.21
(2,1469)	1:A:797:TRP:HE1	1:A:793:LEU:HD22	4	0.21
(2,1469)	1:A:797:TRP:HE1	1:A:793:LEU:HD23	4	0.21
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD21	15	0.21
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD22	15	0.21
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD23	15	0.21
(2,1457)	1:A:785:LEU:HD21	1:A:782:VAL:HA	5	0.21
(2,1457)	1:A:785:LEU:HD22	1:A:782:VAL:HA	5	0.21
(2,1457)	1:A:785:LEU:HD23	1:A:782:VAL:HA	5	0.21
(2,1451)	1:A:785:LEU:H	1:A:782:VAL:HA	3	0.21
(2,1425)	1:A:781:ILE:H	1:A:778:VAL:HA	1	0.21
(2,1415)	1:A:779:THR:H	1:A:776:LEU:HA	12	0.21
(2,1408)	1:A:777:ILE:HG21	1:A:780:ARG:HD2	12	0.21
(2,1408)	1:A:777:ILE:HG21	1:A:780:ARG:HD3	12	0.21
(2,1408)	1:A:777:ILE:HG22	1:A:780:ARG:HD2	12	0.21
(2,1408)	1:A:777:ILE:HG22	1:A:780:ARG:HD3	12	0.21
(2,1408)	1:A:777:ILE:HG23	1:A:780:ARG:HD2	12	0.21
(2,1408)	1:A:777:ILE:HG23	1:A:780:ARG:HD3	12	0.21
(2,1407)	1:A:777:ILE:HD11	1:A:774:LEU:HA	12	0.21
(2,1407)	1:A:777:ILE:HD12	1:A:774:LEU:HA	12	0.21
(2,1407)	1:A:777:ILE:HD13	1:A:774:LEU:HA	12	0.21
(2,1369)	1:A:763:LEU:HD11	1:A:764:SER:HG	1	0.21
(2,1369)	1:A:763:LEU:HD12	1:A:764:SER:HG	1	0.21
(2,1369)	1:A:763:LEU:HD13	1:A:764:SER:HG	1	0.21
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB2	6	0.21
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB3	6	0.21
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB2	11	0.21
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB3	11	0.21
(2,1341)	1:A:753:LEU:HD11	1:A:757:TRP:HB2	14	0.21
(2,1341)	1:A:753:LEU:HD11	1:A:757:TRP:HB3	14	0.21
(2,1341)	1:A:753:LEU:HD12	1:A:757:TRP:HB2	14	0.21
(2,1341)	1:A:753:LEU:HD12	1:A:757:TRP:HB3	14	0.21
(2,1341)	1:A:753:LEU:HD13	1:A:757:TRP:HB2	14	0.21
(2,1341)	1:A:753:LEU:HD13	1:A:757:TRP:HB3	14	0.21
(2,1332)	1:A:749:VAL:H	1:A:746:ILE:HA	5	0.21
(2,1329)	1:A:748:LEU:H	1:A:745:SER:HA	13	0.21
(2,1323)	1:A:746:ILE:HG21	1:A:750:ASN:HD22	15	0.21
(2,1323)	1:A:746:ILE:HG22	1:A:750:ASN:HD22	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1323)	1:A:746:ILE:HG23	1:A:750:ASN:HD22	15	0.21
(2,1319)	1:A:746:ILE:HD11	1:A:742:ARG:HD2	6	0.21
(2,1319)	1:A:746:ILE:HD11	1:A:742:ARG:HD3	6	0.21
(2,1319)	1:A:746:ILE:HD12	1:A:742:ARG:HD2	6	0.21
(2,1319)	1:A:746:ILE:HD12	1:A:742:ARG:HD3	6	0.21
(2,1319)	1:A:746:ILE:HD13	1:A:742:ARG:HD2	6	0.21
(2,1319)	1:A:746:ILE:HD13	1:A:742:ARG:HD3	6	0.21
(2,13)	1:B:666:TRP:HE1	1:A:666:TRP:HD1	8	0.21
(2,1289)	1:A:710:GLN:H	1:A:708:VAL:HA	8	0.21
(2,1289)	1:A:710:GLN:H	1:A:708:VAL:HA	12	0.21
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD2	15	0.21
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD3	15	0.21
(2,1264)	1:A:707:ARG:H	1:A:704:LEU:HA	11	0.21
(2,1246)	1:A:705:VAL:H	1:A:702:LEU:HA	8	0.21
(2,1219)	1:A:701:VAL:H	1:A:698:VAL:HA	11	0.21
(2,1206)	1:A:698:VAL:HG11	1:A:695:LEU:HG	4	0.21
(2,1206)	1:A:698:VAL:HG12	1:A:695:LEU:HG	4	0.21
(2,1206)	1:A:698:VAL:HG13	1:A:695:LEU:HG	4	0.21
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB1	4	0.21
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB2	4	0.21
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB3	4	0.21
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB1	4	0.21
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB2	4	0.21
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB3	4	0.21
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB1	4	0.21
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB2	4	0.21
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB3	4	0.21
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	10	0.21
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	10	0.21
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	10	0.21
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	10	0.21
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	10	0.21
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	10	0.21
(2,1152)	1:A:684:ILE:HD11	1:A:681:TYR:HE1	2	0.21
(2,1152)	1:A:684:ILE:HD11	1:A:681:TYR:HE2	2	0.21
(2,1152)	1:A:684:ILE:HD12	1:A:681:TYR:HE1	2	0.21
(2,1152)	1:A:684:ILE:HD12	1:A:681:TYR:HE2	2	0.21
(2,1152)	1:A:684:ILE:HD13	1:A:681:TYR:HE1	2	0.21
(2,1152)	1:A:684:ILE:HD13	1:A:681:TYR:HE2	2	0.21
(2,1146)	1:A:682:ILE:HD11	1:A:681:TYR:H	6	0.21
(2,1146)	1:A:682:ILE:HD12	1:A:681:TYR:H	6	0.21
(2,1146)	1:A:682:ILE:HD13	1:A:681:TYR:H	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,114)	1:A:781:ILE:HD11	1:B:743:ASP:HA	4	0.21
(2,114)	1:A:781:ILE:HD12	1:B:743:ASP:HA	4	0.21
(2,114)	1:A:781:ILE:HD13	1:B:743:ASP:HA	4	0.21
(2,1130)	1:A:676:THR:HG21	1:A:681:TYR:HH	9	0.21
(2,1130)	1:A:676:THR:HG22	1:A:681:TYR:HH	9	0.21
(2,1130)	1:A:676:THR:HG23	1:A:681:TYR:HH	9	0.21
(2,1127)	1:A:676:THR:HG21	1:A:669:LEU:HA	5	0.21
(2,1127)	1:A:676:THR:HG22	1:A:669:LEU:HA	5	0.21
(2,1127)	1:A:676:THR:HG23	1:A:669:LEU:HA	5	0.21
(2,1126)	1:A:676:THR:HG21	1:A:666:TRP:HZ3	7	0.21
(2,1126)	1:A:676:THR:HG22	1:A:666:TRP:HZ3	7	0.21
(2,1126)	1:A:676:THR:HG23	1:A:666:TRP:HZ3	7	0.21
(2,1122)	1:A:674:ASP:H	1:A:677:ASN:H	15	0.21
(2,1113)	1:A:670:TRP:HE1	1:A:667:ALA:HB1	5	0.21
(2,1113)	1:A:670:TRP:HE1	1:A:667:ALA:HB2	5	0.21
(2,1113)	1:A:670:TRP:HE1	1:A:667:ALA:HB3	5	0.21
(2,1079)	1:A:665:LYS:H	1:A:664:ASP:HA	4	0.21
(2,1079)	1:A:665:LYS:H	1:A:664:ASP:HA	10	0.21
(2,1079)	1:A:665:LYS:H	1:A:664:ASP:HA	15	0.21
(2,1074)	1:A:664:ASP:H	1:A:663:LEU:HA	2	0.21
(2,1074)	1:A:664:ASP:H	1:A:663:LEU:HA	5	0.21
(2,1074)	1:A:664:ASP:H	1:A:663:LEU:HA	13	0.21
(2,1064)	1:A:661:LEU:HD11	1:A:662:GLU:HG2	14	0.21
(2,1064)	1:A:661:LEU:HD11	1:A:662:GLU:HG3	14	0.21
(2,1064)	1:A:661:LEU:HD12	1:A:662:GLU:HG2	14	0.21
(2,1064)	1:A:661:LEU:HD12	1:A:662:GLU:HG3	14	0.21
(2,1064)	1:A:661:LEU:HD13	1:A:662:GLU:HG2	14	0.21
(2,1064)	1:A:661:LEU:HD13	1:A:662:GLU:HG3	14	0.21
(2,1064)	1:A:661:LEU:HD21	1:A:662:GLU:HG2	14	0.21
(2,1064)	1:A:661:LEU:HD21	1:A:662:GLU:HG3	14	0.21
(2,1064)	1:A:661:LEU:HD22	1:A:662:GLU:HG2	14	0.21
(2,1064)	1:A:661:LEU:HD22	1:A:662:GLU:HG3	14	0.21
(2,1064)	1:A:661:LEU:HD23	1:A:662:GLU:HG2	14	0.21
(2,1064)	1:A:661:LEU:HD23	1:A:662:GLU:HG3	14	0.21
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE21	1	0.21
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE22	1	0.21
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE21	3	0.21
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE22	3	0.21
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE21	7	0.21
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE22	7	0.21
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE21	13	0.21
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE22	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1050)	1:A:806:GLU:H	1:A:803:TRP:HB2	1	0.21
(2,1050)	1:A:806:GLU:H	1:A:803:TRP:HB3	1	0.21
(2,1050)	1:A:806:GLU:H	1:A:803:TRP:HB2	9	0.21
(2,1050)	1:A:806:GLU:H	1:A:803:TRP:HB3	9	0.21
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD2	13	0.21
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD3	13	0.21
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	1	0.21
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	1	0.21
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	1	0.21
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	1	0.21
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	1	0.21
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	1	0.21
(2,1044)	1:A:797:TRP:HE1	1:A:793:LEU:HD11	4	0.21
(2,1044)	1:A:797:TRP:HE1	1:A:793:LEU:HD12	4	0.21
(2,1044)	1:A:797:TRP:HE1	1:A:793:LEU:HD13	4	0.21
(2,1044)	1:A:797:TRP:HE1	1:A:793:LEU:HD21	4	0.21
(2,1044)	1:A:797:TRP:HE1	1:A:793:LEU:HD22	4	0.21
(2,1044)	1:A:797:TRP:HE1	1:A:793:LEU:HD23	4	0.21
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD21	15	0.21
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD22	15	0.21
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD23	15	0.21
(2,1032)	1:A:785:LEU:HD21	1:A:782:VAL:HA	5	0.21
(2,1032)	1:A:785:LEU:HD22	1:A:782:VAL:HA	5	0.21
(2,1032)	1:A:785:LEU:HD23	1:A:782:VAL:HA	5	0.21
(2,1026)	1:A:785:LEU:H	1:A:782:VAL:HA	3	0.21
(2,1000)	1:A:781:ILE:H	1:A:778:VAL:HA	1	0.21
(1,96)	1:B:794:LYS:O	1:B:798:ASN:N	13	0.21
(1,47)	1:B:813:SER:O	1:B:817:ALA:H	5	0.21
(1,25)	1:B:802:TYR:O	1:B:806:GLU:H	9	0.21
(1,219)	1:B:813:SER:O	1:B:817:ALA:H	5	0.21
(1,197)	1:B:802:TYR:O	1:B:806:GLU:H	9	0.21
(1,191)	1:B:799:LEU:O	1:B:803:TRP:H	15	0.21
(1,19)	1:B:799:LEU:O	1:B:803:TRP:H	15	0.21
(1,182)	1:B:794:LYS:O	1:B:798:ASN:N	13	0.21
(1,133)	1:B:813:SER:O	1:B:817:ALA:H	5	0.21
(1,111)	1:B:802:TYR:O	1:B:806:GLU:H	9	0.21
(1,105)	1:B:799:LEU:O	1:B:803:TRP:H	15	0.21
(1,10)	1:B:794:LYS:O	1:B:798:ASN:N	13	0.21
(2,989)	1:A:778:VAL:HG21	1:A:775:LEU:HA	11	0.2
(2,989)	1:A:778:VAL:HG22	1:A:775:LEU:HA	11	0.2
(2,989)	1:A:778:VAL:HG23	1:A:775:LEU:HA	11	0.2
(2,977)	1:A:777:ILE:H	1:A:774:LEU:HA	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	9	0.2
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	9	0.2
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	9	0.2
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	9	0.2
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	9	0.2
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	9	0.2
(2,931)	1:A:755:LEU:H	1:A:756:ILE:H	14	0.2
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	1	0.2
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	1	0.2
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	1	0.2
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	1	0.2
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	1	0.2
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	1	0.2
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	14	0.2
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	14	0.2
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	14	0.2
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	14	0.2
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	14	0.2
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	14	0.2
(2,897)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	10	0.2
(2,897)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	10	0.2
(2,897)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	10	0.2
(2,853)	1:A:708:VAL:HG11	1:A:705:VAL:HA	10	0.2
(2,853)	1:A:708:VAL:HG12	1:A:705:VAL:HA	10	0.2
(2,853)	1:A:708:VAL:HG13	1:A:705:VAL:HA	10	0.2
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB2	7	0.2
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB3	7	0.2
(2,798)	1:A:701:VAL:HG21	1:A:698:VAL:HA	13	0.2
(2,798)	1:A:701:VAL:HG22	1:A:698:VAL:HA	13	0.2
(2,798)	1:A:701:VAL:HG23	1:A:698:VAL:HA	13	0.2
(2,794)	1:A:701:VAL:H	1:A:698:VAL:HA	5	0.2
(2,788)	1:A:700:ALA:H	1:A:699:PHE:HA	15	0.2
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD2	7	0.2
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD3	7	0.2
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD2	7	0.2
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD3	7	0.2
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD2	7	0.2
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD3	7	0.2
(2,777)	1:A:697:ILE:HG21	1:A:694:GLY:HA2	3	0.2
(2,777)	1:A:697:ILE:HG21	1:A:694:GLY:HA3	3	0.2
(2,777)	1:A:697:ILE:HG22	1:A:694:GLY:HA2	3	0.2
(2,777)	1:A:697:ILE:HG22	1:A:694:GLY:HA3	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,777)	1:A:697:ILE:HG23	1:A:694:GLY:HA2	3	0.2
(2,777)	1:A:697:ILE:HG23	1:A:694:GLY:HA3	3	0.2
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	5	0.2
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	5	0.2
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	5	0.2
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	5	0.2
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	5	0.2
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	5	0.2
(2,765)	1:A:693:ILE:HG21	1:A:696:ARG:HG2	15	0.2
(2,765)	1:A:693:ILE:HG21	1:A:696:ARG:HG3	15	0.2
(2,765)	1:A:693:ILE:HG22	1:A:696:ARG:HG2	15	0.2
(2,765)	1:A:693:ILE:HG22	1:A:696:ARG:HG3	15	0.2
(2,765)	1:A:693:ILE:HG23	1:A:696:ARG:HG2	15	0.2
(2,765)	1:A:693:ILE:HG23	1:A:696:ARG:HG3	15	0.2
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE1	12	0.2
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE2	12	0.2
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE1	12	0.2
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE2	12	0.2
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE1	12	0.2
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE2	12	0.2
(2,719)	1:A:682:ILE:HG21	1:A:685:PHE:HB2	8	0.2
(2,719)	1:A:682:ILE:HG21	1:A:685:PHE:HB3	8	0.2
(2,719)	1:A:682:ILE:HG22	1:A:685:PHE:HB2	8	0.2
(2,719)	1:A:682:ILE:HG22	1:A:685:PHE:HB3	8	0.2
(2,719)	1:A:682:ILE:HG23	1:A:685:PHE:HB2	8	0.2
(2,719)	1:A:682:ILE:HG23	1:A:685:PHE:HB3	8	0.2
(2,670)	1:A:667:ALA:H	1:A:666:TRP:HD1	6	0.2
(2,667)	1:A:667:ALA:H	1:A:664:ASP:HA	8	0.2
(2,654)	1:A:665:LYS:H	1:A:664:ASP:HA	6	0.2
(2,654)	1:A:665:LYS:H	1:A:664:ASP:HA	7	0.2
(2,653)	1:A:665:LYS:H	1:A:662:GLU:HA	8	0.2
(2,649)	1:A:664:ASP:H	1:A:663:LEU:HA	4	0.2
(2,629)	1:B:835:GLY:H	1:B:834:GLN:HG2	7	0.2
(2,629)	1:B:835:GLY:H	1:B:834:GLN:HG3	7	0.2
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD11	12	0.2
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD12	12	0.2
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD13	12	0.2
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB2	6	0.2
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB3	6	0.2
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB2	6	0.2
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB3	6	0.2
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB2	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB3	6	0.2
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD21	6	0.2
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD22	6	0.2
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD23	6	0.2
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD1	3	0.2
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD2	3	0.2
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD1	3	0.2
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD2	3	0.2
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD1	3	0.2
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD2	3	0.2
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD2	5	0.2
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD3	5	0.2
(2,581)	1:B:782:VAL:H	1:B:779:THR:HA	3	0.2
(2,581)	1:B:782:VAL:H	1:B:779:THR:HA	15	0.2
(2,545)	1:B:775:LEU:HD11	1:B:772:ARG:HA	6	0.2
(2,545)	1:B:775:LEU:HD12	1:B:772:ARG:HA	6	0.2
(2,545)	1:B:775:LEU:HD13	1:B:772:ARG:HA	6	0.2
(2,540)	1:B:775:LEU:H	1:B:772:ARG:HA	6	0.2
(2,531)	1:B:773:ASP:H	1:B:770:ARG:HD2	11	0.2
(2,531)	1:B:773:ASP:H	1:B:770:ARG:HD3	11	0.2
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD11	3	0.2
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD12	3	0.2
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD13	3	0.2
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD11	8	0.2
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD12	8	0.2
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD13	8	0.2
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE1	9	0.2
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE2	9	0.2
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE1	9	0.2
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE2	9	0.2
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE1	9	0.2
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE2	9	0.2
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE1	14	0.2
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE2	14	0.2
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE1	14	0.2
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE2	14	0.2
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE1	14	0.2
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE2	14	0.2
(2,518)	1:B:763:LEU:HD11	1:B:759:ASP:HA	13	0.2
(2,518)	1:B:763:LEU:HD12	1:B:759:ASP:HA	13	0.2
(2,518)	1:B:763:LEU:HD13	1:B:759:ASP:HA	13	0.2
(2,502)	1:B:755:LEU:H	1:B:752:SER:HA	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,501)	1:B:755:LEU:H	1:B:751:GLY:HA2	4	0.2
(2,501)	1:B:755:LEU:H	1:B:751:GLY:HA3	4	0.2
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB2	4	0.2
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB3	4	0.2
(2,482)	1:B:749:VAL:H	1:B:746:ILE:HA	7	0.2
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD2	9	0.2
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD3	9	0.2
(2,472)	1:B:746:ILE:HG21	1:B:750:ASN:HD21	15	0.2
(2,472)	1:B:746:ILE:HG22	1:B:750:ASN:HD21	15	0.2
(2,472)	1:B:746:ILE:HG23	1:B:750:ASN:HD21	15	0.2
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD11	11	0.2
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD12	11	0.2
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD13	11	0.2
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD21	11	0.2
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD22	11	0.2
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD23	11	0.2
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB2	3	0.2
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB3	3	0.2
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB2	4	0.2
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB3	4	0.2
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB2	7	0.2
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB3	7	0.2
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB2	7	0.2
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB3	7	0.2
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB2	7	0.2
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB3	7	0.2
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB2	8	0.2
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB3	8	0.2
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB2	8	0.2
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB3	8	0.2
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB2	8	0.2
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB3	8	0.2
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB2	14	0.2
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB3	14	0.2
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB2	14	0.2
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB3	14	0.2
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB2	14	0.2
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB3	14	0.2
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD1	12	0.2
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD2	12	0.2
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD1	12	0.2
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD2	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD1	12	0.2
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD2	12	0.2
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD1	13	0.2
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD2	13	0.2
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD1	13	0.2
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD2	13	0.2
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD1	13	0.2
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD2	13	0.2
(2,369)	1:B:701:VAL:H	1:B:698:VAL:HA	11	0.2
(2,356)	1:B:698:VAL:HG11	1:B:695:LEU:HG	6	0.2
(2,356)	1:B:698:VAL:HG12	1:B:695:LEU:HG	6	0.2
(2,356)	1:B:698:VAL:HG13	1:B:695:LEU:HG	6	0.2
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD2	2	0.2
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD3	2	0.2
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD2	2	0.2
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD3	2	0.2
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD2	2	0.2
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD3	2	0.2
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD2	12	0.2
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD3	12	0.2
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD2	12	0.2
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD3	12	0.2
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD2	12	0.2
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD3	12	0.2
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD11	8	0.2
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD12	8	0.2
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD13	8	0.2
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB2	4	0.2
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB3	4	0.2
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB2	4	0.2
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB3	4	0.2
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB2	4	0.2
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB3	4	0.2
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD11	10	0.2
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD12	10	0.2
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD13	10	0.2
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD11	2	0.2
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD12	2	0.2
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD13	2	0.2
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD21	2	0.2
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD22	2	0.2
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD23	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,259)	1:B:670:TRP:H	1:B:667:ALA:HA	2	0.2
(2,253)	1:B:669:LEU:H	1:B:666:TRP:HA	8	0.2
(2,229)	1:B:665:LYS:H	1:B:664:ASP:HA	1	0.2
(2,229)	1:B:665:LYS:H	1:B:664:ASP:HA	4	0.2
(2,229)	1:B:665:LYS:H	1:B:664:ASP:HA	8	0.2
(2,229)	1:B:665:LYS:H	1:B:664:ASP:HA	12	0.2
(2,225)	1:B:664:ASP:H	1:B:663:LEU:H	5	0.2
(2,224)	1:B:664:ASP:H	1:B:663:LEU:HA	1	0.2
(2,224)	1:B:664:ASP:H	1:B:663:LEU:HA	15	0.2
(2,222)	1:B:663:LEU:HD21	1:B:667:ALA:HB1	11	0.2
(2,222)	1:B:663:LEU:HD21	1:B:667:ALA:HB2	11	0.2
(2,222)	1:B:663:LEU:HD21	1:B:667:ALA:HB3	11	0.2
(2,222)	1:B:663:LEU:HD22	1:B:667:ALA:HB1	11	0.2
(2,222)	1:B:663:LEU:HD22	1:B:667:ALA:HB2	11	0.2
(2,222)	1:B:663:LEU:HD22	1:B:667:ALA:HB3	11	0.2
(2,222)	1:B:663:LEU:HD23	1:B:667:ALA:HB1	11	0.2
(2,222)	1:B:663:LEU:HD23	1:B:667:ALA:HB2	11	0.2
(2,222)	1:B:663:LEU:HD23	1:B:667:ALA:HB3	11	0.2
(2,219)	1:B:663:LEU:H	1:B:664:ASP:H	5	0.2
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG2	11	0.2
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG3	11	0.2
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG2	15	0.2
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG3	15	0.2
(2,189)	1:A:816:ASN:H	1:A:830:ILE:HD11	2	0.2
(2,189)	1:A:816:ASN:H	1:A:830:ILE:HD12	2	0.2
(2,189)	1:A:816:ASN:H	1:A:830:ILE:HD13	2	0.2
(2,188)	1:A:816:ASN:H	1:A:830:ILE:HD11	2	0.2
(2,188)	1:A:816:ASN:H	1:A:830:ILE:HD12	2	0.2
(2,188)	1:A:816:ASN:H	1:A:830:ILE:HD13	2	0.2
(2,183)	1:A:806:GLU:H	1:B:772:ARG:HE	6	0.2
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	8	0.2
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	8	0.2
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	8	0.2
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	8	0.2
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG12	5	0.2
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG13	5	0.2
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD11	6	0.2
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD12	6	0.2
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD13	6	0.2
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD21	6	0.2
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD22	6	0.2
(2,156)	1:A:792:ALA:H	1:B:753:LEU:HD23	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD2	8	0.2
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD3	8	0.2
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG2	13	0.2
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG3	13	0.2
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD21	1	0.2
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD22	1	0.2
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD23	1	0.2
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD11	14	0.2
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD12	14	0.2
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD13	14	0.2
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD21	14	0.2
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD22	14	0.2
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD23	14	0.2
(2,1431)	1:A:782:VAL:H	1:A:779:THR:HA	2	0.2
(2,1431)	1:A:782:VAL:H	1:A:779:THR:HA	7	0.2
(2,1414)	1:A:778:VAL:HG21	1:A:775:LEU:HA	11	0.2
(2,1414)	1:A:778:VAL:HG22	1:A:775:LEU:HA	11	0.2
(2,1414)	1:A:778:VAL:HG23	1:A:775:LEU:HA	11	0.2
(2,141)	1:B:771:LEU:H	1:A:806:GLU:HB2	9	0.2
(2,141)	1:B:771:LEU:H	1:A:806:GLU:HB3	9	0.2
(2,1402)	1:A:777:ILE:H	1:A:774:LEU:HA	10	0.2
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	9	0.2
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	9	0.2
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	9	0.2
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	9	0.2
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	9	0.2
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	9	0.2
(2,1356)	1:A:755:LEU:H	1:A:756:ILE:H	14	0.2
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	1	0.2
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	1	0.2
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	1	0.2
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	1	0.2
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	1	0.2
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	1	0.2
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	14	0.2
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	14	0.2
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	14	0.2
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	14	0.2
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	14	0.2
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	14	0.2
(2,1322)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	10	0.2
(2,1322)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1322)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	10	0.2
(2,1278)	1:A:708:VAL:HG11	1:A:705:VAL:HA	10	0.2
(2,1278)	1:A:708:VAL:HG12	1:A:705:VAL:HA	10	0.2
(2,1278)	1:A:708:VAL:HG13	1:A:705:VAL:HA	10	0.2
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB2	7	0.2
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB3	7	0.2
(2,126)	1:A:785:LEU:HD21	1:B:749:VAL:HB	1	0.2
(2,126)	1:A:785:LEU:HD22	1:B:749:VAL:HB	1	0.2
(2,126)	1:A:785:LEU:HD23	1:B:749:VAL:HB	1	0.2
(2,123)	1:A:785:LEU:HD21	1:B:747:ARG:HD2	10	0.2
(2,123)	1:A:785:LEU:HD21	1:B:747:ARG:HD3	10	0.2
(2,123)	1:A:785:LEU:HD22	1:B:747:ARG:HD2	10	0.2
(2,123)	1:A:785:LEU:HD22	1:B:747:ARG:HD3	10	0.2
(2,123)	1:A:785:LEU:HD23	1:B:747:ARG:HD2	10	0.2
(2,123)	1:A:785:LEU:HD23	1:B:747:ARG:HD3	10	0.2
(2,1223)	1:A:701:VAL:HG21	1:A:698:VAL:HA	13	0.2
(2,1223)	1:A:701:VAL:HG22	1:A:698:VAL:HA	13	0.2
(2,1223)	1:A:701:VAL:HG23	1:A:698:VAL:HA	13	0.2
(2,1219)	1:A:701:VAL:H	1:A:698:VAL:HA	5	0.2
(2,1213)	1:A:700:ALA:H	1:A:699:PHE:HA	15	0.2
(2,1202)	1:A:697:ILE:HG21	1:A:694:GLY:HA2	3	0.2
(2,1202)	1:A:697:ILE:HG21	1:A:694:GLY:HA3	3	0.2
(2,1202)	1:A:697:ILE:HG22	1:A:694:GLY:HA2	3	0.2
(2,1202)	1:A:697:ILE:HG22	1:A:694:GLY:HA3	3	0.2
(2,1202)	1:A:697:ILE:HG23	1:A:694:GLY:HA2	3	0.2
(2,1202)	1:A:697:ILE:HG23	1:A:694:GLY:HA3	3	0.2
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	5	0.2
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	5	0.2
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	5	0.2
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	5	0.2
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	5	0.2
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	5	0.2
(2,1190)	1:A:693:ILE:HG21	1:A:696:ARG:HG2	15	0.2
(2,1190)	1:A:693:ILE:HG21	1:A:696:ARG:HG3	15	0.2
(2,1190)	1:A:693:ILE:HG22	1:A:696:ARG:HG2	15	0.2
(2,1190)	1:A:693:ILE:HG22	1:A:696:ARG:HG3	15	0.2
(2,1190)	1:A:693:ILE:HG23	1:A:696:ARG:HG2	15	0.2
(2,1190)	1:A:693:ILE:HG23	1:A:696:ARG:HG3	15	0.2
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB2	11	0.2
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB3	11	0.2
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB2	11	0.2
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB3	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB2	11	0.2
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB3	11	0.2
(2,1144)	1:A:682:ILE:HG21	1:A:685:PHE:HB2	8	0.2
(2,1144)	1:A:682:ILE:HG21	1:A:685:PHE:HB3	8	0.2
(2,1144)	1:A:682:ILE:HG22	1:A:685:PHE:HB2	8	0.2
(2,1144)	1:A:682:ILE:HG22	1:A:685:PHE:HB3	8	0.2
(2,1144)	1:A:682:ILE:HG23	1:A:685:PHE:HB2	8	0.2
(2,1144)	1:A:682:ILE:HG23	1:A:685:PHE:HB3	8	0.2
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG21	2	0.2
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG22	2	0.2
(2,111)	1:A:781:ILE:H	1:B:746:ILE:HG23	2	0.2
(2,1095)	1:A:667:ALA:H	1:A:666:TRP:HD1	6	0.2
(2,1092)	1:A:667:ALA:H	1:A:664:ASP:HA	8	0.2
(2,1079)	1:A:665:LYS:H	1:A:664:ASP:HA	6	0.2
(2,1079)	1:A:665:LYS:H	1:A:664:ASP:HA	7	0.2
(2,1078)	1:A:665:LYS:H	1:A:662:GLU:HA	8	0.2
(2,1074)	1:A:664:ASP:H	1:A:663:LEU:HA	4	0.2
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD2	8	0.2
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD3	8	0.2
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG2	13	0.2
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG3	13	0.2
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD21	1	0.2
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD22	1	0.2
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD23	1	0.2
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD11	14	0.2
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD12	14	0.2
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD13	14	0.2
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD21	14	0.2
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD22	14	0.2
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD23	14	0.2
(2,1006)	1:A:782:VAL:H	1:A:779:THR:HA	2	0.2
(2,1006)	1:A:782:VAL:H	1:A:779:THR:HA	7	0.2
(1,75)	1:B:837:SER:O	1:B:841:ARG:H	5	0.2
(1,25)	1:B:802:TYR:O	1:B:806:GLU:H	13	0.2
(1,247)	1:B:837:SER:O	1:B:841:ARG:H	5	0.2
(1,23)	1:B:801:GLN:O	1:B:805:GLN:H	3	0.2
(1,197)	1:B:802:TYR:O	1:B:806:GLU:H	13	0.2
(1,195)	1:B:801:GLN:O	1:B:805:GLN:H	3	0.2
(1,191)	1:B:799:LEU:O	1:B:803:TRP:H	1	0.2
(1,19)	1:B:799:LEU:O	1:B:803:TRP:H	1	0.2
(1,161)	1:B:837:SER:O	1:B:841:ARG:H	5	0.2
(1,111)	1:B:802:TYR:O	1:B:806:GLU:H	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,109)	1:B:801:GLN:O	1:B:805:GLN:H	3	0.2
(1,105)	1:B:799:LEU:O	1:B:803:TRP:H	1	0.2
(2,990)	1:A:779:THR:H	1:A:776:LEU:HA	14	0.19
(2,943)	1:A:763:LEU:HD11	1:A:759:ASP:HA	8	0.19
(2,943)	1:A:763:LEU:HD12	1:A:759:ASP:HA	8	0.19
(2,943)	1:A:763:LEU:HD13	1:A:759:ASP:HA	8	0.19
(2,93)	1:A:754:ALA:H	1:B:716:SER:HB2	4	0.19
(2,93)	1:A:754:ALA:H	1:B:716:SER:HB3	4	0.19
(2,93)	1:A:754:ALA:H	1:B:716:SER:HB2	9	0.19
(2,93)	1:A:754:ALA:H	1:B:716:SER:HB3	9	0.19
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	14	0.19
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	14	0.19
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	14	0.19
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	14	0.19
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	14	0.19
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	14	0.19
(2,904)	1:A:748:LEU:H	1:A:745:SER:HA	8	0.19
(2,897)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	3	0.19
(2,897)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	3	0.19
(2,897)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	3	0.19
(2,895)	1:A:746:ILE:HD11	1:A:743:ASP:HA	6	0.19
(2,895)	1:A:746:ILE:HD12	1:A:743:ASP:HA	6	0.19
(2,895)	1:A:746:ILE:HD13	1:A:743:ASP:HA	6	0.19
(2,890)	1:A:746:ILE:H	1:A:743:ASP:HB2	15	0.19
(2,890)	1:A:746:ILE:H	1:A:743:ASP:HB3	15	0.19
(2,869)	1:A:710:GLN:H	1:A:710:GLN:HB3	13	0.19
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD11	11	0.19
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD12	11	0.19
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD13	11	0.19
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD21	11	0.19
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD22	11	0.19
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD23	11	0.19
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD2	4	0.19
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD3	4	0.19
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	9	0.19
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	9	0.19
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	9	0.19
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	9	0.19
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	9	0.19
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	9	0.19
(2,821)	1:A:705:VAL:H	1:A:702:LEU:HA	12	0.19
(2,788)	1:A:700:ALA:H	1:A:699:PHE:HA	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,788)	1:A:700:ALA:H	1:A:699:PHE:HA	13	0.19
(2,782)	1:A:698:VAL:HG11	1:A:699:PHE:HD1	15	0.19
(2,782)	1:A:698:VAL:HG11	1:A:699:PHE:HD2	15	0.19
(2,782)	1:A:698:VAL:HG12	1:A:699:PHE:HD1	15	0.19
(2,782)	1:A:698:VAL:HG12	1:A:699:PHE:HD2	15	0.19
(2,782)	1:A:698:VAL:HG13	1:A:699:PHE:HD1	15	0.19
(2,782)	1:A:698:VAL:HG13	1:A:699:PHE:HD2	15	0.19
(2,781)	1:A:698:VAL:HG11	1:A:695:LEU:HG	5	0.19
(2,781)	1:A:698:VAL:HG12	1:A:695:LEU:HG	5	0.19
(2,781)	1:A:698:VAL:HG13	1:A:695:LEU:HG	5	0.19
(2,780)	1:A:698:VAL:HG11	1:A:695:LEU:HA	3	0.19
(2,780)	1:A:698:VAL:HG12	1:A:695:LEU:HA	3	0.19
(2,780)	1:A:698:VAL:HG13	1:A:695:LEU:HA	3	0.19
(2,770)	1:A:695:LEU:HD21	1:A:698:VAL:HB	8	0.19
(2,770)	1:A:695:LEU:HD22	1:A:698:VAL:HB	8	0.19
(2,770)	1:A:695:LEU:HD23	1:A:698:VAL:HB	8	0.19
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE1	6	0.19
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE2	6	0.19
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE1	6	0.19
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE2	6	0.19
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE1	6	0.19
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE2	6	0.19
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE1	7	0.19
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE2	7	0.19
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE1	7	0.19
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE2	7	0.19
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE1	7	0.19
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE2	7	0.19
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE1	15	0.19
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE2	15	0.19
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE1	15	0.19
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE2	15	0.19
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE1	15	0.19
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE2	15	0.19
(2,746)	1:A:687:ILE:HD11	1:A:684:ILE:HD11	14	0.19
(2,746)	1:A:687:ILE:HD11	1:A:684:ILE:HD12	14	0.19
(2,746)	1:A:687:ILE:HD11	1:A:684:ILE:HD13	14	0.19
(2,746)	1:A:687:ILE:HD12	1:A:684:ILE:HD11	14	0.19
(2,746)	1:A:687:ILE:HD12	1:A:684:ILE:HD12	14	0.19
(2,746)	1:A:687:ILE:HD12	1:A:684:ILE:HD13	14	0.19
(2,746)	1:A:687:ILE:HD13	1:A:684:ILE:HD11	14	0.19
(2,746)	1:A:687:ILE:HD13	1:A:684:ILE:HD12	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,746)	1:A:687:ILE:HD13	1:A:684:ILE:HD13	14	0.19
(2,744)	1:A:686:ILE:HD11	1:A:685:PHE:HD1	3	0.19
(2,744)	1:A:686:ILE:HD11	1:A:685:PHE:HD2	3	0.19
(2,744)	1:A:686:ILE:HD12	1:A:685:PHE:HD1	3	0.19
(2,744)	1:A:686:ILE:HD12	1:A:685:PHE:HD2	3	0.19
(2,744)	1:A:686:ILE:HD13	1:A:685:PHE:HD1	3	0.19
(2,744)	1:A:686:ILE:HD13	1:A:685:PHE:HD2	3	0.19
(2,721)	1:A:682:ILE:HD11	1:A:681:TYR:H	10	0.19
(2,721)	1:A:682:ILE:HD12	1:A:681:TYR:H	10	0.19
(2,721)	1:A:682:ILE:HD13	1:A:681:TYR:H	10	0.19
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB2	3	0.19
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB3	3	0.19
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB2	3	0.19
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB3	3	0.19
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB2	3	0.19
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB3	3	0.19
(2,718)	1:A:682:ILE:HG21	1:A:679:LEU:H	1	0.19
(2,718)	1:A:682:ILE:HG22	1:A:679:LEU:H	1	0.19
(2,718)	1:A:682:ILE:HG23	1:A:679:LEU:H	1	0.19
(2,711)	1:A:678:TRP:HE1	1:A:682:ILE:H	2	0.19
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD11	1	0.19
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD12	1	0.19
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD13	1	0.19
(2,697)	1:A:674:ASP:H	1:A:677:ASN:H	11	0.19
(2,693)	1:A:672:TRP:H	1:A:673:PHE:H	1	0.19
(2,654)	1:A:665:LYS:H	1:A:664:ASP:HA	2	0.19
(2,654)	1:A:665:LYS:H	1:A:664:ASP:HA	12	0.19
(2,650)	1:A:664:ASP:H	1:A:663:LEU:H	14	0.19
(2,644)	1:A:663:LEU:H	1:A:664:ASP:H	14	0.19
(2,639)	1:A:661:LEU:HD11	1:A:662:GLU:HG2	7	0.19
(2,639)	1:A:661:LEU:HD11	1:A:662:GLU:HG3	7	0.19
(2,639)	1:A:661:LEU:HD12	1:A:662:GLU:HG2	7	0.19
(2,639)	1:A:661:LEU:HD12	1:A:662:GLU:HG3	7	0.19
(2,639)	1:A:661:LEU:HD13	1:A:662:GLU:HG2	7	0.19
(2,639)	1:A:661:LEU:HD13	1:A:662:GLU:HG3	7	0.19
(2,639)	1:A:661:LEU:HD21	1:A:662:GLU:HG2	7	0.19
(2,639)	1:A:661:LEU:HD21	1:A:662:GLU:HG3	7	0.19
(2,639)	1:A:661:LEU:HD22	1:A:662:GLU:HG2	7	0.19
(2,639)	1:A:661:LEU:HD22	1:A:662:GLU:HG3	7	0.19
(2,639)	1:A:661:LEU:HD23	1:A:662:GLU:HG2	7	0.19
(2,639)	1:A:661:LEU:HD23	1:A:662:GLU:HG3	7	0.19
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB2	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB3	1	0.19
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB2	10	0.19
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB3	10	0.19
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB2	11	0.19
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB3	11	0.19
(2,620)	1:B:802:TYR:H	1:B:802:TYR:HB3	6	0.19
(2,601)	1:B:785:LEU:H	1:B:782:VAL:HA	12	0.19
(2,593)	1:B:784:LEU:H	1:B:781:ILE:HA	3	0.19
(2,559)	1:B:778:VAL:H	1:B:775:LEU:HA	2	0.19
(2,545)	1:B:775:LEU:HD11	1:B:772:ARG:HA	7	0.19
(2,545)	1:B:775:LEU:HD12	1:B:772:ARG:HA	7	0.19
(2,545)	1:B:775:LEU:HD13	1:B:772:ARG:HA	7	0.19
(2,540)	1:B:775:LEU:H	1:B:772:ARG:HA	7	0.19
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD11	4	0.19
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD12	4	0.19
(2,53)	1:A:696:ARG:H	1:A:693:ILE:HD13	4	0.19
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH21	9	0.19
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH22	9	0.19
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH21	9	0.19
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH22	9	0.19
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH21	9	0.19
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH22	9	0.19
(2,522)	1:B:764:SER:H	1:B:761:ARG:HA	5	0.19
(2,521)	1:B:763:LEU:HD21	1:B:771:LEU:HB2	12	0.19
(2,521)	1:B:763:LEU:HD21	1:B:771:LEU:HB3	12	0.19
(2,521)	1:B:763:LEU:HD22	1:B:771:LEU:HB2	12	0.19
(2,521)	1:B:763:LEU:HD22	1:B:771:LEU:HB3	12	0.19
(2,521)	1:B:763:LEU:HD23	1:B:771:LEU:HB2	12	0.19
(2,521)	1:B:763:LEU:HD23	1:B:771:LEU:HB3	12	0.19
(2,519)	1:B:763:LEU:HD11	1:B:764:SER:HG	1	0.19
(2,519)	1:B:763:LEU:HD12	1:B:764:SER:HG	1	0.19
(2,519)	1:B:763:LEU:HD13	1:B:764:SER:HG	1	0.19
(2,502)	1:B:755:LEU:H	1:B:752:SER:HA	4	0.19
(2,502)	1:B:755:LEU:H	1:B:752:SER:HA	8	0.19
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA2	8	0.19
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA3	8	0.19
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA2	8	0.19
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA3	8	0.19
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA2	8	0.19
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA3	8	0.19
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA2	14	0.19
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA3	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA2	14	0.19
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA3	14	0.19
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA2	14	0.19
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA3	14	0.19
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB2	6	0.19
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB3	6	0.19
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB2	15	0.19
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB3	15	0.19
(2,396)	1:B:705:VAL:H	1:B:702:LEU:HA	12	0.19
(2,390)	1:B:704:LEU:H	1:B:704:LEU:HB3	7	0.19
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD1	10	0.19
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD2	10	0.19
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD1	10	0.19
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD2	10	0.19
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD1	10	0.19
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD2	10	0.19
(2,363)	1:B:700:ALA:H	1:B:699:PHE:HA	8	0.19
(2,356)	1:B:698:VAL:HG11	1:B:695:LEU:HG	4	0.19
(2,356)	1:B:698:VAL:HG12	1:B:695:LEU:HG	4	0.19
(2,356)	1:B:698:VAL:HG13	1:B:695:LEU:HG	4	0.19
(2,352)	1:B:697:ILE:HG21	1:B:694:GLY:HA2	10	0.19
(2,352)	1:B:697:ILE:HG21	1:B:694:GLY:HA3	10	0.19
(2,352)	1:B:697:ILE:HG22	1:B:694:GLY:HA2	10	0.19
(2,352)	1:B:697:ILE:HG22	1:B:694:GLY:HA3	10	0.19
(2,352)	1:B:697:ILE:HG23	1:B:694:GLY:HA2	10	0.19
(2,352)	1:B:697:ILE:HG23	1:B:694:GLY:HA3	10	0.19
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD2	6	0.19
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD3	6	0.19
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD2	6	0.19
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD3	6	0.19
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD2	6	0.19
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD3	6	0.19
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD2	9	0.19
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD3	9	0.19
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD2	9	0.19
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD3	9	0.19
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD2	9	0.19
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD3	9	0.19
(2,330)	1:B:692:LEU:HD11	1:B:689:VAL:HA	11	0.19
(2,330)	1:B:692:LEU:HD12	1:B:689:VAL:HA	11	0.19
(2,330)	1:B:692:LEU:HD13	1:B:689:VAL:HA	11	0.19
(2,286)	1:B:678:TRP:HE1	1:B:682:ILE:H	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,280)	1:B:676:THR:HG21	1:B:681:TYR:HH	2	0.19
(2,280)	1:B:676:THR:HG22	1:B:681:TYR:HH	2	0.19
(2,280)	1:B:676:THR:HG23	1:B:681:TYR:HH	2	0.19
(2,272)	1:B:674:ASP:H	1:B:677:ASN:H	3	0.19
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD11	5	0.19
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD12	5	0.19
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD13	5	0.19
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD21	5	0.19
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD22	5	0.19
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD23	5	0.19
(2,245)	1:B:667:ALA:H	1:B:666:TRP:HD1	6	0.19
(2,242)	1:B:667:ALA:H	1:B:664:ASP:HA	14	0.19
(2,229)	1:B:665:LYS:H	1:B:664:ASP:HA	5	0.19
(2,229)	1:B:665:LYS:H	1:B:664:ASP:HA	7	0.19
(2,229)	1:B:665:LYS:H	1:B:664:ASP:HA	9	0.19
(2,229)	1:B:665:LYS:H	1:B:664:ASP:HA	10	0.19
(2,229)	1:B:665:LYS:H	1:B:664:ASP:HA	14	0.19
(2,224)	1:B:664:ASP:H	1:B:663:LEU:HA	13	0.19
(2,204)	1:A:827:ASP:H	1:A:820:ILE:HG12	15	0.19
(2,204)	1:A:827:ASP:H	1:A:820:ILE:HG13	15	0.19
(2,203)	1:A:827:ASP:H	1:A:820:ILE:HG12	15	0.19
(2,203)	1:A:827:ASP:H	1:A:820:ILE:HG13	15	0.19
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD11	7	0.19
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD12	7	0.19
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD13	7	0.19
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD11	7	0.19
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD12	7	0.19
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD13	7	0.19
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG12	7	0.19
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG13	7	0.19
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG12	7	0.19
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG13	7	0.19
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG12	13	0.19
(2,193)	1:B:817:ALA:H	1:B:830:ILE:HG13	13	0.19
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD2	1	0.19
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD3	1	0.19
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD2	8	0.19
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD3	8	0.19
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	5	0.19
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	5	0.19
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	5	0.19
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG12	2	0.19
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG13	2	0.19
(2,150)	1:A:790:TRP:HE1	1:A:851:LEU:HD11	5	0.19
(2,150)	1:A:790:TRP:HE1	1:A:851:LEU:HD12	5	0.19
(2,150)	1:A:790:TRP:HE1	1:A:851:LEU:HD13	5	0.19
(2,150)	1:A:790:TRP:HE1	1:A:851:LEU:HD21	5	0.19
(2,150)	1:A:790:TRP:HE1	1:A:851:LEU:HD22	5	0.19
(2,150)	1:A:790:TRP:HE1	1:A:851:LEU:HD23	5	0.19
(2,149)	1:A:790:TRP:HE1	1:A:851:LEU:HD11	5	0.19
(2,149)	1:A:790:TRP:HE1	1:A:851:LEU:HD12	5	0.19
(2,149)	1:A:790:TRP:HE1	1:A:851:LEU:HD13	5	0.19
(2,149)	1:A:790:TRP:HE1	1:A:851:LEU:HD21	5	0.19
(2,149)	1:A:790:TRP:HE1	1:A:851:LEU:HD22	5	0.19
(2,149)	1:A:790:TRP:HE1	1:A:851:LEU:HD23	5	0.19
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE21	2	0.19
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE22	2	0.19
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE21	12	0.19
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE22	12	0.19
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE21	15	0.19
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE22	15	0.19
(2,1457)	1:A:785:LEU:HD21	1:A:782:VAL:HA	11	0.19
(2,1457)	1:A:785:LEU:HD22	1:A:782:VAL:HA	11	0.19
(2,1457)	1:A:785:LEU:HD23	1:A:782:VAL:HA	11	0.19
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD2	9	0.19
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD3	9	0.19
(2,1415)	1:A:779:THR:H	1:A:776:LEU:HA	14	0.19
(2,1368)	1:A:763:LEU:HD11	1:A:759:ASP:HA	8	0.19
(2,1368)	1:A:763:LEU:HD12	1:A:759:ASP:HA	8	0.19
(2,1368)	1:A:763:LEU:HD13	1:A:759:ASP:HA	8	0.19
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	14	0.19
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	14	0.19
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	14	0.19
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	14	0.19
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	14	0.19
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	14	0.19
(2,1329)	1:A:748:LEU:H	1:A:745:SER:HA	8	0.19
(2,1322)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	3	0.19
(2,1322)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	3	0.19
(2,1322)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	3	0.19
(2,1320)	1:A:746:ILE:HD11	1:A:743:ASP:HA	6	0.19
(2,1320)	1:A:746:ILE:HD12	1:A:743:ASP:HA	6	0.19
(2,1320)	1:A:746:ILE:HD13	1:A:743:ASP:HA	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1315)	1:A:746:ILE:H	1:A:743:ASP:HB2	15	0.19
(2,1315)	1:A:746:ILE:H	1:A:743:ASP:HB3	15	0.19
(2,13)	1:B:666:TRP:HE1	1:A:666:TRP:HD1	15	0.19
(2,1294)	1:A:710:GLN:H	1:A:710:GLN:HB3	13	0.19
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD11	11	0.19
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD12	11	0.19
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD13	11	0.19
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD21	11	0.19
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD22	11	0.19
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD23	11	0.19
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD2	4	0.19
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD3	4	0.19
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	9	0.19
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	9	0.19
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	9	0.19
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	9	0.19
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	9	0.19
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	9	0.19
(2,1246)	1:A:705:VAL:H	1:A:702:LEU:HA	12	0.19
(2,1213)	1:A:700:ALA:H	1:A:699:PHE:HA	2	0.19
(2,1213)	1:A:700:ALA:H	1:A:699:PHE:HA	13	0.19
(2,1207)	1:A:698:VAL:HG11	1:A:699:PHE:HD1	15	0.19
(2,1207)	1:A:698:VAL:HG11	1:A:699:PHE:HD2	15	0.19
(2,1207)	1:A:698:VAL:HG12	1:A:699:PHE:HD1	15	0.19
(2,1207)	1:A:698:VAL:HG12	1:A:699:PHE:HD2	15	0.19
(2,1207)	1:A:698:VAL:HG13	1:A:699:PHE:HD1	15	0.19
(2,1207)	1:A:698:VAL:HG13	1:A:699:PHE:HD2	15	0.19
(2,1206)	1:A:698:VAL:HG11	1:A:695:LEU:HG	5	0.19
(2,1206)	1:A:698:VAL:HG12	1:A:695:LEU:HG	5	0.19
(2,1206)	1:A:698:VAL:HG13	1:A:695:LEU:HG	5	0.19
(2,1205)	1:A:698:VAL:HG11	1:A:695:LEU:HA	3	0.19
(2,1205)	1:A:698:VAL:HG12	1:A:695:LEU:HA	3	0.19
(2,1205)	1:A:698:VAL:HG13	1:A:695:LEU:HA	3	0.19
(2,1195)	1:A:695:LEU:HD21	1:A:698:VAL:HB	8	0.19
(2,1195)	1:A:695:LEU:HD22	1:A:698:VAL:HB	8	0.19
(2,1195)	1:A:695:LEU:HD23	1:A:698:VAL:HB	8	0.19
(2,1171)	1:A:687:ILE:HD11	1:A:684:ILE:HD11	14	0.19
(2,1171)	1:A:687:ILE:HD11	1:A:684:ILE:HD12	14	0.19
(2,1171)	1:A:687:ILE:HD11	1:A:684:ILE:HD13	14	0.19
(2,1171)	1:A:687:ILE:HD12	1:A:684:ILE:HD11	14	0.19
(2,1171)	1:A:687:ILE:HD12	1:A:684:ILE:HD12	14	0.19
(2,1171)	1:A:687:ILE:HD12	1:A:684:ILE:HD13	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1171)	1:A:687:ILE:HD13	1:A:684:ILE:HD11	14	0.19
(2,1171)	1:A:687:ILE:HD13	1:A:684:ILE:HD12	14	0.19
(2,1171)	1:A:687:ILE:HD13	1:A:684:ILE:HD13	14	0.19
(2,1169)	1:A:686:ILE:HD11	1:A:685:PHE:HD1	3	0.19
(2,1169)	1:A:686:ILE:HD11	1:A:685:PHE:HD2	3	0.19
(2,1169)	1:A:686:ILE:HD12	1:A:685:PHE:HD1	3	0.19
(2,1169)	1:A:686:ILE:HD12	1:A:685:PHE:HD2	3	0.19
(2,1169)	1:A:686:ILE:HD13	1:A:685:PHE:HD1	3	0.19
(2,1169)	1:A:686:ILE:HD13	1:A:685:PHE:HD2	3	0.19
(2,1146)	1:A:682:ILE:HD11	1:A:681:TYR:H	10	0.19
(2,1146)	1:A:682:ILE:HD12	1:A:681:TYR:H	10	0.19
(2,1146)	1:A:682:ILE:HD13	1:A:681:TYR:H	10	0.19
(2,1143)	1:A:682:ILE:HG21	1:A:679:LEU:H	1	0.19
(2,1143)	1:A:682:ILE:HG22	1:A:679:LEU:H	1	0.19
(2,1143)	1:A:682:ILE:HG23	1:A:679:LEU:H	1	0.19
(2,1136)	1:A:678:TRP:HE1	1:A:682:ILE:H	2	0.19
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD11	1	0.19
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD12	1	0.19
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD13	1	0.19
(2,1122)	1:A:674:ASP:H	1:A:677:ASN:H	11	0.19
(2,1118)	1:A:672:TRP:H	1:A:673:PHE:H	1	0.19
(2,1079)	1:A:665:LYS:H	1:A:664:ASP:HA	2	0.19
(2,1079)	1:A:665:LYS:H	1:A:664:ASP:HA	12	0.19
(2,1075)	1:A:664:ASP:H	1:A:663:LEU:H	14	0.19
(2,1069)	1:A:663:LEU:H	1:A:664:ASP:H	14	0.19
(2,1064)	1:A:661:LEU:HD11	1:A:662:GLU:HG2	7	0.19
(2,1064)	1:A:661:LEU:HD11	1:A:662:GLU:HG3	7	0.19
(2,1064)	1:A:661:LEU:HD12	1:A:662:GLU:HG2	7	0.19
(2,1064)	1:A:661:LEU:HD12	1:A:662:GLU:HG3	7	0.19
(2,1064)	1:A:661:LEU:HD13	1:A:662:GLU:HG2	7	0.19
(2,1064)	1:A:661:LEU:HD13	1:A:662:GLU:HG3	7	0.19
(2,1064)	1:A:661:LEU:HD21	1:A:662:GLU:HG2	7	0.19
(2,1064)	1:A:661:LEU:HD21	1:A:662:GLU:HG3	7	0.19
(2,1064)	1:A:661:LEU:HD22	1:A:662:GLU:HG2	7	0.19
(2,1064)	1:A:661:LEU:HD22	1:A:662:GLU:HG3	7	0.19
(2,1064)	1:A:661:LEU:HD23	1:A:662:GLU:HG2	7	0.19
(2,1064)	1:A:661:LEU:HD23	1:A:662:GLU:HG3	7	0.19
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE21	2	0.19
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE22	2	0.19
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE21	12	0.19
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE22	12	0.19
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE21	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE22	15	0.19
(2,1032)	1:A:785:LEU:HD21	1:A:782:VAL:HA	11	0.19
(2,1032)	1:A:785:LEU:HD22	1:A:782:VAL:HA	11	0.19
(2,1032)	1:A:785:LEU:HD23	1:A:782:VAL:HA	11	0.19
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD2	9	0.19
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD3	9	0.19
(1,96)	1:B:794:LYS:O	1:B:798:ASN:N	12	0.19
(1,95)	1:B:794:LYS:O	1:B:798:ASN:H	5	0.19
(1,95)	1:B:794:LYS:O	1:B:798:ASN:H	7	0.19
(1,95)	1:B:794:LYS:O	1:B:798:ASN:H	15	0.19
(1,9)	1:B:794:LYS:O	1:B:798:ASN:H	5	0.19
(1,9)	1:B:794:LYS:O	1:B:798:ASN:H	7	0.19
(1,9)	1:B:794:LYS:O	1:B:798:ASN:H	15	0.19
(1,24)	1:B:801:GLN:O	1:B:805:GLN:N	13	0.19
(1,23)	1:B:801:GLN:O	1:B:805:GLN:H	11	0.19
(1,21)	1:B:800:LEU:O	1:B:804:SER:H	9	0.19
(1,196)	1:B:801:GLN:O	1:B:805:GLN:N	13	0.19
(1,195)	1:B:801:GLN:O	1:B:805:GLN:H	11	0.19
(1,193)	1:B:800:LEU:O	1:B:804:SER:H	9	0.19
(1,191)	1:B:799:LEU:O	1:B:803:TRP:H	3	0.19
(1,19)	1:B:799:LEU:O	1:B:803:TRP:H	3	0.19
(1,182)	1:B:794:LYS:O	1:B:798:ASN:N	12	0.19
(1,181)	1:B:794:LYS:O	1:B:798:ASN:H	5	0.19
(1,181)	1:B:794:LYS:O	1:B:798:ASN:H	7	0.19
(1,181)	1:B:794:LYS:O	1:B:798:ASN:H	15	0.19
(1,110)	1:B:801:GLN:O	1:B:805:GLN:N	13	0.19
(1,109)	1:B:801:GLN:O	1:B:805:GLN:H	11	0.19
(1,107)	1:B:800:LEU:O	1:B:804:SER:H	9	0.19
(1,105)	1:B:799:LEU:O	1:B:803:TRP:H	3	0.19
(1,10)	1:B:794:LYS:O	1:B:798:ASN:N	12	0.19
(2,989)	1:A:778:VAL:HG21	1:A:775:LEU:HA	8	0.18
(2,989)	1:A:778:VAL:HG22	1:A:775:LEU:HA	8	0.18
(2,989)	1:A:778:VAL:HG23	1:A:775:LEU:HA	8	0.18
(2,984)	1:A:778:VAL:H	1:A:775:LEU:HA	14	0.18
(2,983)	1:A:777:ILE:HG21	1:A:780:ARG:HD2	8	0.18
(2,983)	1:A:777:ILE:HG21	1:A:780:ARG:HD3	8	0.18
(2,983)	1:A:777:ILE:HG22	1:A:780:ARG:HD2	8	0.18
(2,983)	1:A:777:ILE:HG22	1:A:780:ARG:HD3	8	0.18
(2,983)	1:A:777:ILE:HG23	1:A:780:ARG:HD2	8	0.18
(2,983)	1:A:777:ILE:HG23	1:A:780:ARG:HD3	8	0.18
(2,956)	1:A:773:ASP:H	1:A:770:ARG:HD2	9	0.18
(2,956)	1:A:773:ASP:H	1:A:770:ARG:HD3	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,939)	1:A:760:LEU:HD11	1:A:756:ILE:HG12	10	0.18
(2,939)	1:A:760:LEU:HD11	1:A:756:ILE:HG13	10	0.18
(2,939)	1:A:760:LEU:HD12	1:A:756:ILE:HG12	10	0.18
(2,939)	1:A:760:LEU:HD12	1:A:756:ILE:HG13	10	0.18
(2,939)	1:A:760:LEU:HD13	1:A:756:ILE:HG12	10	0.18
(2,939)	1:A:760:LEU:HD13	1:A:756:ILE:HG13	10	0.18
(2,93)	1:A:754:ALA:H	1:B:716:SER:HB2	3	0.18
(2,93)	1:A:754:ALA:H	1:B:716:SER:HB3	3	0.18
(2,93)	1:A:754:ALA:H	1:B:716:SER:HB2	8	0.18
(2,93)	1:A:754:ALA:H	1:B:716:SER:HB3	8	0.18
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD2	3	0.18
(2,903)	1:A:748:LEU:H	1:A:744:ARG:HD3	3	0.18
(2,864)	1:A:710:GLN:H	1:A:708:VAL:HA	5	0.18
(2,864)	1:A:710:GLN:H	1:A:708:VAL:HA	7	0.18
(2,864)	1:A:710:GLN:H	1:A:708:VAL:HA	14	0.18
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB2	5	0.18
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB3	5	0.18
(2,820)	1:A:704:LEU:HD11	1:A:708:VAL:HG21	7	0.18
(2,820)	1:A:704:LEU:HD11	1:A:708:VAL:HG22	7	0.18
(2,820)	1:A:704:LEU:HD11	1:A:708:VAL:HG23	7	0.18
(2,820)	1:A:704:LEU:HD12	1:A:708:VAL:HG21	7	0.18
(2,820)	1:A:704:LEU:HD12	1:A:708:VAL:HG22	7	0.18
(2,820)	1:A:704:LEU:HD12	1:A:708:VAL:HG23	7	0.18
(2,820)	1:A:704:LEU:HD13	1:A:708:VAL:HG21	7	0.18
(2,820)	1:A:704:LEU:HD13	1:A:708:VAL:HG22	7	0.18
(2,820)	1:A:704:LEU:HD13	1:A:708:VAL:HG23	7	0.18
(2,81)	1:A:708:VAL:HG21	1:B:714:PRO:HA	13	0.18
(2,81)	1:A:708:VAL:HG22	1:B:714:PRO:HA	13	0.18
(2,81)	1:A:708:VAL:HG23	1:B:714:PRO:HA	13	0.18
(2,794)	1:A:701:VAL:H	1:A:698:VAL:HA	7	0.18
(2,788)	1:A:700:ALA:H	1:A:699:PHE:HA	1	0.18
(2,788)	1:A:700:ALA:H	1:A:699:PHE:HA	3	0.18
(2,788)	1:A:700:ALA:H	1:A:699:PHE:HA	5	0.18
(2,788)	1:A:700:ALA:H	1:A:699:PHE:HA	6	0.18
(2,788)	1:A:700:ALA:H	1:A:699:PHE:HA	8	0.18
(2,788)	1:A:700:ALA:H	1:A:699:PHE:HA	9	0.18
(2,788)	1:A:700:ALA:H	1:A:699:PHE:HA	10	0.18
(2,788)	1:A:700:ALA:H	1:A:699:PHE:HA	11	0.18
(2,788)	1:A:700:ALA:H	1:A:699:PHE:HA	12	0.18
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB1	15	0.18
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB2	15	0.18
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB3	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB1	15	0.18
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB2	15	0.18
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB3	15	0.18
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB1	15	0.18
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB2	15	0.18
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB3	15	0.18
(2,777)	1:A:697:ILE:HG21	1:A:694:GLY:HA2	6	0.18
(2,777)	1:A:697:ILE:HG21	1:A:694:GLY:HA3	6	0.18
(2,777)	1:A:697:ILE:HG22	1:A:694:GLY:HA2	6	0.18
(2,777)	1:A:697:ILE:HG22	1:A:694:GLY:HA3	6	0.18
(2,777)	1:A:697:ILE:HG23	1:A:694:GLY:HA2	6	0.18
(2,777)	1:A:697:ILE:HG23	1:A:694:GLY:HA3	6	0.18
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	9	0.18
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	9	0.18
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	9	0.18
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	9	0.18
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	9	0.18
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	9	0.18
(2,763)	1:A:693:ILE:HG21	1:A:693:ILE:H	6	0.18
(2,763)	1:A:693:ILE:HG22	1:A:693:ILE:H	6	0.18
(2,763)	1:A:693:ILE:HG23	1:A:693:ILE:H	6	0.18
(2,751)	1:A:689:VAL:HG21	1:A:685:PHE:HD1	3	0.18
(2,751)	1:A:689:VAL:HG21	1:A:685:PHE:HD2	3	0.18
(2,751)	1:A:689:VAL:HG22	1:A:685:PHE:HD1	3	0.18
(2,751)	1:A:689:VAL:HG22	1:A:685:PHE:HD2	3	0.18
(2,751)	1:A:689:VAL:HG23	1:A:685:PHE:HD1	3	0.18
(2,751)	1:A:689:VAL:HG23	1:A:685:PHE:HD2	3	0.18
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE1	9	0.18
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE2	9	0.18
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE1	9	0.18
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE2	9	0.18
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE1	9	0.18
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE2	9	0.18
(2,721)	1:A:682:ILE:HD11	1:A:681:TYR:H	5	0.18
(2,721)	1:A:682:ILE:HD12	1:A:681:TYR:H	5	0.18
(2,721)	1:A:682:ILE:HD13	1:A:681:TYR:H	5	0.18
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB2	9	0.18
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB3	9	0.18
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB2	9	0.18
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB3	9	0.18
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB2	9	0.18
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB3	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,715)	1:A:680:TRP:HE1	1:A:684:ILE:HD11	5	0.18
(2,715)	1:A:680:TRP:HE1	1:A:684:ILE:HD12	5	0.18
(2,715)	1:A:680:TRP:HE1	1:A:684:ILE:HD13	5	0.18
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD11	9	0.18
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD12	9	0.18
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD13	9	0.18
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD21	9	0.18
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD22	9	0.18
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD23	9	0.18
(2,649)	1:A:664:ASP:H	1:A:663:LEU:HA	14	0.18
(2,649)	1:A:664:ASP:H	1:A:663:LEU:HA	15	0.18
(2,639)	1:A:661:LEU:HD11	1:A:662:GLU:HG2	9	0.18
(2,639)	1:A:661:LEU:HD11	1:A:662:GLU:HG3	9	0.18
(2,639)	1:A:661:LEU:HD12	1:A:662:GLU:HG2	9	0.18
(2,639)	1:A:661:LEU:HD12	1:A:662:GLU:HG3	9	0.18
(2,639)	1:A:661:LEU:HD13	1:A:662:GLU:HG2	9	0.18
(2,639)	1:A:661:LEU:HD13	1:A:662:GLU:HG3	9	0.18
(2,639)	1:A:661:LEU:HD21	1:A:662:GLU:HG2	9	0.18
(2,639)	1:A:661:LEU:HD21	1:A:662:GLU:HG3	9	0.18
(2,639)	1:A:661:LEU:HD22	1:A:662:GLU:HG2	9	0.18
(2,639)	1:A:661:LEU:HD22	1:A:662:GLU:HG3	9	0.18
(2,639)	1:A:661:LEU:HD23	1:A:662:GLU:HG2	9	0.18
(2,639)	1:A:661:LEU:HD23	1:A:662:GLU:HG3	9	0.18
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG11	11	0.18
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG12	11	0.18
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG13	11	0.18
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG21	11	0.18
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG22	11	0.18
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG23	11	0.18
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB2	13	0.18
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB3	13	0.18
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD11	3	0.18
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD12	3	0.18
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD13	3	0.18
(2,615)	1:B:796:TRP:HE1	1:B:796:TRP:H	11	0.18
(2,581)	1:B:782:VAL:H	1:B:779:THR:HA	5	0.18
(2,581)	1:B:782:VAL:H	1:B:779:THR:HA	8	0.18
(2,55)	1:B:696:ARG:HE	1:A:694:GLY:HA2	1	0.18
(2,55)	1:B:696:ARG:HE	1:A:694:GLY:HA3	1	0.18
(2,545)	1:B:775:LEU:HD11	1:B:772:ARG:HA	4	0.18
(2,545)	1:B:775:LEU:HD12	1:B:772:ARG:HA	4	0.18
(2,545)	1:B:775:LEU:HD13	1:B:772:ARG:HA	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH21	3	0.18
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH22	3	0.18
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH21	3	0.18
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH22	3	0.18
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH21	3	0.18
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH22	3	0.18
(2,522)	1:B:764:SER:H	1:B:761:ARG:HA	6	0.18
(2,52)	1:B:696:ARG:H	1:A:693:ILE:HD11	11	0.18
(2,52)	1:B:696:ARG:H	1:A:693:ILE:HD12	11	0.18
(2,52)	1:B:696:ARG:H	1:A:693:ILE:HD13	11	0.18
(2,420)	1:B:707:ARG:H	1:B:707:ARG:HG2	11	0.18
(2,420)	1:B:707:ARG:H	1:B:707:ARG:HG3	11	0.18
(2,405)	1:B:705:VAL:HG21	1:B:702:LEU:HG	2	0.18
(2,405)	1:B:705:VAL:HG22	1:B:702:LEU:HG	2	0.18
(2,405)	1:B:705:VAL:HG23	1:B:702:LEU:HG	2	0.18
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB2	12	0.18
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB3	12	0.18
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB2	12	0.18
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB3	12	0.18
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB2	12	0.18
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB3	12	0.18
(2,369)	1:B:701:VAL:H	1:B:698:VAL:HA	6	0.18
(2,363)	1:B:700:ALA:H	1:B:699:PHE:HA	4	0.18
(2,363)	1:B:700:ALA:H	1:B:699:PHE:HA	5	0.18
(2,363)	1:B:700:ALA:H	1:B:699:PHE:HA	9	0.18
(2,363)	1:B:700:ALA:H	1:B:699:PHE:HA	10	0.18
(2,363)	1:B:700:ALA:H	1:B:699:PHE:HA	11	0.18
(2,363)	1:B:700:ALA:H	1:B:699:PHE:HA	13	0.18
(2,357)	1:B:698:VAL:HG11	1:B:699:PHE:HD1	3	0.18
(2,357)	1:B:698:VAL:HG11	1:B:699:PHE:HD2	3	0.18
(2,357)	1:B:698:VAL:HG12	1:B:699:PHE:HD1	3	0.18
(2,357)	1:B:698:VAL:HG12	1:B:699:PHE:HD2	3	0.18
(2,357)	1:B:698:VAL:HG13	1:B:699:PHE:HD1	3	0.18
(2,357)	1:B:698:VAL:HG13	1:B:699:PHE:HD2	3	0.18
(2,356)	1:B:698:VAL:HG11	1:B:695:LEU:HG	1	0.18
(2,356)	1:B:698:VAL:HG12	1:B:695:LEU:HG	1	0.18
(2,356)	1:B:698:VAL:HG13	1:B:695:LEU:HG	1	0.18
(2,356)	1:B:698:VAL:HG11	1:B:695:LEU:HG	14	0.18
(2,356)	1:B:698:VAL:HG12	1:B:695:LEU:HG	14	0.18
(2,356)	1:B:698:VAL:HG13	1:B:695:LEU:HG	14	0.18
(2,340)	1:B:693:ILE:HG21	1:B:696:ARG:HG2	11	0.18
(2,340)	1:B:693:ILE:HG21	1:B:696:ARG:HG3	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,340)	1:B:693:ILE:HG22	1:B:696:ARG:HG2	11	0.18
(2,340)	1:B:693:ILE:HG22	1:B:696:ARG:HG3	11	0.18
(2,340)	1:B:693:ILE:HG23	1:B:696:ARG:HG2	11	0.18
(2,340)	1:B:693:ILE:HG23	1:B:696:ARG:HG3	11	0.18
(2,340)	1:B:693:ILE:HG21	1:B:696:ARG:HG2	14	0.18
(2,340)	1:B:693:ILE:HG21	1:B:696:ARG:HG3	14	0.18
(2,340)	1:B:693:ILE:HG22	1:B:696:ARG:HG2	14	0.18
(2,340)	1:B:693:ILE:HG22	1:B:696:ARG:HG3	14	0.18
(2,340)	1:B:693:ILE:HG23	1:B:696:ARG:HG2	14	0.18
(2,340)	1:B:693:ILE:HG23	1:B:696:ARG:HG3	14	0.18
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD11	4	0.18
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD12	4	0.18
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD13	4	0.18
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD11	4	0.18
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD12	4	0.18
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD13	4	0.18
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD11	4	0.18
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD12	4	0.18
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD13	4	0.18
(2,292)	1:B:681:TYR:H	1:B:682:ILE:H	13	0.18
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD11	15	0.18
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD12	15	0.18
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD13	15	0.18
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD21	15	0.18
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD22	15	0.18
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD23	15	0.18
(2,272)	1:B:674:ASP:H	1:B:677:ASN:H	11	0.18
(2,245)	1:B:667:ALA:H	1:B:666:TRP:HD1	2	0.18
(2,242)	1:B:667:ALA:H	1:B:664:ASP:HA	13	0.18
(2,225)	1:B:664:ASP:H	1:B:663:LEU:H	2	0.18
(2,224)	1:B:664:ASP:H	1:B:663:LEU:HA	2	0.18
(2,224)	1:B:664:ASP:H	1:B:663:LEU:HA	5	0.18
(2,224)	1:B:664:ASP:H	1:B:663:LEU:HA	7	0.18
(2,219)	1:B:663:LEU:H	1:B:664:ASP:H	2	0.18
(2,177)	1:A:803:TRP:HE1	1:B:764:SER:HG	5	0.18
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG12	15	0.18
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG13	15	0.18
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG12	15	0.18
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG13	15	0.18
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG12	4	0.18
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG13	4	0.18
(2,153)	1:A:792:ALA:H	1:B:752:SER:HB2	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,153)	1:A:792:ALA:H	1:B:752:SER:HB3	1	0.18
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	2	0.18
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	2	0.18
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	2	0.18
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	2	0.18
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	2	0.18
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	2	0.18
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	2	0.18
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	2	0.18
(2,1475)	1:A:806:GLU:H	1:A:803:TRP:HB2	8	0.18
(2,1475)	1:A:806:GLU:H	1:A:803:TRP:HB3	8	0.18
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	12	0.18
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	12	0.18
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	12	0.18
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	12	0.18
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	12	0.18
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	12	0.18
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD21	3	0.18
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD22	3	0.18
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD23	3	0.18
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD21	7	0.18
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD22	7	0.18
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD23	7	0.18
(2,1451)	1:A:785:LEU:H	1:A:782:VAL:HA	13	0.18
(2,1443)	1:A:784:LEU:H	1:A:781:ILE:HA	6	0.18
(2,1443)	1:A:784:LEU:H	1:A:781:ILE:HA	13	0.18
(2,1425)	1:A:781:ILE:H	1:A:778:VAL:HA	7	0.18
(2,142)	1:A:781:ILE:H	1:B:746:ILE:HG12	5	0.18
(2,142)	1:A:781:ILE:H	1:B:746:ILE:HG13	5	0.18
(2,142)	1:A:781:ILE:H	1:B:746:ILE:HG12	14	0.18
(2,142)	1:A:781:ILE:H	1:B:746:ILE:HG13	14	0.18
(2,1414)	1:A:778:VAL:HG21	1:A:775:LEU:HA	8	0.18
(2,1414)	1:A:778:VAL:HG22	1:A:775:LEU:HA	8	0.18
(2,1414)	1:A:778:VAL:HG23	1:A:775:LEU:HA	8	0.18
(2,1409)	1:A:778:VAL:H	1:A:775:LEU:HA	14	0.18
(2,1408)	1:A:777:ILE:HG21	1:A:780:ARG:HD2	8	0.18
(2,1408)	1:A:777:ILE:HG21	1:A:780:ARG:HD3	8	0.18
(2,1408)	1:A:777:ILE:HG22	1:A:780:ARG:HD2	8	0.18
(2,1408)	1:A:777:ILE:HG22	1:A:780:ARG:HD3	8	0.18
(2,1408)	1:A:777:ILE:HG23	1:A:780:ARG:HD2	8	0.18
(2,1408)	1:A:777:ILE:HG23	1:A:780:ARG:HD3	8	0.18
(2,1381)	1:A:773:ASP:H	1:A:770:ARG:HD2	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1381)	1:A:773:ASP:H	1:A:770:ARG:HD3	9	0.18
(2,1364)	1:A:760:LEU:HD11	1:A:756:ILE:HG12	10	0.18
(2,1364)	1:A:760:LEU:HD11	1:A:756:ILE:HG13	10	0.18
(2,1364)	1:A:760:LEU:HD12	1:A:756:ILE:HG12	10	0.18
(2,1364)	1:A:760:LEU:HD12	1:A:756:ILE:HG13	10	0.18
(2,1364)	1:A:760:LEU:HD13	1:A:756:ILE:HG12	10	0.18
(2,1364)	1:A:760:LEU:HD13	1:A:756:ILE:HG13	10	0.18
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD2	3	0.18
(2,1328)	1:A:748:LEU:H	1:A:744:ARG:HD3	3	0.18
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD1	7	0.18
(2,132)	1:B:756:ILE:H	1:A:795:TYR:HD2	7	0.18
(2,1289)	1:A:710:GLN:H	1:A:708:VAL:HA	5	0.18
(2,1289)	1:A:710:GLN:H	1:A:708:VAL:HA	7	0.18
(2,1289)	1:A:710:GLN:H	1:A:708:VAL:HA	14	0.18
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB2	5	0.18
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB3	5	0.18
(2,1245)	1:A:704:LEU:HD11	1:A:708:VAL:HG21	7	0.18
(2,1245)	1:A:704:LEU:HD11	1:A:708:VAL:HG22	7	0.18
(2,1245)	1:A:704:LEU:HD11	1:A:708:VAL:HG23	7	0.18
(2,1245)	1:A:704:LEU:HD12	1:A:708:VAL:HG21	7	0.18
(2,1245)	1:A:704:LEU:HD12	1:A:708:VAL:HG22	7	0.18
(2,1245)	1:A:704:LEU:HD12	1:A:708:VAL:HG23	7	0.18
(2,1245)	1:A:704:LEU:HD13	1:A:708:VAL:HG21	7	0.18
(2,1245)	1:A:704:LEU:HD13	1:A:708:VAL:HG22	7	0.18
(2,1245)	1:A:704:LEU:HD13	1:A:708:VAL:HG23	7	0.18
(2,1219)	1:A:701:VAL:H	1:A:698:VAL:HA	7	0.18
(2,1213)	1:A:700:ALA:H	1:A:699:PHE:HA	1	0.18
(2,1213)	1:A:700:ALA:H	1:A:699:PHE:HA	3	0.18
(2,1213)	1:A:700:ALA:H	1:A:699:PHE:HA	5	0.18
(2,1213)	1:A:700:ALA:H	1:A:699:PHE:HA	6	0.18
(2,1213)	1:A:700:ALA:H	1:A:699:PHE:HA	8	0.18
(2,1213)	1:A:700:ALA:H	1:A:699:PHE:HA	9	0.18
(2,1213)	1:A:700:ALA:H	1:A:699:PHE:HA	10	0.18
(2,1213)	1:A:700:ALA:H	1:A:699:PHE:HA	11	0.18
(2,1213)	1:A:700:ALA:H	1:A:699:PHE:HA	12	0.18
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB1	15	0.18
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB2	15	0.18
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB3	15	0.18
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB1	15	0.18
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB2	15	0.18
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB3	15	0.18
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB1	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB2	15	0.18
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB3	15	0.18
(2,1202)	1:A:697:ILE:HG21	1:A:694:GLY:HA2	6	0.18
(2,1202)	1:A:697:ILE:HG21	1:A:694:GLY:HA3	6	0.18
(2,1202)	1:A:697:ILE:HG22	1:A:694:GLY:HA2	6	0.18
(2,1202)	1:A:697:ILE:HG22	1:A:694:GLY:HA3	6	0.18
(2,1202)	1:A:697:ILE:HG23	1:A:694:GLY:HA2	6	0.18
(2,1202)	1:A:697:ILE:HG23	1:A:694:GLY:HA3	6	0.18
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	9	0.18
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	9	0.18
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	9	0.18
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	9	0.18
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	9	0.18
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	9	0.18
(2,1188)	1:A:693:ILE:HG21	1:A:693:ILE:H	6	0.18
(2,1188)	1:A:693:ILE:HG22	1:A:693:ILE:H	6	0.18
(2,1188)	1:A:693:ILE:HG23	1:A:693:ILE:H	6	0.18
(2,1176)	1:A:689:VAL:HG21	1:A:685:PHE:HD1	3	0.18
(2,1176)	1:A:689:VAL:HG21	1:A:685:PHE:HD2	3	0.18
(2,1176)	1:A:689:VAL:HG22	1:A:685:PHE:HD1	3	0.18
(2,1176)	1:A:689:VAL:HG22	1:A:685:PHE:HD2	3	0.18
(2,1176)	1:A:689:VAL:HG23	1:A:685:PHE:HD1	3	0.18
(2,1176)	1:A:689:VAL:HG23	1:A:685:PHE:HD2	3	0.18
(2,1146)	1:A:682:ILE:HD11	1:A:681:TYR:H	5	0.18
(2,1146)	1:A:682:ILE:HD12	1:A:681:TYR:H	5	0.18
(2,1146)	1:A:682:ILE:HD13	1:A:681:TYR:H	5	0.18
(2,1140)	1:A:680:TRP:HE1	1:A:684:ILE:HD11	5	0.18
(2,1140)	1:A:680:TRP:HE1	1:A:684:ILE:HD12	5	0.18
(2,1140)	1:A:680:TRP:HE1	1:A:684:ILE:HD13	5	0.18
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD11	9	0.18
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD12	9	0.18
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD13	9	0.18
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD21	9	0.18
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD22	9	0.18
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD23	9	0.18
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD2	12	0.18
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD3	12	0.18
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD2	12	0.18
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD3	12	0.18
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD2	12	0.18
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD3	12	0.18
(2,1074)	1:A:664:ASP:H	1:A:663:LEU:HA	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1074)	1:A:664:ASP:H	1:A:663:LEU:HA	15	0.18
(2,1064)	1:A:661:LEU:HD11	1:A:662:GLU:HG2	9	0.18
(2,1064)	1:A:661:LEU:HD11	1:A:662:GLU:HG3	9	0.18
(2,1064)	1:A:661:LEU:HD12	1:A:662:GLU:HG2	9	0.18
(2,1064)	1:A:661:LEU:HD12	1:A:662:GLU:HG3	9	0.18
(2,1064)	1:A:661:LEU:HD13	1:A:662:GLU:HG2	9	0.18
(2,1064)	1:A:661:LEU:HD13	1:A:662:GLU:HG3	9	0.18
(2,1064)	1:A:661:LEU:HD21	1:A:662:GLU:HG2	9	0.18
(2,1064)	1:A:661:LEU:HD21	1:A:662:GLU:HG3	9	0.18
(2,1064)	1:A:661:LEU:HD22	1:A:662:GLU:HG2	9	0.18
(2,1064)	1:A:661:LEU:HD22	1:A:662:GLU:HG3	9	0.18
(2,1064)	1:A:661:LEU:HD23	1:A:662:GLU:HG2	9	0.18
(2,1064)	1:A:661:LEU:HD23	1:A:662:GLU:HG3	9	0.18
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	2	0.18
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	2	0.18
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	2	0.18
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	2	0.18
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	2	0.18
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	2	0.18
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	2	0.18
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	2	0.18
(2,1050)	1:A:806:GLU:H	1:A:803:TRP:HB2	8	0.18
(2,1050)	1:A:806:GLU:H	1:A:803:TRP:HB3	8	0.18
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	12	0.18
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	12	0.18
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	12	0.18
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	12	0.18
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	12	0.18
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	12	0.18
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD21	3	0.18
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD22	3	0.18
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD23	3	0.18
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD21	7	0.18
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD22	7	0.18
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD23	7	0.18
(2,1026)	1:A:785:LEU:H	1:A:782:VAL:HA	13	0.18
(2,1018)	1:A:784:LEU:H	1:A:781:ILE:HA	6	0.18
(2,1018)	1:A:784:LEU:H	1:A:781:ILE:HA	13	0.18
(2,1000)	1:A:781:ILE:H	1:A:778:VAL:HA	7	0.18
(1,23)	1:B:801:GLN:O	1:B:805:GLN:H	6	0.18
(1,20)	1:B:799:LEU:O	1:B:803:TRP:N	4	0.18
(1,195)	1:B:801:GLN:O	1:B:805:GLN:H	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:B:799:LEU:O	1:B:803:TRP:N	4	0.18
(1,109)	1:B:801:GLN:O	1:B:805:GLN:H	6	0.18
(1,106)	1:B:799:LEU:O	1:B:803:TRP:N	4	0.18
(2,977)	1:A:777:ILE:H	1:A:774:LEU:HA	1	0.17
(2,976)	1:A:776:LEU:HD11	1:A:773:ASP:HB2	10	0.17
(2,976)	1:A:776:LEU:HD11	1:A:773:ASP:HB3	10	0.17
(2,976)	1:A:776:LEU:HD12	1:A:773:ASP:HB2	10	0.17
(2,976)	1:A:776:LEU:HD12	1:A:773:ASP:HB3	10	0.17
(2,976)	1:A:776:LEU:HD13	1:A:773:ASP:HB2	10	0.17
(2,976)	1:A:776:LEU:HD13	1:A:773:ASP:HB3	10	0.17
(2,952)	1:A:771:LEU:HD21	1:A:772:ARG:HH21	6	0.17
(2,952)	1:A:771:LEU:HD21	1:A:772:ARG:HH22	6	0.17
(2,952)	1:A:771:LEU:HD22	1:A:772:ARG:HH21	6	0.17
(2,952)	1:A:771:LEU:HD22	1:A:772:ARG:HH22	6	0.17
(2,952)	1:A:771:LEU:HD23	1:A:772:ARG:HH21	6	0.17
(2,952)	1:A:771:LEU:HD23	1:A:772:ARG:HH22	6	0.17
(2,948)	1:A:764:SER:H	1:A:771:LEU:HB2	2	0.17
(2,948)	1:A:764:SER:H	1:A:771:LEU:HB3	2	0.17
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	15	0.17
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	15	0.17
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	15	0.17
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	15	0.17
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	15	0.17
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	15	0.17
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB1	8	0.17
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB2	8	0.17
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB3	8	0.17
(2,925)	1:A:754:ALA:HB1	1:A:758:ASP:H	8	0.17
(2,925)	1:A:754:ALA:HB2	1:A:758:ASP:H	8	0.17
(2,925)	1:A:754:ALA:HB3	1:A:758:ASP:H	8	0.17
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	15	0.17
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	15	0.17
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	15	0.17
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	15	0.17
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	15	0.17
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	15	0.17
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	7	0.17
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	7	0.17
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	7	0.17
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	7	0.17
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	7	0.17
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,916)	1:A:753:LEU:HD11	1:A:757:TRP:HB2	10	0.17
(2,916)	1:A:753:LEU:HD11	1:A:757:TRP:HB3	10	0.17
(2,916)	1:A:753:LEU:HD12	1:A:757:TRP:HB2	10	0.17
(2,916)	1:A:753:LEU:HD12	1:A:757:TRP:HB3	10	0.17
(2,916)	1:A:753:LEU:HD13	1:A:757:TRP:HB2	10	0.17
(2,916)	1:A:753:LEU:HD13	1:A:757:TRP:HB3	10	0.17
(2,907)	1:A:749:VAL:H	1:A:746:ILE:HA	15	0.17
(2,896)	1:A:746:ILE:HD11	1:A:743:ASP:HB2	12	0.17
(2,896)	1:A:746:ILE:HD11	1:A:743:ASP:HB3	12	0.17
(2,896)	1:A:746:ILE:HD12	1:A:743:ASP:HB2	12	0.17
(2,896)	1:A:746:ILE:HD12	1:A:743:ASP:HB3	12	0.17
(2,896)	1:A:746:ILE:HD13	1:A:743:ASP:HB2	12	0.17
(2,896)	1:A:746:ILE:HD13	1:A:743:ASP:HB3	12	0.17
(2,864)	1:A:710:GLN:H	1:A:708:VAL:HA	11	0.17
(2,845)	1:A:707:ARG:H	1:A:707:ARG:HG2	7	0.17
(2,845)	1:A:707:ARG:H	1:A:707:ARG:HG3	7	0.17
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB2	15	0.17
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB3	15	0.17
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	8	0.17
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	8	0.17
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	8	0.17
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	8	0.17
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	8	0.17
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	8	0.17
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	1	0.17
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	1	0.17
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	1	0.17
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	1	0.17
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	1	0.17
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	1	0.17
(2,804)	1:A:702:LEU:HD21	1:A:706:ASN:HB2	12	0.17
(2,804)	1:A:702:LEU:HD21	1:A:706:ASN:HB3	12	0.17
(2,804)	1:A:702:LEU:HD22	1:A:706:ASN:HB2	12	0.17
(2,804)	1:A:702:LEU:HD22	1:A:706:ASN:HB3	12	0.17
(2,804)	1:A:702:LEU:HD23	1:A:706:ASN:HB2	12	0.17
(2,804)	1:A:702:LEU:HD23	1:A:706:ASN:HB3	12	0.17
(2,788)	1:A:700:ALA:H	1:A:699:PHE:HA	4	0.17
(2,788)	1:A:700:ALA:H	1:A:699:PHE:HA	7	0.17
(2,788)	1:A:700:ALA:H	1:A:699:PHE:HA	14	0.17
(2,781)	1:A:698:VAL:HG11	1:A:695:LEU:HG	8	0.17
(2,781)	1:A:698:VAL:HG12	1:A:695:LEU:HG	8	0.17
(2,781)	1:A:698:VAL:HG13	1:A:695:LEU:HG	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,781)	1:A:698:VAL:HG11	1:A:695:LEU:HG	10	0.17
(2,781)	1:A:698:VAL:HG12	1:A:695:LEU:HG	10	0.17
(2,781)	1:A:698:VAL:HG13	1:A:695:LEU:HG	10	0.17
(2,773)	1:A:695:LEU:HD21	1:A:696:ARG:HH11	8	0.17
(2,773)	1:A:695:LEU:HD21	1:A:696:ARG:HH12	8	0.17
(2,773)	1:A:695:LEU:HD22	1:A:696:ARG:HH11	8	0.17
(2,773)	1:A:695:LEU:HD22	1:A:696:ARG:HH12	8	0.17
(2,773)	1:A:695:LEU:HD23	1:A:696:ARG:HH11	8	0.17
(2,773)	1:A:695:LEU:HD23	1:A:696:ARG:HH12	8	0.17
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	2	0.17
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	2	0.17
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	2	0.17
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	2	0.17
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	2	0.17
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	2	0.17
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	13	0.17
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	13	0.17
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	13	0.17
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	13	0.17
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	13	0.17
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	13	0.17
(2,715)	1:A:680:TRP:HE1	1:A:684:ILE:HD11	14	0.17
(2,715)	1:A:680:TRP:HE1	1:A:684:ILE:HD12	14	0.17
(2,715)	1:A:680:TRP:HE1	1:A:684:ILE:HD13	14	0.17
(2,701)	1:A:676:THR:HG21	1:A:666:TRP:HZ3	15	0.17
(2,701)	1:A:676:THR:HG22	1:A:666:TRP:HZ3	15	0.17
(2,701)	1:A:676:THR:HG23	1:A:666:TRP:HZ3	15	0.17
(2,693)	1:A:672:TRP:H	1:A:673:PHE:H	6	0.17
(2,693)	1:A:672:TRP:H	1:A:673:PHE:H	12	0.17
(2,670)	1:A:667:ALA:H	1:A:666:TRP:HD1	2	0.17
(2,654)	1:A:665:LYS:H	1:A:664:ASP:HA	1	0.17
(2,654)	1:A:665:LYS:H	1:A:664:ASP:HA	5	0.17
(2,649)	1:A:664:ASP:H	1:A:663:LEU:HA	10	0.17
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB2	4	0.17
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB3	4	0.17
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB2	14	0.17
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB3	14	0.17
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB2	14	0.17
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB3	14	0.17
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB2	14	0.17
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB3	14	0.17
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD11	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD12	8	0.17
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD13	8	0.17
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD1	10	0.17
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD2	10	0.17
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD1	10	0.17
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD2	10	0.17
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD1	10	0.17
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD2	10	0.17
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD1	11	0.17
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD2	11	0.17
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD1	11	0.17
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD2	11	0.17
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD1	11	0.17
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD2	11	0.17
(2,546)	1:B:776:LEU:H	1:B:773:ASP:HA	15	0.17
(2,545)	1:B:775:LEU:HD11	1:B:772:ARG:HA	1	0.17
(2,545)	1:B:775:LEU:HD12	1:B:772:ARG:HA	1	0.17
(2,545)	1:B:775:LEU:HD13	1:B:772:ARG:HA	1	0.17
(2,531)	1:B:773:ASP:H	1:B:770:ARG:HD2	15	0.17
(2,531)	1:B:773:ASP:H	1:B:770:ARG:HD3	15	0.17
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH21	11	0.17
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH22	11	0.17
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH21	11	0.17
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH22	11	0.17
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH21	11	0.17
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH22	11	0.17
(2,522)	1:B:764:SER:H	1:B:761:ARG:HA	9	0.17
(2,522)	1:B:764:SER:H	1:B:761:ARG:HA	13	0.17
(2,516)	1:B:760:LEU:HD21	1:B:768:TYR:HE1	10	0.17
(2,516)	1:B:760:LEU:HD21	1:B:768:TYR:HE2	10	0.17
(2,516)	1:B:760:LEU:HD22	1:B:768:TYR:HE1	10	0.17
(2,516)	1:B:760:LEU:HD22	1:B:768:TYR:HE2	10	0.17
(2,516)	1:B:760:LEU:HD23	1:B:768:TYR:HE1	10	0.17
(2,516)	1:B:760:LEU:HD23	1:B:768:TYR:HE2	10	0.17
(2,509)	1:B:758:ASP:H	1:B:754:ALA:HB1	12	0.17
(2,509)	1:B:758:ASP:H	1:B:754:ALA:HB2	12	0.17
(2,509)	1:B:758:ASP:H	1:B:754:ALA:HB3	12	0.17
(2,500)	1:B:754:ALA:HB1	1:B:758:ASP:H	12	0.17
(2,500)	1:B:754:ALA:HB2	1:B:758:ASP:H	12	0.17
(2,500)	1:B:754:ALA:HB3	1:B:758:ASP:H	12	0.17
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA2	12	0.17
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA3	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA2	12	0.17
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA3	12	0.17
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA2	12	0.17
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA3	12	0.17
(2,492)	1:B:753:LEU:HD21	1:B:750:ASN:HB2	1	0.17
(2,492)	1:B:753:LEU:HD21	1:B:750:ASN:HB3	1	0.17
(2,492)	1:B:753:LEU:HD22	1:B:750:ASN:HB2	1	0.17
(2,492)	1:B:753:LEU:HD22	1:B:750:ASN:HB3	1	0.17
(2,492)	1:B:753:LEU:HD23	1:B:750:ASN:HB2	1	0.17
(2,492)	1:B:753:LEU:HD23	1:B:750:ASN:HB3	1	0.17
(2,472)	1:B:746:ILE:HG21	1:B:750:ASN:HD21	7	0.17
(2,472)	1:B:746:ILE:HG22	1:B:750:ASN:HD21	7	0.17
(2,472)	1:B:746:ILE:HG23	1:B:750:ASN:HD21	7	0.17
(2,465)	1:B:746:ILE:H	1:B:743:ASP:HB2	14	0.17
(2,465)	1:B:746:ILE:H	1:B:743:ASP:HB3	14	0.17
(2,421)	1:B:707:ARG:H	1:B:707:ARG:HD2	8	0.17
(2,421)	1:B:707:ARG:H	1:B:707:ARG:HD3	8	0.17
(2,414)	1:B:707:ARG:H	1:B:704:LEU:HA	12	0.17
(2,395)	1:B:704:LEU:HD11	1:B:708:VAL:HG21	8	0.17
(2,395)	1:B:704:LEU:HD11	1:B:708:VAL:HG22	8	0.17
(2,395)	1:B:704:LEU:HD11	1:B:708:VAL:HG23	8	0.17
(2,395)	1:B:704:LEU:HD12	1:B:708:VAL:HG21	8	0.17
(2,395)	1:B:704:LEU:HD12	1:B:708:VAL:HG22	8	0.17
(2,395)	1:B:704:LEU:HD12	1:B:708:VAL:HG23	8	0.17
(2,395)	1:B:704:LEU:HD13	1:B:708:VAL:HG21	8	0.17
(2,395)	1:B:704:LEU:HD13	1:B:708:VAL:HG22	8	0.17
(2,395)	1:B:704:LEU:HD13	1:B:708:VAL:HG23	8	0.17
(2,395)	1:B:704:LEU:HD11	1:B:708:VAL:HG21	15	0.17
(2,395)	1:B:704:LEU:HD11	1:B:708:VAL:HG22	15	0.17
(2,395)	1:B:704:LEU:HD11	1:B:708:VAL:HG23	15	0.17
(2,395)	1:B:704:LEU:HD12	1:B:708:VAL:HG21	15	0.17
(2,395)	1:B:704:LEU:HD12	1:B:708:VAL:HG22	15	0.17
(2,395)	1:B:704:LEU:HD12	1:B:708:VAL:HG23	15	0.17
(2,395)	1:B:704:LEU:HD13	1:B:708:VAL:HG21	15	0.17
(2,395)	1:B:704:LEU:HD13	1:B:708:VAL:HG22	15	0.17
(2,395)	1:B:704:LEU:HD13	1:B:708:VAL:HG23	15	0.17
(2,393)	1:B:704:LEU:HD11	1:B:707:ARG:HD2	10	0.17
(2,393)	1:B:704:LEU:HD11	1:B:707:ARG:HD3	10	0.17
(2,393)	1:B:704:LEU:HD12	1:B:707:ARG:HD2	10	0.17
(2,393)	1:B:704:LEU:HD12	1:B:707:ARG:HD3	10	0.17
(2,393)	1:B:704:LEU:HD13	1:B:707:ARG:HD2	10	0.17
(2,393)	1:B:704:LEU:HD13	1:B:707:ARG:HD3	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB2	11	0.17
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB3	11	0.17
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB2	11	0.17
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB3	11	0.17
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB2	11	0.17
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB3	11	0.17
(2,363)	1:B:700:ALA:H	1:B:699:PHE:HA	2	0.17
(2,363)	1:B:700:ALA:H	1:B:699:PHE:HA	3	0.17
(2,363)	1:B:700:ALA:H	1:B:699:PHE:HA	6	0.17
(2,363)	1:B:700:ALA:H	1:B:699:PHE:HA	7	0.17
(2,363)	1:B:700:ALA:H	1:B:699:PHE:HA	15	0.17
(2,356)	1:B:698:VAL:HG11	1:B:695:LEU:HG	9	0.17
(2,356)	1:B:698:VAL:HG12	1:B:695:LEU:HG	9	0.17
(2,356)	1:B:698:VAL:HG13	1:B:695:LEU:HG	9	0.17
(2,356)	1:B:698:VAL:HG11	1:B:695:LEU:HG	12	0.17
(2,356)	1:B:698:VAL:HG12	1:B:695:LEU:HG	12	0.17
(2,356)	1:B:698:VAL:HG13	1:B:695:LEU:HG	12	0.17
(2,354)	1:B:697:ILE:HG21	1:B:700:ALA:HB1	15	0.17
(2,354)	1:B:697:ILE:HG21	1:B:700:ALA:HB2	15	0.17
(2,354)	1:B:697:ILE:HG21	1:B:700:ALA:HB3	15	0.17
(2,354)	1:B:697:ILE:HG22	1:B:700:ALA:HB1	15	0.17
(2,354)	1:B:697:ILE:HG22	1:B:700:ALA:HB2	15	0.17
(2,354)	1:B:697:ILE:HG22	1:B:700:ALA:HB3	15	0.17
(2,354)	1:B:697:ILE:HG23	1:B:700:ALA:HB1	15	0.17
(2,354)	1:B:697:ILE:HG23	1:B:700:ALA:HB2	15	0.17
(2,354)	1:B:697:ILE:HG23	1:B:700:ALA:HB3	15	0.17
(2,338)	1:B:693:ILE:HG21	1:B:693:ILE:H	6	0.17
(2,338)	1:B:693:ILE:HG22	1:B:693:ILE:H	6	0.17
(2,338)	1:B:693:ILE:HG23	1:B:693:ILE:H	6	0.17
(2,336)	1:B:693:ILE:HD11	1:B:697:ILE:H	6	0.17
(2,336)	1:B:693:ILE:HD12	1:B:697:ILE:H	6	0.17
(2,336)	1:B:693:ILE:HD13	1:B:697:ILE:H	6	0.17
(2,332)	1:B:692:LEU:HD11	1:B:691:SER:HB2	11	0.17
(2,332)	1:B:692:LEU:HD11	1:B:691:SER:HB3	11	0.17
(2,332)	1:B:692:LEU:HD12	1:B:691:SER:HB2	11	0.17
(2,332)	1:B:692:LEU:HD12	1:B:691:SER:HB3	11	0.17
(2,332)	1:B:692:LEU:HD13	1:B:691:SER:HB2	11	0.17
(2,332)	1:B:692:LEU:HD13	1:B:691:SER:HB3	11	0.17
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD11	10	0.17
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD12	10	0.17
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD13	10	0.17
(2,288)	1:B:679:LEU:HD11	1:B:678:TRP:HH2	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,288)	1:B:679:LEU:HD12	1:B:678:TRP:HH2	2	0.17
(2,288)	1:B:679:LEU:HD13	1:B:678:TRP:HH2	2	0.17
(2,288)	1:B:679:LEU:HD21	1:B:678:TRP:HH2	2	0.17
(2,288)	1:B:679:LEU:HD22	1:B:678:TRP:HH2	2	0.17
(2,288)	1:B:679:LEU:HD23	1:B:678:TRP:HH2	2	0.17
(2,277)	1:B:676:THR:HG21	1:B:669:LEU:HA	9	0.17
(2,277)	1:B:676:THR:HG22	1:B:669:LEU:HA	9	0.17
(2,277)	1:B:676:THR:HG23	1:B:669:LEU:HA	9	0.17
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD11	12	0.17
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD12	12	0.17
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD13	12	0.17
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD21	12	0.17
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD22	12	0.17
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD23	12	0.17
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD11	12	0.17
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD12	12	0.17
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD13	12	0.17
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD21	12	0.17
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD22	12	0.17
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD23	12	0.17
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD11	12	0.17
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD12	12	0.17
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD13	12	0.17
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD21	12	0.17
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD22	12	0.17
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD23	12	0.17
(2,229)	1:B:665:LYS:H	1:B:664:ASP:HA	3	0.17
(2,225)	1:B:664:ASP:H	1:B:663:LEU:H	14	0.17
(2,224)	1:B:664:ASP:H	1:B:663:LEU:HA	10	0.17
(2,224)	1:B:664:ASP:H	1:B:663:LEU:HA	14	0.17
(2,219)	1:B:663:LEU:H	1:B:664:ASP:H	14	0.17
(2,214)	1:B:661:LEU:HD11	1:B:662:GLU:HG2	8	0.17
(2,214)	1:B:661:LEU:HD11	1:B:662:GLU:HG3	8	0.17
(2,214)	1:B:661:LEU:HD12	1:B:662:GLU:HG2	8	0.17
(2,214)	1:B:661:LEU:HD12	1:B:662:GLU:HG3	8	0.17
(2,214)	1:B:661:LEU:HD13	1:B:662:GLU:HG2	8	0.17
(2,214)	1:B:661:LEU:HD13	1:B:662:GLU:HG3	8	0.17
(2,214)	1:B:661:LEU:HD21	1:B:662:GLU:HG2	8	0.17
(2,214)	1:B:661:LEU:HD21	1:B:662:GLU:HG3	8	0.17
(2,214)	1:B:661:LEU:HD22	1:B:662:GLU:HG2	8	0.17
(2,214)	1:B:661:LEU:HD22	1:B:662:GLU:HG3	8	0.17
(2,214)	1:B:661:LEU:HD23	1:B:662:GLU:HG2	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,214)	1:B:661:LEU:HD23	1:B:662:GLU:HG3	8	0.17
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD11	1	0.17
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD12	1	0.17
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD13	1	0.17
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD11	2	0.17
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD12	2	0.17
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD13	2	0.17
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD11	10	0.17
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD12	10	0.17
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD13	10	0.17
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD11	1	0.17
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD12	1	0.17
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD13	1	0.17
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD11	2	0.17
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD12	2	0.17
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD13	2	0.17
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD11	10	0.17
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD12	10	0.17
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD13	10	0.17
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD11	2	0.17
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD12	2	0.17
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD13	2	0.17
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG2	13	0.17
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG3	13	0.17
(2,189)	1:A:816:ASN:H	1:A:830:ILE:HD11	6	0.17
(2,189)	1:A:816:ASN:H	1:A:830:ILE:HD12	6	0.17
(2,189)	1:A:816:ASN:H	1:A:830:ILE:HD13	6	0.17
(2,188)	1:A:816:ASN:H	1:A:830:ILE:HD11	6	0.17
(2,188)	1:A:816:ASN:H	1:A:830:ILE:HD12	6	0.17
(2,188)	1:A:816:ASN:H	1:A:830:ILE:HD13	6	0.17
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD2	12	0.17
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD3	12	0.17
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD2	14	0.17
(2,184)	1:B:808:LYS:H	1:B:838:ARG:HD3	14	0.17
(2,177)	1:A:803:TRP:HE1	1:B:764:SER:HG	14	0.17
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB2	5	0.17
(2,174)	1:A:803:TRP:HE1	1:B:764:SER:HB3	5	0.17
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	14	0.17
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	14	0.17
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	14	0.17
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	14	0.17
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE21	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE22	4	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG11	10	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG12	10	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG13	10	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG21	10	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG22	10	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG23	10	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG11	14	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG12	14	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG13	14	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG21	14	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG22	14	0.17
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG23	14	0.17
(2,1477)	1:A:819:ALA:H	1:A:820:ILE:HD11	1	0.17
(2,1477)	1:A:819:ALA:H	1:A:820:ILE:HD12	1	0.17
(2,1477)	1:A:819:ALA:H	1:A:820:ILE:HD13	1	0.17
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	2	0.17
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	2	0.17
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	2	0.17
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	2	0.17
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	2	0.17
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	2	0.17
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	8	0.17
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	8	0.17
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	8	0.17
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	8	0.17
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	8	0.17
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	8	0.17
(2,1457)	1:A:785:LEU:HD21	1:A:782:VAL:HA	14	0.17
(2,1457)	1:A:785:LEU:HD22	1:A:782:VAL:HA	14	0.17
(2,1457)	1:A:785:LEU:HD23	1:A:782:VAL:HA	14	0.17
(2,1436)	1:A:782:VAL:HG21	1:A:779:THR:HA	4	0.17
(2,1436)	1:A:782:VAL:HG22	1:A:779:THR:HA	4	0.17
(2,1436)	1:A:782:VAL:HG23	1:A:779:THR:HA	4	0.17
(2,1431)	1:A:782:VAL:H	1:A:779:THR:HA	12	0.17
(2,1430)	1:A:781:ILE:HG21	1:A:778:VAL:HA	12	0.17
(2,1430)	1:A:781:ILE:HG22	1:A:778:VAL:HA	12	0.17
(2,1430)	1:A:781:ILE:HG23	1:A:778:VAL:HA	12	0.17
(2,1430)	1:A:781:ILE:HG21	1:A:778:VAL:HA	14	0.17
(2,1430)	1:A:781:ILE:HG22	1:A:778:VAL:HA	14	0.17
(2,1430)	1:A:781:ILE:HG23	1:A:778:VAL:HA	14	0.17
(2,1402)	1:A:777:ILE:H	1:A:774:LEU:HA	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1401)	1:A:776:LEU:HD11	1:A:773:ASP:HB2	10	0.17
(2,1401)	1:A:776:LEU:HD11	1:A:773:ASP:HB3	10	0.17
(2,1401)	1:A:776:LEU:HD12	1:A:773:ASP:HB2	10	0.17
(2,1401)	1:A:776:LEU:HD12	1:A:773:ASP:HB3	10	0.17
(2,1401)	1:A:776:LEU:HD13	1:A:773:ASP:HB2	10	0.17
(2,1401)	1:A:776:LEU:HD13	1:A:773:ASP:HB3	10	0.17
(2,1377)	1:A:771:LEU:HD21	1:A:772:ARG:HH21	6	0.17
(2,1377)	1:A:771:LEU:HD21	1:A:772:ARG:HH22	6	0.17
(2,1377)	1:A:771:LEU:HD22	1:A:772:ARG:HH21	6	0.17
(2,1377)	1:A:771:LEU:HD22	1:A:772:ARG:HH22	6	0.17
(2,1377)	1:A:771:LEU:HD23	1:A:772:ARG:HH21	6	0.17
(2,1377)	1:A:771:LEU:HD23	1:A:772:ARG:HH22	6	0.17
(2,1373)	1:A:764:SER:H	1:A:771:LEU:HB2	2	0.17
(2,1373)	1:A:764:SER:H	1:A:771:LEU:HB3	2	0.17
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	15	0.17
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	15	0.17
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	15	0.17
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	15	0.17
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	15	0.17
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	15	0.17
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB1	8	0.17
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB2	8	0.17
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB3	8	0.17
(2,1350)	1:A:754:ALA:HB1	1:A:758:ASP:H	8	0.17
(2,1350)	1:A:754:ALA:HB2	1:A:758:ASP:H	8	0.17
(2,1350)	1:A:754:ALA:HB3	1:A:758:ASP:H	8	0.17
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	15	0.17
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	15	0.17
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	15	0.17
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	15	0.17
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	15	0.17
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	15	0.17
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	7	0.17
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	7	0.17
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	7	0.17
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	7	0.17
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	7	0.17
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	7	0.17
(2,1341)	1:A:753:LEU:HD11	1:A:757:TRP:HB2	10	0.17
(2,1341)	1:A:753:LEU:HD11	1:A:757:TRP:HB3	10	0.17
(2,1341)	1:A:753:LEU:HD12	1:A:757:TRP:HB2	10	0.17
(2,1341)	1:A:753:LEU:HD12	1:A:757:TRP:HB3	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1341)	1:A:753:LEU:HD13	1:A:757:TRP:HB2	10	0.17
(2,1341)	1:A:753:LEU:HD13	1:A:757:TRP:HB3	10	0.17
(2,1332)	1:A:749:VAL:H	1:A:746:ILE:HA	15	0.17
(2,1321)	1:A:746:ILE:HD11	1:A:743:ASP:HB2	12	0.17
(2,1321)	1:A:746:ILE:HD11	1:A:743:ASP:HB3	12	0.17
(2,1321)	1:A:746:ILE:HD12	1:A:743:ASP:HB2	12	0.17
(2,1321)	1:A:746:ILE:HD12	1:A:743:ASP:HB3	12	0.17
(2,1321)	1:A:746:ILE:HD13	1:A:743:ASP:HB2	12	0.17
(2,1321)	1:A:746:ILE:HD13	1:A:743:ASP:HB3	12	0.17
(2,1289)	1:A:710:GLN:H	1:A:708:VAL:HA	11	0.17
(2,1270)	1:A:707:ARG:H	1:A:707:ARG:HG2	7	0.17
(2,1270)	1:A:707:ARG:H	1:A:707:ARG:HG3	7	0.17
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB2	15	0.17
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB3	15	0.17
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	8	0.17
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	8	0.17
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	8	0.17
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	8	0.17
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	8	0.17
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	8	0.17
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	1	0.17
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	1	0.17
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	1	0.17
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	1	0.17
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	1	0.17
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	1	0.17
(2,1229)	1:A:702:LEU:HD21	1:A:706:ASN:HB2	12	0.17
(2,1229)	1:A:702:LEU:HD21	1:A:706:ASN:HB3	12	0.17
(2,1229)	1:A:702:LEU:HD22	1:A:706:ASN:HB2	12	0.17
(2,1229)	1:A:702:LEU:HD22	1:A:706:ASN:HB3	12	0.17
(2,1229)	1:A:702:LEU:HD23	1:A:706:ASN:HB2	12	0.17
(2,1229)	1:A:702:LEU:HD23	1:A:706:ASN:HB3	12	0.17
(2,1213)	1:A:700:ALA:H	1:A:699:PHE:HA	4	0.17
(2,1213)	1:A:700:ALA:H	1:A:699:PHE:HA	7	0.17
(2,1213)	1:A:700:ALA:H	1:A:699:PHE:HA	14	0.17
(2,1206)	1:A:698:VAL:HG11	1:A:695:LEU:HG	8	0.17
(2,1206)	1:A:698:VAL:HG12	1:A:695:LEU:HG	8	0.17
(2,1206)	1:A:698:VAL:HG13	1:A:695:LEU:HG	8	0.17
(2,1206)	1:A:698:VAL:HG11	1:A:695:LEU:HG	10	0.17
(2,1206)	1:A:698:VAL:HG12	1:A:695:LEU:HG	10	0.17
(2,1206)	1:A:698:VAL:HG13	1:A:695:LEU:HG	10	0.17
(2,1198)	1:A:695:LEU:HD21	1:A:696:ARG:HH11	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1198)	1:A:695:LEU:HD21	1:A:696:ARG:HH12	8	0.17
(2,1198)	1:A:695:LEU:HD22	1:A:696:ARG:HH11	8	0.17
(2,1198)	1:A:695:LEU:HD22	1:A:696:ARG:HH12	8	0.17
(2,1198)	1:A:695:LEU:HD23	1:A:696:ARG:HH11	8	0.17
(2,1198)	1:A:695:LEU:HD23	1:A:696:ARG:HH12	8	0.17
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	2	0.17
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	2	0.17
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	2	0.17
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	2	0.17
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	2	0.17
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	2	0.17
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	13	0.17
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	13	0.17
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	13	0.17
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	13	0.17
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	13	0.17
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	13	0.17
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB2	7	0.17
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB3	7	0.17
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB2	7	0.17
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB3	7	0.17
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB2	7	0.17
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB3	7	0.17
(2,1140)	1:A:680:TRP:HE1	1:A:684:ILE:HD11	14	0.17
(2,1140)	1:A:680:TRP:HE1	1:A:684:ILE:HD12	14	0.17
(2,1140)	1:A:680:TRP:HE1	1:A:684:ILE:HD13	14	0.17
(2,1126)	1:A:676:THR:HG21	1:A:666:TRP:HZ3	15	0.17
(2,1126)	1:A:676:THR:HG22	1:A:666:TRP:HZ3	15	0.17
(2,1126)	1:A:676:THR:HG23	1:A:666:TRP:HZ3	15	0.17
(2,1118)	1:A:672:TRP:H	1:A:673:PHE:H	6	0.17
(2,1118)	1:A:672:TRP:H	1:A:673:PHE:H	12	0.17
(2,1095)	1:A:667:ALA:H	1:A:666:TRP:HD1	2	0.17
(2,1079)	1:A:665:LYS:H	1:A:664:ASP:HA	1	0.17
(2,1079)	1:A:665:LYS:H	1:A:664:ASP:HA	5	0.17
(2,1074)	1:A:664:ASP:H	1:A:663:LEU:HA	10	0.17
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE21	4	0.17
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE22	4	0.17
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG11	10	0.17
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG12	10	0.17
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG13	10	0.17
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG21	10	0.17
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG22	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG23	10	0.17
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG11	14	0.17
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG12	14	0.17
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG13	14	0.17
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG21	14	0.17
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG22	14	0.17
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG23	14	0.17
(2,1052)	1:A:819:ALA:H	1:A:820:ILE:HD11	1	0.17
(2,1052)	1:A:819:ALA:H	1:A:820:ILE:HD12	1	0.17
(2,1052)	1:A:819:ALA:H	1:A:820:ILE:HD13	1	0.17
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	2	0.17
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	2	0.17
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	2	0.17
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	2	0.17
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	2	0.17
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	2	0.17
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	8	0.17
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	8	0.17
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	8	0.17
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	8	0.17
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	8	0.17
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	8	0.17
(2,1032)	1:A:785:LEU:HD21	1:A:782:VAL:HA	14	0.17
(2,1032)	1:A:785:LEU:HD22	1:A:782:VAL:HA	14	0.17
(2,1032)	1:A:785:LEU:HD23	1:A:782:VAL:HA	14	0.17
(2,1011)	1:A:782:VAL:HG21	1:A:779:THR:HA	4	0.17
(2,1011)	1:A:782:VAL:HG22	1:A:779:THR:HA	4	0.17
(2,1011)	1:A:782:VAL:HG23	1:A:779:THR:HA	4	0.17
(2,1006)	1:A:782:VAL:H	1:A:779:THR:HA	12	0.17
(2,1005)	1:A:781:ILE:HG21	1:A:778:VAL:HA	12	0.17
(2,1005)	1:A:781:ILE:HG22	1:A:778:VAL:HA	12	0.17
(2,1005)	1:A:781:ILE:HG23	1:A:778:VAL:HA	12	0.17
(2,1005)	1:A:781:ILE:HG21	1:A:778:VAL:HA	14	0.17
(2,1005)	1:A:781:ILE:HG22	1:A:778:VAL:HA	14	0.17
(2,1005)	1:A:781:ILE:HG23	1:A:778:VAL:HA	14	0.17
(1,96)	1:B:794:LYS:O	1:B:798:ASN:N	10	0.17
(1,75)	1:B:837:SER:O	1:B:841:ARG:H	4	0.17
(1,247)	1:B:837:SER:O	1:B:841:ARG:H	4	0.17
(1,20)	1:B:799:LEU:O	1:B:803:TRP:N	15	0.17
(1,192)	1:B:799:LEU:O	1:B:803:TRP:N	15	0.17
(1,191)	1:B:799:LEU:O	1:B:803:TRP:H	6	0.17
(1,19)	1:B:799:LEU:O	1:B:803:TRP:H	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:B:794:LYS:O	1:B:798:ASN:N	10	0.17
(1,161)	1:B:837:SER:O	1:B:841:ARG:H	4	0.17
(1,106)	1:B:799:LEU:O	1:B:803:TRP:N	15	0.17
(1,105)	1:B:799:LEU:O	1:B:803:TRP:H	6	0.17
(1,10)	1:B:794:LYS:O	1:B:798:ASN:N	10	0.17
(2,940)	1:A:760:LEU:HD11	1:A:757:TRP:HA	3	0.16
(2,940)	1:A:760:LEU:HD12	1:A:757:TRP:HA	3	0.16
(2,940)	1:A:760:LEU:HD13	1:A:757:TRP:HA	3	0.16
(2,93)	1:A:754:ALA:H	1:B:716:SER:HB2	10	0.16
(2,93)	1:A:754:ALA:H	1:B:716:SER:HB3	10	0.16
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	12	0.16
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	12	0.16
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	12	0.16
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	12	0.16
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	12	0.16
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	12	0.16
(2,904)	1:A:748:LEU:H	1:A:745:SER:HA	14	0.16
(2,898)	1:A:746:ILE:HG21	1:A:750:ASN:HD22	13	0.16
(2,898)	1:A:746:ILE:HG22	1:A:750:ASN:HD22	13	0.16
(2,898)	1:A:746:ILE:HG23	1:A:750:ASN:HD22	13	0.16
(2,889)	1:A:746:ILE:H	1:A:743:ASP:HA	8	0.16
(2,839)	1:A:707:ARG:H	1:A:704:LEU:HA	8	0.16
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	7	0.16
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	7	0.16
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	7	0.16
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	7	0.16
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	7	0.16
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	7	0.16
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	4	0.16
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	4	0.16
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	4	0.16
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	4	0.16
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	4	0.16
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	4	0.16
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	12	0.16
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	12	0.16
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	12	0.16
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	12	0.16
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	12	0.16
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	12	0.16
(2,803)	1:A:702:LEU:HD11	1:A:699:PHE:HE1	13	0.16
(2,803)	1:A:702:LEU:HD11	1:A:699:PHE:HE2	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,803)	1:A:702:LEU:HD12	1:A:699:PHE:HE1	13	0.16
(2,803)	1:A:702:LEU:HD12	1:A:699:PHE:HE2	13	0.16
(2,803)	1:A:702:LEU:HD13	1:A:699:PHE:HE1	13	0.16
(2,803)	1:A:702:LEU:HD13	1:A:699:PHE:HE2	13	0.16
(2,802)	1:A:702:LEU:HD11	1:A:699:PHE:HD1	15	0.16
(2,802)	1:A:702:LEU:HD11	1:A:699:PHE:HD2	15	0.16
(2,802)	1:A:702:LEU:HD12	1:A:699:PHE:HD1	15	0.16
(2,802)	1:A:702:LEU:HD12	1:A:699:PHE:HD2	15	0.16
(2,802)	1:A:702:LEU:HD13	1:A:699:PHE:HD1	15	0.16
(2,802)	1:A:702:LEU:HD13	1:A:699:PHE:HD2	15	0.16
(2,792)	1:A:700:ALA:HB1	1:A:697:ILE:HA	11	0.16
(2,792)	1:A:700:ALA:HB2	1:A:697:ILE:HA	11	0.16
(2,792)	1:A:700:ALA:HB3	1:A:697:ILE:HA	11	0.16
(2,782)	1:A:698:VAL:HG11	1:A:699:PHE:HD1	7	0.16
(2,782)	1:A:698:VAL:HG11	1:A:699:PHE:HD2	7	0.16
(2,782)	1:A:698:VAL:HG12	1:A:699:PHE:HD1	7	0.16
(2,782)	1:A:698:VAL:HG12	1:A:699:PHE:HD2	7	0.16
(2,782)	1:A:698:VAL:HG13	1:A:699:PHE:HD1	7	0.16
(2,782)	1:A:698:VAL:HG13	1:A:699:PHE:HD2	7	0.16
(2,781)	1:A:698:VAL:HG11	1:A:695:LEU:HG	11	0.16
(2,781)	1:A:698:VAL:HG12	1:A:695:LEU:HG	11	0.16
(2,781)	1:A:698:VAL:HG13	1:A:695:LEU:HG	11	0.16
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD2	3	0.16
(2,78)	1:A:708:VAL:HG21	1:B:714:PRO:HD3	3	0.16
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD2	3	0.16
(2,78)	1:A:708:VAL:HG22	1:B:714:PRO:HD3	3	0.16
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD2	3	0.16
(2,78)	1:A:708:VAL:HG23	1:B:714:PRO:HD3	3	0.16
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	7	0.16
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	7	0.16
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	7	0.16
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	7	0.16
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	7	0.16
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	7	0.16
(2,760)	1:A:693:ILE:HD11	1:A:694:GLY:HA2	3	0.16
(2,760)	1:A:693:ILE:HD11	1:A:694:GLY:HA3	3	0.16
(2,760)	1:A:693:ILE:HD12	1:A:694:GLY:HA2	3	0.16
(2,760)	1:A:693:ILE:HD12	1:A:694:GLY:HA3	3	0.16
(2,760)	1:A:693:ILE:HD13	1:A:694:GLY:HA2	3	0.16
(2,760)	1:A:693:ILE:HD13	1:A:694:GLY:HA3	3	0.16
(2,756)	1:A:692:LEU:HD11	1:A:689:VAL:HG21	6	0.16
(2,756)	1:A:692:LEU:HD11	1:A:689:VAL:HG22	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,756)	1:A:692:LEU:HD11	1:A:689:VAL:HG23	6	0.16
(2,756)	1:A:692:LEU:HD12	1:A:689:VAL:HG21	6	0.16
(2,756)	1:A:692:LEU:HD12	1:A:689:VAL:HG22	6	0.16
(2,756)	1:A:692:LEU:HD12	1:A:689:VAL:HG23	6	0.16
(2,756)	1:A:692:LEU:HD13	1:A:689:VAL:HG21	6	0.16
(2,756)	1:A:692:LEU:HD13	1:A:689:VAL:HG22	6	0.16
(2,756)	1:A:692:LEU:HD13	1:A:689:VAL:HG23	6	0.16
(2,752)	1:A:689:VAL:HG21	1:A:685:PHE:HE1	10	0.16
(2,752)	1:A:689:VAL:HG21	1:A:685:PHE:HE2	10	0.16
(2,752)	1:A:689:VAL:HG22	1:A:685:PHE:HE1	10	0.16
(2,752)	1:A:689:VAL:HG22	1:A:685:PHE:HE2	10	0.16
(2,752)	1:A:689:VAL:HG23	1:A:685:PHE:HE1	10	0.16
(2,752)	1:A:689:VAL:HG23	1:A:685:PHE:HE2	10	0.16
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE1	1	0.16
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE2	1	0.16
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE1	1	0.16
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE2	1	0.16
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE1	1	0.16
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE2	1	0.16
(2,743)	1:A:686:ILE:HD11	1:A:685:PHE:H	6	0.16
(2,743)	1:A:686:ILE:HD12	1:A:685:PHE:H	6	0.16
(2,743)	1:A:686:ILE:HD13	1:A:685:PHE:H	6	0.16
(2,722)	1:A:682:ILE:HD11	1:A:685:PHE:HB2	6	0.16
(2,722)	1:A:682:ILE:HD11	1:A:685:PHE:HB3	6	0.16
(2,722)	1:A:682:ILE:HD12	1:A:685:PHE:HB2	6	0.16
(2,722)	1:A:682:ILE:HD12	1:A:685:PHE:HB3	6	0.16
(2,722)	1:A:682:ILE:HD13	1:A:685:PHE:HB2	6	0.16
(2,722)	1:A:682:ILE:HD13	1:A:685:PHE:HB3	6	0.16
(2,722)	1:A:682:ILE:HD11	1:A:685:PHE:HB2	13	0.16
(2,722)	1:A:682:ILE:HD11	1:A:685:PHE:HB3	13	0.16
(2,722)	1:A:682:ILE:HD12	1:A:685:PHE:HB2	13	0.16
(2,722)	1:A:682:ILE:HD12	1:A:685:PHE:HB3	13	0.16
(2,722)	1:A:682:ILE:HD13	1:A:685:PHE:HB2	13	0.16
(2,722)	1:A:682:ILE:HD13	1:A:685:PHE:HB3	13	0.16
(2,721)	1:A:682:ILE:HD11	1:A:681:TYR:H	3	0.16
(2,721)	1:A:682:ILE:HD12	1:A:681:TYR:H	3	0.16
(2,721)	1:A:682:ILE:HD13	1:A:681:TYR:H	3	0.16
(2,718)	1:A:682:ILE:HG21	1:A:679:LEU:H	7	0.16
(2,718)	1:A:682:ILE:HG22	1:A:679:LEU:H	7	0.16
(2,718)	1:A:682:ILE:HG23	1:A:679:LEU:H	7	0.16
(2,697)	1:A:674:ASP:H	1:A:677:ASN:H	14	0.16
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD11	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD12	15	0.16
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD13	15	0.16
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD21	15	0.16
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD22	15	0.16
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD23	15	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD11	2	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD12	2	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD13	2	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD21	2	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD22	2	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD23	2	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD11	2	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD12	2	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD13	2	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD21	2	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD22	2	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD23	2	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD11	2	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD12	2	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD13	2	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD21	2	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD22	2	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD23	2	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD11	8	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD12	8	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD13	8	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD21	8	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD22	8	0.16
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD23	8	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD11	8	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD12	8	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD13	8	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD21	8	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD22	8	0.16
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD23	8	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD11	8	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD12	8	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD13	8	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD21	8	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD22	8	0.16
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD23	8	0.16
(2,654)	1:A:665:LYS:H	1:A:664:ASP:HA	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,649)	1:A:664:ASP:H	1:A:663:LEU:HA	8	0.16
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD2	6	0.16
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD3	6	0.16
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD11	15	0.16
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD12	15	0.16
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD13	15	0.16
(2,601)	1:B:785:LEU:H	1:B:782:VAL:HA	3	0.16
(2,599)	1:B:784:LEU:HD11	1:B:787:ARG:HD2	3	0.16
(2,599)	1:B:784:LEU:HD11	1:B:787:ARG:HD3	3	0.16
(2,599)	1:B:784:LEU:HD12	1:B:787:ARG:HD2	3	0.16
(2,599)	1:B:784:LEU:HD12	1:B:787:ARG:HD3	3	0.16
(2,599)	1:B:784:LEU:HD13	1:B:787:ARG:HD2	3	0.16
(2,599)	1:B:784:LEU:HD13	1:B:787:ARG:HD3	3	0.16
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD1	1	0.16
(2,59)	1:A:700:ALA:HB1	1:A:699:PHE:HD2	1	0.16
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD1	1	0.16
(2,59)	1:A:700:ALA:HB2	1:A:699:PHE:HD2	1	0.16
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD1	1	0.16
(2,59)	1:A:700:ALA:HB3	1:A:699:PHE:HD2	1	0.16
(2,575)	1:B:781:ILE:H	1:B:778:VAL:HA	12	0.16
(2,55)	1:B:696:ARG:HE	1:A:694:GLY:HA2	15	0.16
(2,55)	1:B:696:ARG:HE	1:A:694:GLY:HA3	15	0.16
(2,546)	1:B:776:LEU:H	1:B:773:ASP:HA	3	0.16
(2,522)	1:B:764:SER:H	1:B:761:ARG:HA	11	0.16
(2,515)	1:B:760:LEU:HD11	1:B:757:TRP:HA	2	0.16
(2,515)	1:B:760:LEU:HD12	1:B:757:TRP:HA	2	0.16
(2,515)	1:B:760:LEU:HD13	1:B:757:TRP:HA	2	0.16
(2,515)	1:B:760:LEU:HD11	1:B:757:TRP:HA	11	0.16
(2,515)	1:B:760:LEU:HD12	1:B:757:TRP:HA	11	0.16
(2,515)	1:B:760:LEU:HD13	1:B:757:TRP:HA	11	0.16
(2,502)	1:B:755:LEU:H	1:B:752:SER:HA	10	0.16
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA2	5	0.16
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA3	5	0.16
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA2	5	0.16
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA3	5	0.16
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA2	5	0.16
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA3	5	0.16
(2,482)	1:B:749:VAL:H	1:B:746:ILE:HA	14	0.16
(2,479)	1:B:748:LEU:H	1:B:745:SER:HA	13	0.16
(2,473)	1:B:746:ILE:HG21	1:B:750:ASN:HD22	8	0.16
(2,473)	1:B:746:ILE:HG22	1:B:750:ASN:HD22	8	0.16
(2,473)	1:B:746:ILE:HG23	1:B:750:ASN:HD22	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,473)	1:B:746:ILE:HG21	1:B:750:ASN:HD22	10	0.16
(2,473)	1:B:746:ILE:HG22	1:B:750:ASN:HD22	10	0.16
(2,473)	1:B:746:ILE:HG23	1:B:750:ASN:HD22	10	0.16
(2,470)	1:B:746:ILE:HD11	1:B:743:ASP:HA	15	0.16
(2,470)	1:B:746:ILE:HD12	1:B:743:ASP:HA	15	0.16
(2,470)	1:B:746:ILE:HD13	1:B:743:ASP:HA	15	0.16
(2,428)	1:B:708:VAL:HG11	1:B:705:VAL:HA	9	0.16
(2,428)	1:B:708:VAL:HG12	1:B:705:VAL:HA	9	0.16
(2,428)	1:B:708:VAL:HG13	1:B:705:VAL:HA	9	0.16
(2,414)	1:B:707:ARG:H	1:B:704:LEU:HA	15	0.16
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB2	12	0.16
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB3	12	0.16
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD1	3	0.16
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD2	3	0.16
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD1	3	0.16
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD2	3	0.16
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD1	3	0.16
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD2	3	0.16
(2,372)	1:B:701:VAL:HG11	1:B:698:VAL:HA	5	0.16
(2,372)	1:B:701:VAL:HG12	1:B:698:VAL:HA	5	0.16
(2,372)	1:B:701:VAL:HG13	1:B:698:VAL:HA	5	0.16
(2,37)	1:B:692:LEU:HD21	1:A:694:GLY:H	3	0.16
(2,37)	1:B:692:LEU:HD22	1:A:694:GLY:H	3	0.16
(2,37)	1:B:692:LEU:HD23	1:A:694:GLY:H	3	0.16
(2,363)	1:B:700:ALA:H	1:B:699:PHE:HA	1	0.16
(2,363)	1:B:700:ALA:H	1:B:699:PHE:HA	12	0.16
(2,363)	1:B:700:ALA:H	1:B:699:PHE:HA	14	0.16
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD2	13	0.16
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD3	13	0.16
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD2	13	0.16
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD3	13	0.16
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD2	13	0.16
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD3	13	0.16
(2,333)	1:B:692:LEU:HD11	1:B:696:ARG:HH11	11	0.16
(2,333)	1:B:692:LEU:HD11	1:B:696:ARG:HH12	11	0.16
(2,333)	1:B:692:LEU:HD11	1:B:696:ARG:HH21	11	0.16
(2,333)	1:B:692:LEU:HD11	1:B:696:ARG:HH22	11	0.16
(2,333)	1:B:692:LEU:HD12	1:B:696:ARG:HH11	11	0.16
(2,333)	1:B:692:LEU:HD12	1:B:696:ARG:HH12	11	0.16
(2,333)	1:B:692:LEU:HD12	1:B:696:ARG:HH21	11	0.16
(2,333)	1:B:692:LEU:HD12	1:B:696:ARG:HH22	11	0.16
(2,333)	1:B:692:LEU:HD13	1:B:696:ARG:HH11	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,333)	1:B:692:LEU:HD13	1:B:696:ARG:HH12	11	0.16
(2,333)	1:B:692:LEU:HD13	1:B:696:ARG:HH21	11	0.16
(2,333)	1:B:692:LEU:HD13	1:B:696:ARG:HH22	11	0.16
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG21	9	0.16
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG22	9	0.16
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG23	9	0.16
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG21	9	0.16
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG22	9	0.16
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG23	9	0.16
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG21	9	0.16
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG22	9	0.16
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG23	9	0.16
(2,326)	1:B:689:VAL:HG21	1:B:685:PHE:HD1	14	0.16
(2,326)	1:B:689:VAL:HG21	1:B:685:PHE:HD2	14	0.16
(2,326)	1:B:689:VAL:HG22	1:B:685:PHE:HD1	14	0.16
(2,326)	1:B:689:VAL:HG22	1:B:685:PHE:HD2	14	0.16
(2,326)	1:B:689:VAL:HG23	1:B:685:PHE:HD1	14	0.16
(2,326)	1:B:689:VAL:HG23	1:B:685:PHE:HD2	14	0.16
(2,296)	1:B:682:ILE:HD11	1:B:681:TYR:H	2	0.16
(2,296)	1:B:682:ILE:HD12	1:B:681:TYR:H	2	0.16
(2,296)	1:B:682:ILE:HD13	1:B:681:TYR:H	2	0.16
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD11	3	0.16
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD12	3	0.16
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD13	3	0.16
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD11	9	0.16
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD12	9	0.16
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD13	9	0.16
(2,280)	1:B:676:THR:HG21	1:B:681:TYR:HH	6	0.16
(2,280)	1:B:676:THR:HG22	1:B:681:TYR:HH	6	0.16
(2,280)	1:B:676:THR:HG23	1:B:681:TYR:HH	6	0.16
(2,273)	1:B:675:ILE:H	1:B:674:ASP:H	15	0.16
(2,271)	1:B:673:PHE:H	1:B:672:TRP:H	6	0.16
(2,259)	1:B:670:TRP:H	1:B:667:ALA:HA	3	0.16
(2,253)	1:B:669:LEU:H	1:B:666:TRP:HA	13	0.16
(2,253)	1:B:669:LEU:H	1:B:666:TRP:HA	15	0.16
(2,229)	1:B:665:LYS:H	1:B:664:ASP:HA	15	0.16
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG12	15	0.16
(2,195)	1:A:817:ALA:H	1:A:830:ILE:HG13	15	0.16
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG12	15	0.16
(2,194)	1:A:817:ALA:H	1:A:830:ILE:HG13	15	0.16
(2,187)	1:B:816:ASN:H	1:B:830:ILE:HD11	5	0.16
(2,187)	1:B:816:ASN:H	1:B:830:ILE:HD12	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,187)	1:B:816:ASN:H	1:B:830:ILE:HD13	5	0.16
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG11	4	0.16
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG12	4	0.16
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG13	4	0.16
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG21	4	0.16
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG22	4	0.16
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG23	4	0.16
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	14	0.16
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	14	0.16
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	14	0.16
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	14	0.16
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	14	0.16
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	14	0.16
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG12	9	0.16
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG13	9	0.16
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG12	14	0.16
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG13	14	0.16
(2,1465)	1:A:796:TRP:HE1	1:A:796:TRP:H	3	0.16
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD11	9	0.16
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD12	9	0.16
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD13	9	0.16
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD21	9	0.16
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD22	9	0.16
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD23	9	0.16
(2,1458)	1:A:786:GLY:H	1:A:782:VAL:HA	9	0.16
(2,1451)	1:A:785:LEU:H	1:A:782:VAL:HA	4	0.16
(2,1443)	1:A:784:LEU:H	1:A:781:ILE:HA	5	0.16
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD2	12	0.16
(2,1438)	1:A:783:GLU:H	1:A:780:ARG:HD3	12	0.16
(2,1437)	1:A:783:GLU:H	1:A:780:ARG:HA	11	0.16
(2,1436)	1:A:782:VAL:HG21	1:A:779:THR:HA	15	0.16
(2,1436)	1:A:782:VAL:HG22	1:A:779:THR:HA	15	0.16
(2,1436)	1:A:782:VAL:HG23	1:A:779:THR:HA	15	0.16
(2,1431)	1:A:782:VAL:H	1:A:779:THR:HA	9	0.16
(2,1365)	1:A:760:LEU:HD11	1:A:757:TRP:HA	3	0.16
(2,1365)	1:A:760:LEU:HD12	1:A:757:TRP:HA	3	0.16
(2,1365)	1:A:760:LEU:HD13	1:A:757:TRP:HA	3	0.16
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	12	0.16
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	12	0.16
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	12	0.16
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	12	0.16
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	12	0.16
(2,1329)	1:A:748:LEU:H	1:A:745:SER:HA	14	0.16
(2,1323)	1:A:746:ILE:HG21	1:A:750:ASN:HD22	13	0.16
(2,1323)	1:A:746:ILE:HG22	1:A:750:ASN:HD22	13	0.16
(2,1323)	1:A:746:ILE:HG23	1:A:750:ASN:HD22	13	0.16
(2,1314)	1:A:746:ILE:H	1:A:743:ASP:HA	8	0.16
(2,13)	1:B:666:TRP:HE1	1:A:666:TRP:HD1	14	0.16
(2,1264)	1:A:707:ARG:H	1:A:704:LEU:HA	8	0.16
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	7	0.16
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	7	0.16
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	7	0.16
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	7	0.16
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	7	0.16
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	7	0.16
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	4	0.16
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	4	0.16
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	4	0.16
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	4	0.16
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	4	0.16
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	4	0.16
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	12	0.16
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	12	0.16
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	12	0.16
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	12	0.16
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	12	0.16
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	12	0.16
(2,1228)	1:A:702:LEU:HD11	1:A:699:PHE:HE1	13	0.16
(2,1228)	1:A:702:LEU:HD11	1:A:699:PHE:HE2	13	0.16
(2,1228)	1:A:702:LEU:HD12	1:A:699:PHE:HE1	13	0.16
(2,1228)	1:A:702:LEU:HD12	1:A:699:PHE:HE2	13	0.16
(2,1228)	1:A:702:LEU:HD13	1:A:699:PHE:HE1	13	0.16
(2,1228)	1:A:702:LEU:HD13	1:A:699:PHE:HE2	13	0.16
(2,1227)	1:A:702:LEU:HD11	1:A:699:PHE:HD1	15	0.16
(2,1227)	1:A:702:LEU:HD11	1:A:699:PHE:HD2	15	0.16
(2,1227)	1:A:702:LEU:HD12	1:A:699:PHE:HD1	15	0.16
(2,1227)	1:A:702:LEU:HD12	1:A:699:PHE:HD2	15	0.16
(2,1227)	1:A:702:LEU:HD13	1:A:699:PHE:HD1	15	0.16
(2,1227)	1:A:702:LEU:HD13	1:A:699:PHE:HD2	15	0.16
(2,1217)	1:A:700:ALA:HB1	1:A:697:ILE:HA	11	0.16
(2,1217)	1:A:700:ALA:HB2	1:A:697:ILE:HA	11	0.16
(2,1217)	1:A:700:ALA:HB3	1:A:697:ILE:HA	11	0.16
(2,1207)	1:A:698:VAL:HG11	1:A:699:PHE:HD1	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1207)	1:A:698:VAL:HG11	1:A:699:PHE:HD2	7	0.16
(2,1207)	1:A:698:VAL:HG12	1:A:699:PHE:HD1	7	0.16
(2,1207)	1:A:698:VAL:HG12	1:A:699:PHE:HD2	7	0.16
(2,1207)	1:A:698:VAL:HG13	1:A:699:PHE:HD1	7	0.16
(2,1207)	1:A:698:VAL:HG13	1:A:699:PHE:HD2	7	0.16
(2,1206)	1:A:698:VAL:HG11	1:A:695:LEU:HG	11	0.16
(2,1206)	1:A:698:VAL:HG12	1:A:695:LEU:HG	11	0.16
(2,1206)	1:A:698:VAL:HG13	1:A:695:LEU:HG	11	0.16
(2,12)	1:A:666:TRP:HE1	1:B:666:TRP:HZ2	4	0.16
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	7	0.16
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	7	0.16
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	7	0.16
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	7	0.16
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	7	0.16
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	7	0.16
(2,1185)	1:A:693:ILE:HD11	1:A:694:GLY:HA2	3	0.16
(2,1185)	1:A:693:ILE:HD11	1:A:694:GLY:HA3	3	0.16
(2,1185)	1:A:693:ILE:HD12	1:A:694:GLY:HA2	3	0.16
(2,1185)	1:A:693:ILE:HD12	1:A:694:GLY:HA3	3	0.16
(2,1185)	1:A:693:ILE:HD13	1:A:694:GLY:HA2	3	0.16
(2,1185)	1:A:693:ILE:HD13	1:A:694:GLY:HA3	3	0.16
(2,1181)	1:A:692:LEU:HD11	1:A:689:VAL:HG21	6	0.16
(2,1181)	1:A:692:LEU:HD11	1:A:689:VAL:HG22	6	0.16
(2,1181)	1:A:692:LEU:HD11	1:A:689:VAL:HG23	6	0.16
(2,1181)	1:A:692:LEU:HD12	1:A:689:VAL:HG21	6	0.16
(2,1181)	1:A:692:LEU:HD12	1:A:689:VAL:HG22	6	0.16
(2,1181)	1:A:692:LEU:HD12	1:A:689:VAL:HG23	6	0.16
(2,1181)	1:A:692:LEU:HD13	1:A:689:VAL:HG21	6	0.16
(2,1181)	1:A:692:LEU:HD13	1:A:689:VAL:HG22	6	0.16
(2,1181)	1:A:692:LEU:HD13	1:A:689:VAL:HG23	6	0.16
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB2	9	0.16
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB3	9	0.16
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB2	9	0.16
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB3	9	0.16
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB2	9	0.16
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB3	9	0.16
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB2	13	0.16
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB3	13	0.16
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB2	13	0.16
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB3	13	0.16
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB2	13	0.16
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB3	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1177)	1:A:689:VAL:HG21	1:A:685:PHE:HE1	10	0.16
(2,1177)	1:A:689:VAL:HG21	1:A:685:PHE:HE2	10	0.16
(2,1177)	1:A:689:VAL:HG22	1:A:685:PHE:HE1	10	0.16
(2,1177)	1:A:689:VAL:HG22	1:A:685:PHE:HE2	10	0.16
(2,1177)	1:A:689:VAL:HG23	1:A:685:PHE:HE1	10	0.16
(2,1177)	1:A:689:VAL:HG23	1:A:685:PHE:HE2	10	0.16
(2,1168)	1:A:686:ILE:HD11	1:A:685:PHE:H	6	0.16
(2,1168)	1:A:686:ILE:HD12	1:A:685:PHE:H	6	0.16
(2,1168)	1:A:686:ILE:HD13	1:A:685:PHE:H	6	0.16
(2,1147)	1:A:682:ILE:HD11	1:A:685:PHE:HB2	6	0.16
(2,1147)	1:A:682:ILE:HD11	1:A:685:PHE:HB3	6	0.16
(2,1147)	1:A:682:ILE:HD12	1:A:685:PHE:HB2	6	0.16
(2,1147)	1:A:682:ILE:HD12	1:A:685:PHE:HB3	6	0.16
(2,1147)	1:A:682:ILE:HD13	1:A:685:PHE:HB2	6	0.16
(2,1147)	1:A:682:ILE:HD13	1:A:685:PHE:HB3	6	0.16
(2,1147)	1:A:682:ILE:HD11	1:A:685:PHE:HB2	13	0.16
(2,1147)	1:A:682:ILE:HD11	1:A:685:PHE:HB3	13	0.16
(2,1147)	1:A:682:ILE:HD12	1:A:685:PHE:HB2	13	0.16
(2,1147)	1:A:682:ILE:HD12	1:A:685:PHE:HB3	13	0.16
(2,1147)	1:A:682:ILE:HD13	1:A:685:PHE:HB2	13	0.16
(2,1147)	1:A:682:ILE:HD13	1:A:685:PHE:HB3	13	0.16
(2,1146)	1:A:682:ILE:HD11	1:A:681:TYR:H	3	0.16
(2,1146)	1:A:682:ILE:HD12	1:A:681:TYR:H	3	0.16
(2,1146)	1:A:682:ILE:HD13	1:A:681:TYR:H	3	0.16
(2,1143)	1:A:682:ILE:HG21	1:A:679:LEU:H	7	0.16
(2,1143)	1:A:682:ILE:HG22	1:A:679:LEU:H	7	0.16
(2,1143)	1:A:682:ILE:HG23	1:A:679:LEU:H	7	0.16
(2,1114)	1:A:781:ILE:HD11	1:B:743:ASP:HA	5	0.16
(2,1114)	1:A:781:ILE:HD12	1:B:743:ASP:HA	5	0.16
(2,1114)	1:A:781:ILE:HD13	1:B:743:ASP:HA	5	0.16
(2,1122)	1:A:674:ASP:H	1:A:677:ASN:H	14	0.16
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD11	15	0.16
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD12	15	0.16
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD13	15	0.16
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD21	15	0.16
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD22	15	0.16
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD23	15	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD11	2	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD12	2	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD13	2	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD21	2	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD22	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD23	2	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD11	2	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD12	2	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD13	2	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD21	2	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD22	2	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD23	2	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD11	2	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD12	2	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD13	2	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD21	2	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD22	2	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD23	2	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD11	8	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD12	8	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD13	8	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD21	8	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD22	8	0.16
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD23	8	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD11	8	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD12	8	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD13	8	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD21	8	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD22	8	0.16
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD23	8	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD11	8	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD12	8	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD13	8	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD21	8	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD22	8	0.16
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD23	8	0.16
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD2	1	0.16
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD3	1	0.16
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD2	1	0.16
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD3	1	0.16
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD2	1	0.16
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD3	1	0.16
(2,1079)	1:A:665:LYS:H	1:A:664:ASP:HA	14	0.16
(2,1074)	1:A:664:ASP:H	1:A:663:LEU:HA	8	0.16
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG11	4	0.16
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG12	4	0.16
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG13	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG21	4	0.16
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG22	4	0.16
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG23	4	0.16
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD2	8	0.16
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD3	8	0.16
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	14	0.16
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	14	0.16
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	14	0.16
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	14	0.16
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	14	0.16
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	14	0.16
(2,1040)	1:A:796:TRP:HE1	1:A:796:TRP:H	3	0.16
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD11	9	0.16
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD12	9	0.16
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD13	9	0.16
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD21	9	0.16
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD22	9	0.16
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD23	9	0.16
(2,1033)	1:A:786:GLY:H	1:A:782:VAL:HA	9	0.16
(2,1026)	1:A:785:LEU:H	1:A:782:VAL:HA	4	0.16
(2,1018)	1:A:784:LEU:H	1:A:781:ILE:HA	5	0.16
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD2	12	0.16
(2,1013)	1:A:783:GLU:H	1:A:780:ARG:HD3	12	0.16
(2,1012)	1:A:783:GLU:H	1:A:780:ARG:HA	11	0.16
(2,1011)	1:A:782:VAL:HG21	1:A:779:THR:HA	15	0.16
(2,1011)	1:A:782:VAL:HG22	1:A:779:THR:HA	15	0.16
(2,1011)	1:A:782:VAL:HG23	1:A:779:THR:HA	15	0.16
(2,1006)	1:A:782:VAL:H	1:A:779:THR:HA	9	0.16
(1,95)	1:B:794:LYS:O	1:B:798:ASN:H	4	0.16
(1,9)	1:B:794:LYS:O	1:B:798:ASN:H	4	0.16
(1,89)	1:B:791:GLU:O	1:B:795:TYR:H	1	0.16
(1,89)	1:B:791:GLU:O	1:B:795:TYR:H	7	0.16
(1,89)	1:B:791:GLU:O	1:B:795:TYR:H	10	0.16
(1,61)	1:B:830:ILE:O	1:B:834:GLN:H	14	0.16
(1,3)	1:B:791:GLU:O	1:B:795:TYR:H	1	0.16
(1,3)	1:B:791:GLU:O	1:B:795:TYR:H	7	0.16
(1,3)	1:B:791:GLU:O	1:B:795:TYR:H	10	0.16
(1,233)	1:B:830:ILE:O	1:B:834:GLN:H	14	0.16
(1,23)	1:B:801:GLN:O	1:B:805:GLN:H	12	0.16
(1,195)	1:B:801:GLN:O	1:B:805:GLN:H	12	0.16
(1,191)	1:B:799:LEU:O	1:B:803:TRP:H	7	0.16
(1,19)	1:B:799:LEU:O	1:B:803:TRP:H	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:B:794:LYS:O	1:B:798:ASN:H	4	0.16
(1,175)	1:B:791:GLU:O	1:B:795:TYR:H	1	0.16
(1,175)	1:B:791:GLU:O	1:B:795:TYR:H	7	0.16
(1,175)	1:B:791:GLU:O	1:B:795:TYR:H	10	0.16
(1,147)	1:B:830:ILE:O	1:B:834:GLN:H	14	0.16
(1,109)	1:B:801:GLN:O	1:B:805:GLN:H	12	0.16
(1,105)	1:B:799:LEU:O	1:B:803:TRP:H	7	0.16
(2,96)	1:A:755:LEU:HD11	1:B:710:GLN:HE21	8	0.15
(2,96)	1:A:755:LEU:HD11	1:B:710:GLN:HE22	8	0.15
(2,96)	1:A:755:LEU:HD12	1:B:710:GLN:HE21	8	0.15
(2,96)	1:A:755:LEU:HD12	1:B:710:GLN:HE22	8	0.15
(2,96)	1:A:755:LEU:HD13	1:B:710:GLN:HE21	8	0.15
(2,96)	1:A:755:LEU:HD13	1:B:710:GLN:HE22	8	0.15
(2,951)	1:A:771:LEU:HD11	1:A:768:TYR:HE1	3	0.15
(2,951)	1:A:771:LEU:HD11	1:A:768:TYR:HE2	3	0.15
(2,951)	1:A:771:LEU:HD12	1:A:768:TYR:HE1	3	0.15
(2,951)	1:A:771:LEU:HD12	1:A:768:TYR:HE2	3	0.15
(2,951)	1:A:771:LEU:HD13	1:A:768:TYR:HE1	3	0.15
(2,951)	1:A:771:LEU:HD13	1:A:768:TYR:HE2	3	0.15
(2,948)	1:A:764:SER:H	1:A:771:LEU:HB2	1	0.15
(2,948)	1:A:764:SER:H	1:A:771:LEU:HB3	1	0.15
(2,948)	1:A:764:SER:H	1:A:771:LEU:HB2	10	0.15
(2,948)	1:A:764:SER:H	1:A:771:LEU:HB3	10	0.15
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	12	0.15
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	12	0.15
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	12	0.15
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	12	0.15
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	12	0.15
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	12	0.15
(2,939)	1:A:760:LEU:HD11	1:A:756:ILE:HG12	14	0.15
(2,939)	1:A:760:LEU:HD11	1:A:756:ILE:HG13	14	0.15
(2,939)	1:A:760:LEU:HD12	1:A:756:ILE:HG12	14	0.15
(2,939)	1:A:760:LEU:HD12	1:A:756:ILE:HG13	14	0.15
(2,939)	1:A:760:LEU:HD13	1:A:756:ILE:HG12	14	0.15
(2,939)	1:A:760:LEU:HD13	1:A:756:ILE:HG13	14	0.15
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB2	2	0.15
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB3	2	0.15
(2,863)	1:A:709:ARG:HE	1:A:709:ARG:H	13	0.15
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB2	5	0.15
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB3	5	0.15
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB2	5	0.15
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB3	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB2	5	0.15
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB3	5	0.15
(2,839)	1:A:707:ARG:H	1:A:704:LEU:HA	6	0.15
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB2	11	0.15
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB3	11	0.15
(2,810)	1:A:704:LEU:H	1:A:701:VAL:HA	14	0.15
(2,81)	1:A:708:VAL:HG21	1:B:714:PRO:HA	7	0.15
(2,81)	1:A:708:VAL:HG22	1:B:714:PRO:HA	7	0.15
(2,81)	1:A:708:VAL:HG23	1:B:714:PRO:HA	7	0.15
(2,802)	1:A:702:LEU:HD11	1:A:699:PHE:HD1	9	0.15
(2,802)	1:A:702:LEU:HD11	1:A:699:PHE:HD2	9	0.15
(2,802)	1:A:702:LEU:HD12	1:A:699:PHE:HD1	9	0.15
(2,802)	1:A:702:LEU:HD12	1:A:699:PHE:HD2	9	0.15
(2,802)	1:A:702:LEU:HD13	1:A:699:PHE:HD1	9	0.15
(2,802)	1:A:702:LEU:HD13	1:A:699:PHE:HD2	9	0.15
(2,799)	1:A:702:LEU:H	1:A:699:PHE:HA	14	0.15
(2,793)	1:A:700:ALA:HB1	1:A:703:SER:HB2	11	0.15
(2,793)	1:A:700:ALA:HB1	1:A:703:SER:HB3	11	0.15
(2,793)	1:A:700:ALA:HB2	1:A:703:SER:HB2	11	0.15
(2,793)	1:A:700:ALA:HB2	1:A:703:SER:HB3	11	0.15
(2,793)	1:A:700:ALA:HB3	1:A:703:SER:HB2	11	0.15
(2,793)	1:A:700:ALA:HB3	1:A:703:SER:HB3	11	0.15
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB1	3	0.15
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB2	3	0.15
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB3	3	0.15
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB1	3	0.15
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB2	3	0.15
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB3	3	0.15
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB1	3	0.15
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB2	3	0.15
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB3	3	0.15
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB1	14	0.15
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB2	14	0.15
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB3	14	0.15
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB1	14	0.15
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB2	14	0.15
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB3	14	0.15
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB1	14	0.15
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB2	14	0.15
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB3	14	0.15
(2,773)	1:A:695:LEU:HD21	1:A:696:ARG:HH11	10	0.15
(2,773)	1:A:695:LEU:HD21	1:A:696:ARG:HH12	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,773)	1:A:695:LEU:HD22	1:A:696:ARG:HH11	10	0.15
(2,773)	1:A:695:LEU:HD22	1:A:696:ARG:HH12	10	0.15
(2,773)	1:A:695:LEU:HD23	1:A:696:ARG:HH11	10	0.15
(2,773)	1:A:695:LEU:HD23	1:A:696:ARG:HH12	10	0.15
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	6	0.15
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	6	0.15
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	6	0.15
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	6	0.15
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	6	0.15
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	6	0.15
(2,713)	1:A:679:LEU:HD11	1:A:678:TRP:HH2	6	0.15
(2,713)	1:A:679:LEU:HD12	1:A:678:TRP:HH2	6	0.15
(2,713)	1:A:679:LEU:HD13	1:A:678:TRP:HH2	6	0.15
(2,713)	1:A:679:LEU:HD21	1:A:678:TRP:HH2	6	0.15
(2,713)	1:A:679:LEU:HD22	1:A:678:TRP:HH2	6	0.15
(2,713)	1:A:679:LEU:HD23	1:A:678:TRP:HH2	6	0.15
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD11	6	0.15
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD12	6	0.15
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD13	6	0.15
(2,701)	1:A:676:THR:HG21	1:A:666:TRP:HZ3	10	0.15
(2,701)	1:A:676:THR:HG22	1:A:666:TRP:HZ3	10	0.15
(2,701)	1:A:676:THR:HG23	1:A:666:TRP:HZ3	10	0.15
(2,684)	1:A:670:TRP:H	1:A:667:ALA:HA	11	0.15
(2,683)	1:A:669:LEU:HD11	1:A:672:TRP:HZ3	6	0.15
(2,683)	1:A:669:LEU:HD12	1:A:672:TRP:HZ3	6	0.15
(2,683)	1:A:669:LEU:HD13	1:A:672:TRP:HZ3	6	0.15
(2,683)	1:A:669:LEU:HD21	1:A:672:TRP:HZ3	6	0.15
(2,683)	1:A:669:LEU:HD22	1:A:672:TRP:HZ3	6	0.15
(2,683)	1:A:669:LEU:HD23	1:A:672:TRP:HZ3	6	0.15
(2,670)	1:A:667:ALA:H	1:A:666:TRP:HD1	4	0.15
(2,659)	1:A:666:TRP:H	1:A:663:LEU:HA	9	0.15
(2,654)	1:A:665:LYS:H	1:A:664:ASP:HA	11	0.15
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB1	8	0.15
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB2	8	0.15
(2,64)	1:B:702:LEU:HD21	1:A:700:ALA:HB3	8	0.15
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB1	8	0.15
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB2	8	0.15
(2,64)	1:B:702:LEU:HD22	1:A:700:ALA:HB3	8	0.15
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB1	8	0.15
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB2	8	0.15
(2,64)	1:B:702:LEU:HD23	1:A:700:ALA:HB3	8	0.15
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD2	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD3	15	0.15
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD11	13	0.15
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD12	13	0.15
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD13	13	0.15
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD11	3	0.15
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD12	3	0.15
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD13	3	0.15
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD21	3	0.15
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD22	3	0.15
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD23	3	0.15
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD11	5	0.15
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD12	5	0.15
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD13	5	0.15
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD21	5	0.15
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD22	5	0.15
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD23	5	0.15
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD21	12	0.15
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD22	12	0.15
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD23	12	0.15
(2,608)	1:B:786:GLY:H	1:B:782:VAL:HA	3	0.15
(2,608)	1:B:786:GLY:H	1:B:782:VAL:HA	9	0.15
(2,60)	1:A:700:ALA:HB1	1:B:699:PHE:HD1	4	0.15
(2,60)	1:A:700:ALA:HB1	1:B:699:PHE:HD2	4	0.15
(2,60)	1:A:700:ALA:HB2	1:B:699:PHE:HD1	4	0.15
(2,60)	1:A:700:ALA:HB2	1:B:699:PHE:HD2	4	0.15
(2,60)	1:A:700:ALA:HB3	1:B:699:PHE:HD1	4	0.15
(2,60)	1:A:700:ALA:HB3	1:B:699:PHE:HD2	4	0.15
(2,593)	1:B:784:LEU:H	1:B:781:ILE:HA	7	0.15
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD2	7	0.15
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD3	7	0.15
(2,581)	1:B:782:VAL:H	1:B:779:THR:HA	7	0.15
(2,558)	1:B:777:ILE:HG21	1:B:780:ARG:HD2	5	0.15
(2,558)	1:B:777:ILE:HG21	1:B:780:ARG:HD3	5	0.15
(2,558)	1:B:777:ILE:HG22	1:B:780:ARG:HD2	5	0.15
(2,558)	1:B:777:ILE:HG22	1:B:780:ARG:HD3	5	0.15
(2,558)	1:B:777:ILE:HG23	1:B:780:ARG:HD2	5	0.15
(2,558)	1:B:777:ILE:HG23	1:B:780:ARG:HD3	5	0.15
(2,557)	1:B:777:ILE:HD11	1:B:774:LEU:HA	1	0.15
(2,557)	1:B:777:ILE:HD12	1:B:774:LEU:HA	1	0.15
(2,557)	1:B:777:ILE:HD13	1:B:774:LEU:HA	1	0.15
(2,55)	1:B:696:ARG:HE	1:A:694:GLY:HA2	14	0.15
(2,55)	1:B:696:ARG:HE	1:A:694:GLY:HA3	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,546)	1:B:776:LEU:H	1:B:773:ASP:HA	8	0.15
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH21	6	0.15
(2,527)	1:B:771:LEU:HD21	1:B:772:ARG:HH22	6	0.15
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH21	6	0.15
(2,527)	1:B:771:LEU:HD22	1:B:772:ARG:HH22	6	0.15
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH21	6	0.15
(2,527)	1:B:771:LEU:HD23	1:B:772:ARG:HH22	6	0.15
(2,522)	1:B:764:SER:H	1:B:761:ARG:HA	2	0.15
(2,5)	1:A:663:LEU:H	1:A:661:LEU:HB2	13	0.15
(2,5)	1:A:663:LEU:H	1:A:661:LEU:HB3	13	0.15
(2,479)	1:B:748:LEU:H	1:B:745:SER:HA	12	0.15
(2,472)	1:B:746:ILE:HG21	1:B:750:ASN:HD21	12	0.15
(2,472)	1:B:746:ILE:HG22	1:B:750:ASN:HD21	12	0.15
(2,472)	1:B:746:ILE:HG23	1:B:750:ASN:HD21	12	0.15
(2,437)	1:B:709:ARG:HE	1:B:705:VAL:HG11	6	0.15
(2,437)	1:B:709:ARG:HE	1:B:705:VAL:HG12	6	0.15
(2,437)	1:B:709:ARG:HE	1:B:705:VAL:HG13	6	0.15
(2,437)	1:B:709:ARG:HE	1:B:705:VAL:HG11	11	0.15
(2,437)	1:B:709:ARG:HE	1:B:705:VAL:HG12	11	0.15
(2,437)	1:B:709:ARG:HE	1:B:705:VAL:HG13	11	0.15
(2,429)	1:B:708:VAL:HG21	1:B:707:ARG:HD2	9	0.15
(2,429)	1:B:708:VAL:HG21	1:B:707:ARG:HD3	9	0.15
(2,429)	1:B:708:VAL:HG22	1:B:707:ARG:HD2	9	0.15
(2,429)	1:B:708:VAL:HG22	1:B:707:ARG:HD3	9	0.15
(2,429)	1:B:708:VAL:HG23	1:B:707:ARG:HD2	9	0.15
(2,429)	1:B:708:VAL:HG23	1:B:707:ARG:HD3	9	0.15
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB2	10	0.15
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB3	10	0.15
(2,395)	1:B:704:LEU:HD11	1:B:708:VAL:HG21	3	0.15
(2,395)	1:B:704:LEU:HD11	1:B:708:VAL:HG22	3	0.15
(2,395)	1:B:704:LEU:HD11	1:B:708:VAL:HG23	3	0.15
(2,395)	1:B:704:LEU:HD12	1:B:708:VAL:HG21	3	0.15
(2,395)	1:B:704:LEU:HD12	1:B:708:VAL:HG22	3	0.15
(2,395)	1:B:704:LEU:HD12	1:B:708:VAL:HG23	3	0.15
(2,395)	1:B:704:LEU:HD13	1:B:708:VAL:HG21	3	0.15
(2,395)	1:B:704:LEU:HD13	1:B:708:VAL:HG22	3	0.15
(2,395)	1:B:704:LEU:HD13	1:B:708:VAL:HG23	3	0.15
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB2	15	0.15
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB3	15	0.15
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB2	15	0.15
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB3	15	0.15
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB2	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB3	15	0.15
(2,378)	1:B:702:LEU:HD11	1:B:699:PHE:HE1	3	0.15
(2,378)	1:B:702:LEU:HD11	1:B:699:PHE:HE2	3	0.15
(2,378)	1:B:702:LEU:HD12	1:B:699:PHE:HE1	3	0.15
(2,378)	1:B:702:LEU:HD12	1:B:699:PHE:HE2	3	0.15
(2,378)	1:B:702:LEU:HD13	1:B:699:PHE:HE1	3	0.15
(2,378)	1:B:702:LEU:HD13	1:B:699:PHE:HE2	3	0.15
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD1	2	0.15
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD2	2	0.15
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD1	2	0.15
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD2	2	0.15
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD1	2	0.15
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD2	2	0.15
(2,372)	1:B:701:VAL:HG11	1:B:698:VAL:HA	4	0.15
(2,372)	1:B:701:VAL:HG12	1:B:698:VAL:HA	4	0.15
(2,372)	1:B:701:VAL:HG13	1:B:698:VAL:HA	4	0.15
(2,367)	1:B:700:ALA:HB1	1:B:697:ILE:HA	6	0.15
(2,367)	1:B:700:ALA:HB2	1:B:697:ILE:HA	6	0.15
(2,367)	1:B:700:ALA:HB3	1:B:697:ILE:HA	6	0.15
(2,367)	1:B:700:ALA:HB1	1:B:697:ILE:HA	7	0.15
(2,367)	1:B:700:ALA:HB2	1:B:697:ILE:HA	7	0.15
(2,367)	1:B:700:ALA:HB3	1:B:697:ILE:HA	7	0.15
(2,357)	1:B:698:VAL:HG11	1:B:699:PHE:HD1	14	0.15
(2,357)	1:B:698:VAL:HG11	1:B:699:PHE:HD2	14	0.15
(2,357)	1:B:698:VAL:HG12	1:B:699:PHE:HD1	14	0.15
(2,357)	1:B:698:VAL:HG12	1:B:699:PHE:HD2	14	0.15
(2,357)	1:B:698:VAL:HG13	1:B:699:PHE:HD1	14	0.15
(2,357)	1:B:698:VAL:HG13	1:B:699:PHE:HD2	14	0.15
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD2	1	0.15
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD3	1	0.15
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD2	1	0.15
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD3	1	0.15
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD2	1	0.15
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD3	1	0.15
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD2	7	0.15
(2,344)	1:B:695:LEU:HD21	1:B:696:ARG:HD3	7	0.15
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD2	7	0.15
(2,344)	1:B:695:LEU:HD22	1:B:696:ARG:HD3	7	0.15
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD2	7	0.15
(2,344)	1:B:695:LEU:HD23	1:B:696:ARG:HD3	7	0.15
(2,343)	1:B:695:LEU:HD11	1:B:691:SER:HB2	7	0.15
(2,343)	1:B:695:LEU:HD11	1:B:691:SER:HB3	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,343)	1:B:695:LEU:HD12	1:B:691:SER:HB2	7	0.15
(2,343)	1:B:695:LEU:HD12	1:B:691:SER:HB3	7	0.15
(2,343)	1:B:695:LEU:HD13	1:B:691:SER:HB2	7	0.15
(2,343)	1:B:695:LEU:HD13	1:B:691:SER:HB3	7	0.15
(2,326)	1:B:689:VAL:HG21	1:B:685:PHE:HD1	13	0.15
(2,326)	1:B:689:VAL:HG21	1:B:685:PHE:HD2	13	0.15
(2,326)	1:B:689:VAL:HG22	1:B:685:PHE:HD1	13	0.15
(2,326)	1:B:689:VAL:HG22	1:B:685:PHE:HD2	13	0.15
(2,326)	1:B:689:VAL:HG23	1:B:685:PHE:HD1	13	0.15
(2,326)	1:B:689:VAL:HG23	1:B:685:PHE:HD2	13	0.15
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD11	2	0.15
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD12	2	0.15
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD13	2	0.15
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD11	2	0.15
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD12	2	0.15
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD13	2	0.15
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD11	2	0.15
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD12	2	0.15
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD13	2	0.15
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD11	3	0.15
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD12	3	0.15
(2,323)	1:B:688:ILE:HD11	1:B:684:ILE:HD13	3	0.15
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD11	3	0.15
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD12	3	0.15
(2,323)	1:B:688:ILE:HD12	1:B:684:ILE:HD13	3	0.15
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD11	3	0.15
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD12	3	0.15
(2,323)	1:B:688:ILE:HD13	1:B:684:ILE:HD13	3	0.15
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD11	2	0.15
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD12	2	0.15
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD13	2	0.15
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB2	12	0.15
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB3	12	0.15
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB2	12	0.15
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB3	12	0.15
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB2	12	0.15
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB3	12	0.15
(2,259)	1:B:670:TRP:H	1:B:667:ALA:HA	8	0.15
(2,245)	1:B:667:ALA:H	1:B:666:TRP:HD1	12	0.15
(2,242)	1:B:667:ALA:H	1:B:664:ASP:HA	7	0.15
(2,242)	1:B:667:ALA:H	1:B:664:ASP:HA	12	0.15
(2,228)	1:B:665:LYS:H	1:B:662:GLU:HA	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:B:678:TRP:HE1	1:A:683:ARG:HE	13	0.15
(2,180)	1:A:806:GLU:H	1:B:771:LEU:HG	10	0.15
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG12	14	0.15
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG13	14	0.15
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG12	14	0.15
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG13	14	0.15
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG12	11	0.15
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG13	11	0.15
(2,153)	1:A:792:ALA:H	1:B:752:SER:HB2	12	0.15
(2,153)	1:A:792:ALA:H	1:B:752:SER:HB3	12	0.15
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE21	6	0.15
(2,1480)	1:A:835:GLY:H	1:A:834:GLN:HE22	6	0.15
(2,1475)	1:A:806:GLU:H	1:A:803:TRP:HB2	5	0.15
(2,1475)	1:A:806:GLU:H	1:A:803:TRP:HB3	5	0.15
(2,1475)	1:A:806:GLU:H	1:A:803:TRP:HB2	7	0.15
(2,1475)	1:A:806:GLU:H	1:A:803:TRP:HB3	7	0.15
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG12	4	0.15
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG13	4	0.15
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD21	4	0.15
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD22	4	0.15
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD23	4	0.15
(2,1458)	1:A:786:GLY:H	1:A:782:VAL:HA	8	0.15
(2,1457)	1:A:785:LEU:HD21	1:A:782:VAL:HA	12	0.15
(2,1457)	1:A:785:LEU:HD22	1:A:782:VAL:HA	12	0.15
(2,1457)	1:A:785:LEU:HD23	1:A:782:VAL:HA	12	0.15
(2,1425)	1:A:781:ILE:H	1:A:778:VAL:HA	6	0.15
(2,1425)	1:A:781:ILE:H	1:A:778:VAL:HA	10	0.15
(2,1376)	1:A:771:LEU:HD11	1:A:768:TYR:HE1	3	0.15
(2,1376)	1:A:771:LEU:HD11	1:A:768:TYR:HE2	3	0.15
(2,1376)	1:A:771:LEU:HD12	1:A:768:TYR:HE1	3	0.15
(2,1376)	1:A:771:LEU:HD12	1:A:768:TYR:HE2	3	0.15
(2,1376)	1:A:771:LEU:HD13	1:A:768:TYR:HE1	3	0.15
(2,1376)	1:A:771:LEU:HD13	1:A:768:TYR:HE2	3	0.15
(2,1373)	1:A:764:SER:H	1:A:771:LEU:HB2	1	0.15
(2,1373)	1:A:764:SER:H	1:A:771:LEU:HB3	1	0.15
(2,1373)	1:A:764:SER:H	1:A:771:LEU:HB2	10	0.15
(2,1373)	1:A:764:SER:H	1:A:771:LEU:HB3	10	0.15
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	12	0.15
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	12	0.15
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	12	0.15
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	12	0.15
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	12	0.15
(2,1364)	1:A:760:LEU:HD11	1:A:756:ILE:HG12	14	0.15
(2,1364)	1:A:760:LEU:HD11	1:A:756:ILE:HG13	14	0.15
(2,1364)	1:A:760:LEU:HD12	1:A:756:ILE:HG12	14	0.15
(2,1364)	1:A:760:LEU:HD12	1:A:756:ILE:HG13	14	0.15
(2,1364)	1:A:760:LEU:HD13	1:A:756:ILE:HG12	14	0.15
(2,1364)	1:A:760:LEU:HD13	1:A:756:ILE:HG13	14	0.15
(2,135)	1:B:756:ILE:H	1:A:796:TRP:HE1	1	0.15
(2,13)	1:B:666:TRP:HE1	1:A:666:TRP:HD1	1	0.15
(2,13)	1:B:666:TRP:HE1	1:A:666:TRP:HD1	2	0.15
(2,1288)	1:A:709:ARG:HE	1:A:709:ARG:H	13	0.15
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB2	5	0.15
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB3	5	0.15
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB2	5	0.15
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB3	5	0.15
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB2	5	0.15
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB3	5	0.15
(2,1264)	1:A:707:ARG:H	1:A:704:LEU:HA	6	0.15
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB2	11	0.15
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB3	11	0.15
(2,1235)	1:A:704:LEU:H	1:A:701:VAL:HA	14	0.15
(2,123)	1:A:785:LEU:HD21	1:B:747:ARG:HD2	15	0.15
(2,123)	1:A:785:LEU:HD21	1:B:747:ARG:HD3	15	0.15
(2,123)	1:A:785:LEU:HD22	1:B:747:ARG:HD2	15	0.15
(2,123)	1:A:785:LEU:HD22	1:B:747:ARG:HD3	15	0.15
(2,123)	1:A:785:LEU:HD23	1:B:747:ARG:HD2	15	0.15
(2,123)	1:A:785:LEU:HD23	1:B:747:ARG:HD3	15	0.15
(2,1227)	1:A:702:LEU:HD11	1:A:699:PHE:HD1	9	0.15
(2,1227)	1:A:702:LEU:HD11	1:A:699:PHE:HD2	9	0.15
(2,1227)	1:A:702:LEU:HD12	1:A:699:PHE:HD1	9	0.15
(2,1227)	1:A:702:LEU:HD12	1:A:699:PHE:HD2	9	0.15
(2,1227)	1:A:702:LEU:HD13	1:A:699:PHE:HD1	9	0.15
(2,1227)	1:A:702:LEU:HD13	1:A:699:PHE:HD2	9	0.15
(2,1224)	1:A:702:LEU:H	1:A:699:PHE:HA	14	0.15
(2,1218)	1:A:700:ALA:HB1	1:A:703:SER:HB2	11	0.15
(2,1218)	1:A:700:ALA:HB1	1:A:703:SER:HB3	11	0.15
(2,1218)	1:A:700:ALA:HB2	1:A:703:SER:HB2	11	0.15
(2,1218)	1:A:700:ALA:HB2	1:A:703:SER:HB3	11	0.15
(2,1218)	1:A:700:ALA:HB3	1:A:703:SER:HB2	11	0.15
(2,1218)	1:A:700:ALA:HB3	1:A:703:SER:HB3	11	0.15
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB1	3	0.15
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB2	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB3	3	0.15
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB1	3	0.15
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB2	3	0.15
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB3	3	0.15
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB1	3	0.15
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB2	3	0.15
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB3	3	0.15
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB1	14	0.15
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB2	14	0.15
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB3	14	0.15
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB1	14	0.15
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB2	14	0.15
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB3	14	0.15
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB1	14	0.15
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB2	14	0.15
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB3	14	0.15
(2,1198)	1:A:695:LEU:HD21	1:A:696:ARG:HH11	10	0.15
(2,1198)	1:A:695:LEU:HD21	1:A:696:ARG:HH12	10	0.15
(2,1198)	1:A:695:LEU:HD22	1:A:696:ARG:HH11	10	0.15
(2,1198)	1:A:695:LEU:HD22	1:A:696:ARG:HH12	10	0.15
(2,1198)	1:A:695:LEU:HD23	1:A:696:ARG:HH11	10	0.15
(2,1198)	1:A:695:LEU:HD23	1:A:696:ARG:HH12	10	0.15
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	6	0.15
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	6	0.15
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	6	0.15
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	6	0.15
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	6	0.15
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	6	0.15
(2,1138)	1:A:679:LEU:HD11	1:A:678:TRP:HH2	6	0.15
(2,1138)	1:A:679:LEU:HD12	1:A:678:TRP:HH2	6	0.15
(2,1138)	1:A:679:LEU:HD13	1:A:678:TRP:HH2	6	0.15
(2,1138)	1:A:679:LEU:HD21	1:A:678:TRP:HH2	6	0.15
(2,1138)	1:A:679:LEU:HD22	1:A:678:TRP:HH2	6	0.15
(2,1138)	1:A:679:LEU:HD23	1:A:678:TRP:HH2	6	0.15
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD11	6	0.15
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD12	6	0.15
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD13	6	0.15
(2,1126)	1:A:676:THR:HG21	1:A:666:TRP:HZ3	10	0.15
(2,1126)	1:A:676:THR:HG22	1:A:666:TRP:HZ3	10	0.15
(2,1126)	1:A:676:THR:HG23	1:A:666:TRP:HZ3	10	0.15
(2,1109)	1:A:670:TRP:H	1:A:667:ALA:HA	11	0.15
(2,1108)	1:A:669:LEU:HD11	1:A:672:TRP:HZ3	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1108)	1:A:669:LEU:HD12	1:A:672:TRP:HZ3	6	0.15
(2,1108)	1:A:669:LEU:HD13	1:A:672:TRP:HZ3	6	0.15
(2,1108)	1:A:669:LEU:HD21	1:A:672:TRP:HZ3	6	0.15
(2,1108)	1:A:669:LEU:HD22	1:A:672:TRP:HZ3	6	0.15
(2,1108)	1:A:669:LEU:HD23	1:A:672:TRP:HZ3	6	0.15
(2,1095)	1:A:667:ALA:H	1:A:666:TRP:HD1	4	0.15
(2,1084)	1:A:666:TRP:H	1:A:663:LEU:HA	9	0.15
(2,1079)	1:A:665:LYS:H	1:A:664:ASP:HA	11	0.15
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE21	6	0.15
(2,1055)	1:A:835:GLY:H	1:A:834:GLN:HE22	6	0.15
(2,1050)	1:A:806:GLU:H	1:A:803:TRP:HB2	5	0.15
(2,1050)	1:A:806:GLU:H	1:A:803:TRP:HB3	5	0.15
(2,1050)	1:A:806:GLU:H	1:A:803:TRP:HB2	7	0.15
(2,1050)	1:A:806:GLU:H	1:A:803:TRP:HB3	7	0.15
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD2	6	0.15
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD3	6	0.15
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD2	9	0.15
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD3	9	0.15
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD21	4	0.15
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD22	4	0.15
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD23	4	0.15
(2,1033)	1:A:786:GLY:H	1:A:782:VAL:HA	8	0.15
(2,1032)	1:A:785:LEU:HD21	1:A:782:VAL:HA	12	0.15
(2,1032)	1:A:785:LEU:HD22	1:A:782:VAL:HA	12	0.15
(2,1032)	1:A:785:LEU:HD23	1:A:782:VAL:HA	12	0.15
(2,1000)	1:A:781:ILE:H	1:A:778:VAL:HA	6	0.15
(2,1000)	1:A:781:ILE:H	1:A:778:VAL:HA	10	0.15
(1,95)	1:B:794:LYS:O	1:B:798:ASN:H	1	0.15
(1,95)	1:B:794:LYS:O	1:B:798:ASN:H	11	0.15
(1,91)	1:B:792:ALA:O	1:B:796:TRP:H	5	0.15
(1,90)	1:B:791:GLU:O	1:B:795:TYR:N	1	0.15
(1,9)	1:B:794:LYS:O	1:B:798:ASN:H	1	0.15
(1,9)	1:B:794:LYS:O	1:B:798:ASN:H	11	0.15
(1,75)	1:B:837:SER:O	1:B:841:ARG:H	13	0.15
(1,73)	1:B:836:ALA:O	1:B:840:ILE:H	5	0.15
(1,71)	1:B:835:GLY:O	1:B:839:ALA:H	4	0.15
(1,61)	1:B:830:ILE:O	1:B:834:GLN:H	8	0.15
(1,53)	1:B:826:THR:O	1:B:830:ILE:H	1	0.15
(1,5)	1:B:792:ALA:O	1:B:796:TRP:H	5	0.15
(1,47)	1:B:813:SER:O	1:B:817:ALA:H	11	0.15
(1,4)	1:B:791:GLU:O	1:B:795:TYR:N	1	0.15
(1,27)	1:B:803:TRP:O	1:B:807:LEU:H	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,247)	1:B:837:SER:O	1:B:841:ARG:H	13	0.15
(1,245)	1:B:836:ALA:O	1:B:840:ILE:H	5	0.15
(1,243)	1:B:835:GLY:O	1:B:839:ALA:H	4	0.15
(1,233)	1:B:830:ILE:O	1:B:834:GLN:H	8	0.15
(1,225)	1:B:826:THR:O	1:B:830:ILE:H	1	0.15
(1,219)	1:B:813:SER:O	1:B:817:ALA:H	11	0.15
(1,20)	1:B:799:LEU:O	1:B:803:TRP:N	1	0.15
(1,199)	1:B:803:TRP:O	1:B:807:LEU:H	15	0.15
(1,192)	1:B:799:LEU:O	1:B:803:TRP:N	1	0.15
(1,181)	1:B:794:LYS:O	1:B:798:ASN:H	1	0.15
(1,181)	1:B:794:LYS:O	1:B:798:ASN:H	11	0.15
(1,177)	1:B:792:ALA:O	1:B:796:TRP:H	5	0.15
(1,176)	1:B:791:GLU:O	1:B:795:TYR:N	1	0.15
(1,161)	1:B:837:SER:O	1:B:841:ARG:H	13	0.15
(1,159)	1:B:836:ALA:O	1:B:840:ILE:H	5	0.15
(1,157)	1:B:835:GLY:O	1:B:839:ALA:H	4	0.15
(1,147)	1:B:830:ILE:O	1:B:834:GLN:H	8	0.15
(1,139)	1:B:826:THR:O	1:B:830:ILE:H	1	0.15
(1,133)	1:B:813:SER:O	1:B:817:ALA:H	11	0.15
(1,113)	1:B:803:TRP:O	1:B:807:LEU:H	15	0.15
(1,106)	1:B:799:LEU:O	1:B:803:TRP:N	1	0.15
(2,989)	1:A:778:VAL:HG21	1:A:775:LEU:HA	1	0.14
(2,989)	1:A:778:VAL:HG22	1:A:775:LEU:HA	1	0.14
(2,989)	1:A:778:VAL:HG23	1:A:775:LEU:HA	1	0.14
(2,970)	1:A:775:LEU:HD11	1:A:772:ARG:HA	8	0.14
(2,970)	1:A:775:LEU:HD12	1:A:772:ARG:HA	8	0.14
(2,970)	1:A:775:LEU:HD13	1:A:772:ARG:HA	8	0.14
(2,970)	1:A:775:LEU:HD11	1:A:772:ARG:HA	15	0.14
(2,970)	1:A:775:LEU:HD12	1:A:772:ARG:HA	15	0.14
(2,970)	1:A:775:LEU:HD13	1:A:772:ARG:HA	15	0.14
(2,96)	1:A:755:LEU:HD11	1:B:710:GLN:HE21	3	0.14
(2,96)	1:A:755:LEU:HD11	1:B:710:GLN:HE22	3	0.14
(2,96)	1:A:755:LEU:HD12	1:B:710:GLN:HE21	3	0.14
(2,96)	1:A:755:LEU:HD12	1:B:710:GLN:HE22	3	0.14
(2,96)	1:A:755:LEU:HD13	1:B:710:GLN:HE21	3	0.14
(2,96)	1:A:755:LEU:HD13	1:B:710:GLN:HE22	3	0.14
(2,948)	1:A:764:SER:H	1:A:771:LEU:HB2	3	0.14
(2,948)	1:A:764:SER:H	1:A:771:LEU:HB3	3	0.14
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB1	6	0.14
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB2	6	0.14
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB3	6	0.14
(2,93)	1:A:754:ALA:H	1:B:716:SER:HB2	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,93)	1:A:754:ALA:H	1:B:716:SER:HB3	14	0.14
(2,927)	1:A:755:LEU:H	1:A:752:SER:HA	5	0.14
(2,925)	1:A:754:ALA:HB1	1:A:758:ASP:H	6	0.14
(2,925)	1:A:754:ALA:HB2	1:A:758:ASP:H	6	0.14
(2,925)	1:A:754:ALA:HB3	1:A:758:ASP:H	6	0.14
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	3	0.14
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	3	0.14
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	3	0.14
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	3	0.14
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	3	0.14
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	3	0.14
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB2	13	0.14
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB3	13	0.14
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB2	15	0.14
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB3	15	0.14
(2,898)	1:A:746:ILE:HG21	1:A:750:ASN:HD22	6	0.14
(2,898)	1:A:746:ILE:HG22	1:A:750:ASN:HD22	6	0.14
(2,898)	1:A:746:ILE:HG23	1:A:750:ASN:HD22	6	0.14
(2,896)	1:A:746:ILE:HD11	1:A:743:ASP:HB2	4	0.14
(2,896)	1:A:746:ILE:HD11	1:A:743:ASP:HB3	4	0.14
(2,896)	1:A:746:ILE:HD12	1:A:743:ASP:HB2	4	0.14
(2,896)	1:A:746:ILE:HD12	1:A:743:ASP:HB3	4	0.14
(2,896)	1:A:746:ILE:HD13	1:A:743:ASP:HB2	4	0.14
(2,896)	1:A:746:ILE:HD13	1:A:743:ASP:HB3	4	0.14
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD11	14	0.14
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD12	14	0.14
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD13	14	0.14
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD21	14	0.14
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD22	14	0.14
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD23	14	0.14
(2,839)	1:A:707:ARG:H	1:A:704:LEU:HA	3	0.14
(2,839)	1:A:707:ARG:H	1:A:704:LEU:HA	15	0.14
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	12	0.14
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	12	0.14
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	12	0.14
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	12	0.14
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	12	0.14
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	12	0.14
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	13	0.14
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	13	0.14
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	13	0.14
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	13	0.14
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	13	0.14
(2,820)	1:A:704:LEU:HD11	1:A:708:VAL:HG21	3	0.14
(2,820)	1:A:704:LEU:HD11	1:A:708:VAL:HG22	3	0.14
(2,820)	1:A:704:LEU:HD11	1:A:708:VAL:HG23	3	0.14
(2,820)	1:A:704:LEU:HD12	1:A:708:VAL:HG21	3	0.14
(2,820)	1:A:704:LEU:HD12	1:A:708:VAL:HG22	3	0.14
(2,820)	1:A:704:LEU:HD12	1:A:708:VAL:HG23	3	0.14
(2,820)	1:A:704:LEU:HD13	1:A:708:VAL:HG21	3	0.14
(2,820)	1:A:704:LEU:HD13	1:A:708:VAL:HG22	3	0.14
(2,820)	1:A:704:LEU:HD13	1:A:708:VAL:HG23	3	0.14
(2,804)	1:A:702:LEU:HD21	1:A:706:ASN:HB2	4	0.14
(2,804)	1:A:702:LEU:HD21	1:A:706:ASN:HB3	4	0.14
(2,804)	1:A:702:LEU:HD22	1:A:706:ASN:HB2	4	0.14
(2,804)	1:A:702:LEU:HD22	1:A:706:ASN:HB3	4	0.14
(2,804)	1:A:702:LEU:HD23	1:A:706:ASN:HB2	4	0.14
(2,804)	1:A:702:LEU:HD23	1:A:706:ASN:HB3	4	0.14
(2,804)	1:A:702:LEU:HD21	1:A:706:ASN:HB2	8	0.14
(2,804)	1:A:702:LEU:HD21	1:A:706:ASN:HB3	8	0.14
(2,804)	1:A:702:LEU:HD22	1:A:706:ASN:HB2	8	0.14
(2,804)	1:A:702:LEU:HD22	1:A:706:ASN:HB3	8	0.14
(2,804)	1:A:702:LEU:HD23	1:A:706:ASN:HB2	8	0.14
(2,804)	1:A:702:LEU:HD23	1:A:706:ASN:HB3	8	0.14
(2,803)	1:A:702:LEU:HD11	1:A:699:PHE:HE1	7	0.14
(2,803)	1:A:702:LEU:HD11	1:A:699:PHE:HE2	7	0.14
(2,803)	1:A:702:LEU:HD12	1:A:699:PHE:HE1	7	0.14
(2,803)	1:A:702:LEU:HD12	1:A:699:PHE:HE2	7	0.14
(2,803)	1:A:702:LEU:HD13	1:A:699:PHE:HE1	7	0.14
(2,803)	1:A:702:LEU:HD13	1:A:699:PHE:HE2	7	0.14
(2,803)	1:A:702:LEU:HD11	1:A:699:PHE:HE1	9	0.14
(2,803)	1:A:702:LEU:HD11	1:A:699:PHE:HE2	9	0.14
(2,803)	1:A:702:LEU:HD12	1:A:699:PHE:HE1	9	0.14
(2,803)	1:A:702:LEU:HD12	1:A:699:PHE:HE2	9	0.14
(2,803)	1:A:702:LEU:HD13	1:A:699:PHE:HE1	9	0.14
(2,803)	1:A:702:LEU:HD13	1:A:699:PHE:HE2	9	0.14
(2,799)	1:A:702:LEU:H	1:A:699:PHE:HA	7	0.14
(2,794)	1:A:701:VAL:H	1:A:698:VAL:HA	9	0.14
(2,794)	1:A:701:VAL:H	1:A:698:VAL:HA	13	0.14
(2,792)	1:A:700:ALA:HB1	1:A:697:ILE:HA	15	0.14
(2,792)	1:A:700:ALA:HB2	1:A:697:ILE:HA	15	0.14
(2,792)	1:A:700:ALA:HB3	1:A:697:ILE:HA	15	0.14
(2,781)	1:A:698:VAL:HG11	1:A:695:LEU:HG	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,781)	1:A:698:VAL:HG12	1:A:695:LEU:HG	1	0.14
(2,781)	1:A:698:VAL:HG13	1:A:695:LEU:HG	1	0.14
(2,770)	1:A:695:LEU:HD21	1:A:698:VAL:HB	13	0.14
(2,770)	1:A:695:LEU:HD22	1:A:698:VAL:HB	13	0.14
(2,770)	1:A:695:LEU:HD23	1:A:698:VAL:HB	13	0.14
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	4	0.14
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	4	0.14
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	4	0.14
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	4	0.14
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	4	0.14
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	4	0.14
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	11	0.14
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	11	0.14
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	11	0.14
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	11	0.14
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	11	0.14
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	11	0.14
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	12	0.14
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	12	0.14
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	12	0.14
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	12	0.14
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	12	0.14
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	12	0.14
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	15	0.14
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	15	0.14
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	15	0.14
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	15	0.14
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	15	0.14
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	15	0.14
(2,768)	1:A:695:LEU:HD11	1:A:691:SER:HB2	8	0.14
(2,768)	1:A:695:LEU:HD11	1:A:691:SER:HB3	8	0.14
(2,768)	1:A:695:LEU:HD12	1:A:691:SER:HB2	8	0.14
(2,768)	1:A:695:LEU:HD12	1:A:691:SER:HB3	8	0.14
(2,768)	1:A:695:LEU:HD13	1:A:691:SER:HB2	8	0.14
(2,768)	1:A:695:LEU:HD13	1:A:691:SER:HB3	8	0.14
(2,718)	1:A:682:ILE:HG21	1:A:679:LEU:H	12	0.14
(2,718)	1:A:682:ILE:HG22	1:A:679:LEU:H	12	0.14
(2,718)	1:A:682:ILE:HG23	1:A:679:LEU:H	12	0.14
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD11	8	0.14
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD12	8	0.14
(2,709)	1:A:678:TRP:HE1	1:A:675:ILE:HD13	8	0.14
(2,705)	1:A:676:THR:HG21	1:A:681:TYR:HH	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,705)	1:A:676:THR:HG22	1:A:681:TYR:HH	4	0.14
(2,705)	1:A:676:THR:HG23	1:A:681:TYR:HH	4	0.14
(2,684)	1:A:670:TRP:H	1:A:667:ALA:HA	6	0.14
(2,683)	1:A:669:LEU:HD11	1:A:672:TRP:HZ3	5	0.14
(2,683)	1:A:669:LEU:HD12	1:A:672:TRP:HZ3	5	0.14
(2,683)	1:A:669:LEU:HD13	1:A:672:TRP:HZ3	5	0.14
(2,683)	1:A:669:LEU:HD21	1:A:672:TRP:HZ3	5	0.14
(2,683)	1:A:669:LEU:HD22	1:A:672:TRP:HZ3	5	0.14
(2,683)	1:A:669:LEU:HD23	1:A:672:TRP:HZ3	5	0.14
(2,683)	1:A:669:LEU:HD11	1:A:672:TRP:HZ3	7	0.14
(2,683)	1:A:669:LEU:HD12	1:A:672:TRP:HZ3	7	0.14
(2,683)	1:A:669:LEU:HD13	1:A:672:TRP:HZ3	7	0.14
(2,683)	1:A:669:LEU:HD21	1:A:672:TRP:HZ3	7	0.14
(2,683)	1:A:669:LEU:HD22	1:A:672:TRP:HZ3	7	0.14
(2,683)	1:A:669:LEU:HD23	1:A:672:TRP:HZ3	7	0.14
(2,670)	1:A:667:ALA:H	1:A:666:TRP:HD1	13	0.14
(2,667)	1:A:667:ALA:H	1:A:664:ASP:HA	12	0.14
(2,666)	1:A:666:TRP:HE1	1:A:662:GLU:H	14	0.14
(2,666)	1:A:666:TRP:HE1	1:A:662:GLU:H	15	0.14
(2,654)	1:A:665:LYS:H	1:A:664:ASP:HA	3	0.14
(2,654)	1:A:665:LYS:H	1:A:664:ASP:HA	13	0.14
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB2	1	0.14
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB3	1	0.14
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB2	1	0.14
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB3	1	0.14
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB2	1	0.14
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB3	1	0.14
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD11	15	0.14
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD12	15	0.14
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD13	15	0.14
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD21	15	0.14
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD22	15	0.14
(2,619)	1:B:797:TRP:HE1	1:B:793:LEU:HD23	15	0.14
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD21	7	0.14
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD22	7	0.14
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD23	7	0.14
(2,615)	1:B:796:TRP:HE1	1:B:796:TRP:H	15	0.14
(2,599)	1:B:784:LEU:HD11	1:B:787:ARG:HD2	14	0.14
(2,599)	1:B:784:LEU:HD11	1:B:787:ARG:HD3	14	0.14
(2,599)	1:B:784:LEU:HD12	1:B:787:ARG:HD2	14	0.14
(2,599)	1:B:784:LEU:HD12	1:B:787:ARG:HD3	14	0.14
(2,599)	1:B:784:LEU:HD13	1:B:787:ARG:HD2	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,599)	1:B:784:LEU:HD13	1:B:787:ARG:HD3	14	0.14
(2,580)	1:B:781:ILE:HG21	1:B:778:VAL:HA	3	0.14
(2,580)	1:B:781:ILE:HG22	1:B:778:VAL:HA	3	0.14
(2,580)	1:B:781:ILE:HG23	1:B:778:VAL:HA	3	0.14
(2,576)	1:B:781:ILE:H	1:B:780:ARG:HA	5	0.14
(2,575)	1:B:781:ILE:H	1:B:778:VAL:HA	3	0.14
(2,519)	1:B:763:LEU:HD11	1:B:764:SER:HG	3	0.14
(2,519)	1:B:763:LEU:HD12	1:B:764:SER:HG	3	0.14
(2,519)	1:B:763:LEU:HD13	1:B:764:SER:HG	3	0.14
(2,519)	1:B:763:LEU:HD11	1:B:764:SER:HG	15	0.14
(2,519)	1:B:763:LEU:HD12	1:B:764:SER:HG	15	0.14
(2,519)	1:B:763:LEU:HD13	1:B:764:SER:HG	15	0.14
(2,515)	1:B:760:LEU:HD11	1:B:757:TRP:HA	5	0.14
(2,515)	1:B:760:LEU:HD12	1:B:757:TRP:HA	5	0.14
(2,515)	1:B:760:LEU:HD13	1:B:757:TRP:HA	5	0.14
(2,515)	1:B:760:LEU:HD11	1:B:757:TRP:HA	15	0.14
(2,515)	1:B:760:LEU:HD12	1:B:757:TRP:HA	15	0.14
(2,515)	1:B:760:LEU:HD13	1:B:757:TRP:HA	15	0.14
(2,509)	1:B:758:ASP:H	1:B:754:ALA:HB1	8	0.14
(2,509)	1:B:758:ASP:H	1:B:754:ALA:HB2	8	0.14
(2,509)	1:B:758:ASP:H	1:B:754:ALA:HB3	8	0.14
(2,502)	1:B:755:LEU:H	1:B:752:SER:HA	12	0.14
(2,500)	1:B:754:ALA:HB1	1:B:758:ASP:H	8	0.14
(2,500)	1:B:754:ALA:HB2	1:B:758:ASP:H	8	0.14
(2,500)	1:B:754:ALA:HB3	1:B:758:ASP:H	8	0.14
(2,5)	1:A:663:LEU:H	1:A:661:LEU:HB2	9	0.14
(2,5)	1:A:663:LEU:H	1:A:661:LEU:HB3	9	0.14
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA2	1	0.14
(2,498)	1:B:754:ALA:HB1	1:B:751:GLY:HA3	1	0.14
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA2	1	0.14
(2,498)	1:B:754:ALA:HB2	1:B:751:GLY:HA3	1	0.14
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA2	1	0.14
(2,498)	1:B:754:ALA:HB3	1:B:751:GLY:HA3	1	0.14
(2,482)	1:B:749:VAL:H	1:B:746:ILE:HA	1	0.14
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD2	5	0.14
(2,478)	1:B:748:LEU:H	1:B:744:ARG:HD3	5	0.14
(2,471)	1:B:746:ILE:HD11	1:B:743:ASP:HB2	4	0.14
(2,471)	1:B:746:ILE:HD11	1:B:743:ASP:HB3	4	0.14
(2,471)	1:B:746:ILE:HD12	1:B:743:ASP:HB2	4	0.14
(2,471)	1:B:746:ILE:HD12	1:B:743:ASP:HB3	4	0.14
(2,471)	1:B:746:ILE:HD13	1:B:743:ASP:HB2	4	0.14
(2,471)	1:B:746:ILE:HD13	1:B:743:ASP:HB3	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,471)	1:B:746:ILE:HD11	1:B:743:ASP:HB2	9	0.14
(2,471)	1:B:746:ILE:HD11	1:B:743:ASP:HB3	9	0.14
(2,471)	1:B:746:ILE:HD12	1:B:743:ASP:HB2	9	0.14
(2,471)	1:B:746:ILE:HD12	1:B:743:ASP:HB3	9	0.14
(2,471)	1:B:746:ILE:HD13	1:B:743:ASP:HB2	9	0.14
(2,471)	1:B:746:ILE:HD13	1:B:743:ASP:HB3	9	0.14
(2,446)	1:B:710:GLN:HE21	1:B:706:ASN:HB2	8	0.14
(2,446)	1:B:710:GLN:HE21	1:B:706:ASN:HB3	8	0.14
(2,446)	1:B:710:GLN:HE22	1:B:706:ASN:HB2	8	0.14
(2,446)	1:B:710:GLN:HE22	1:B:706:ASN:HB3	8	0.14
(2,43)	1:B:693:ILE:H	1:A:693:ILE:HD11	13	0.14
(2,43)	1:B:693:ILE:H	1:A:693:ILE:HD12	13	0.14
(2,43)	1:B:693:ILE:H	1:A:693:ILE:HD13	13	0.14
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD11	7	0.14
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD12	7	0.14
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD13	7	0.14
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD21	7	0.14
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD22	7	0.14
(2,422)	1:B:707:ARG:HE	1:B:704:LEU:HD23	7	0.14
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG12	6	0.14
(2,42)	1:A:693:ILE:H	1:B:693:ILE:HG13	6	0.14
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB2	11	0.14
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB3	11	0.14
(2,407)	1:B:706:ASN:H	1:B:703:SER:HA	12	0.14
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB2	5	0.14
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB3	5	0.14
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB2	5	0.14
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB3	5	0.14
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB2	5	0.14
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB3	5	0.14
(2,405)	1:B:705:VAL:HG21	1:B:702:LEU:HG	5	0.14
(2,405)	1:B:705:VAL:HG22	1:B:702:LEU:HG	5	0.14
(2,405)	1:B:705:VAL:HG23	1:B:702:LEU:HG	5	0.14
(2,403)	1:B:705:VAL:HG11	1:B:709:ARG:HD2	9	0.14
(2,403)	1:B:705:VAL:HG11	1:B:709:ARG:HD3	9	0.14
(2,403)	1:B:705:VAL:HG12	1:B:709:ARG:HD2	9	0.14
(2,403)	1:B:705:VAL:HG12	1:B:709:ARG:HD3	9	0.14
(2,403)	1:B:705:VAL:HG13	1:B:709:ARG:HD2	9	0.14
(2,403)	1:B:705:VAL:HG13	1:B:709:ARG:HD3	9	0.14
(2,395)	1:B:704:LEU:HD11	1:B:708:VAL:HG21	7	0.14
(2,395)	1:B:704:LEU:HD11	1:B:708:VAL:HG22	7	0.14
(2,395)	1:B:704:LEU:HD11	1:B:708:VAL:HG23	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,395)	1:B:704:LEU:HD12	1:B:708:VAL:HG21	7	0.14
(2,395)	1:B:704:LEU:HD12	1:B:708:VAL:HG22	7	0.14
(2,395)	1:B:704:LEU:HD12	1:B:708:VAL:HG23	7	0.14
(2,395)	1:B:704:LEU:HD13	1:B:708:VAL:HG21	7	0.14
(2,395)	1:B:704:LEU:HD13	1:B:708:VAL:HG22	7	0.14
(2,395)	1:B:704:LEU:HD13	1:B:708:VAL:HG23	7	0.14
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB2	1	0.14
(2,379)	1:B:702:LEU:HD21	1:B:706:ASN:HB3	1	0.14
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB2	1	0.14
(2,379)	1:B:702:LEU:HD22	1:B:706:ASN:HB3	1	0.14
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB2	1	0.14
(2,379)	1:B:702:LEU:HD23	1:B:706:ASN:HB3	1	0.14
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD1	7	0.14
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD2	7	0.14
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD1	7	0.14
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD2	7	0.14
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD1	7	0.14
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD2	7	0.14
(2,374)	1:B:702:LEU:H	1:B:699:PHE:HA	7	0.14
(2,37)	1:B:692:LEU:HD21	1:A:694:GLY:H	6	0.14
(2,37)	1:B:692:LEU:HD22	1:A:694:GLY:H	6	0.14
(2,37)	1:B:692:LEU:HD23	1:A:694:GLY:H	6	0.14
(2,37)	1:B:692:LEU:HD21	1:A:694:GLY:H	13	0.14
(2,37)	1:B:692:LEU:HD22	1:A:694:GLY:H	13	0.14
(2,37)	1:B:692:LEU:HD23	1:A:694:GLY:H	13	0.14
(2,356)	1:B:698:VAL:HG11	1:B:695:LEU:HG	10	0.14
(2,356)	1:B:698:VAL:HG12	1:B:695:LEU:HG	10	0.14
(2,356)	1:B:698:VAL:HG13	1:B:695:LEU:HG	10	0.14
(2,345)	1:B:695:LEU:HD21	1:B:698:VAL:HB	15	0.14
(2,345)	1:B:695:LEU:HD22	1:B:698:VAL:HB	15	0.14
(2,345)	1:B:695:LEU:HD23	1:B:698:VAL:HB	15	0.14
(2,335)	1:B:693:ILE:HD11	1:B:694:GLY:HA2	3	0.14
(2,335)	1:B:693:ILE:HD11	1:B:694:GLY:HA3	3	0.14
(2,335)	1:B:693:ILE:HD12	1:B:694:GLY:HA2	3	0.14
(2,335)	1:B:693:ILE:HD12	1:B:694:GLY:HA3	3	0.14
(2,335)	1:B:693:ILE:HD13	1:B:694:GLY:HA2	3	0.14
(2,335)	1:B:693:ILE:HD13	1:B:694:GLY:HA3	3	0.14
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG21	10	0.14
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG22	10	0.14
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG23	10	0.14
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG21	10	0.14
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG22	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG23	10	0.14
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG21	10	0.14
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG22	10	0.14
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG23	10	0.14
(2,307)	1:B:684:ILE:HG21	1:B:688:ILE:H	1	0.14
(2,307)	1:B:684:ILE:HG22	1:B:688:ILE:H	1	0.14
(2,307)	1:B:684:ILE:HG23	1:B:688:ILE:H	1	0.14
(2,305)	1:B:684:ILE:HG21	1:B:685:PHE:HD1	13	0.14
(2,305)	1:B:684:ILE:HG21	1:B:685:PHE:HD2	13	0.14
(2,305)	1:B:684:ILE:HG22	1:B:685:PHE:HD1	13	0.14
(2,305)	1:B:684:ILE:HG22	1:B:685:PHE:HD2	13	0.14
(2,305)	1:B:684:ILE:HG23	1:B:685:PHE:HD1	13	0.14
(2,305)	1:B:684:ILE:HG23	1:B:685:PHE:HD2	13	0.14
(2,301)	1:B:684:ILE:HD11	1:B:681:TYR:HA	4	0.14
(2,301)	1:B:684:ILE:HD12	1:B:681:TYR:HA	4	0.14
(2,301)	1:B:684:ILE:HD13	1:B:681:TYR:HA	4	0.14
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB2	15	0.14
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB3	15	0.14
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB2	15	0.14
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB3	15	0.14
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB2	15	0.14
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB3	15	0.14
(2,292)	1:B:681:TYR:H	1:B:682:ILE:H	11	0.14
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD11	9	0.14
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD12	9	0.14
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD13	9	0.14
(2,286)	1:B:678:TRP:HE1	1:B:682:ILE:H	2	0.14
(2,280)	1:B:676:THR:HG21	1:B:681:TYR:HH	1	0.14
(2,280)	1:B:676:THR:HG22	1:B:681:TYR:HH	1	0.14
(2,280)	1:B:676:THR:HG23	1:B:681:TYR:HH	1	0.14
(2,272)	1:B:674:ASP:H	1:B:677:ASN:H	10	0.14
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD11	7	0.14
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD12	7	0.14
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD13	7	0.14
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD21	7	0.14
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD22	7	0.14
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD23	7	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD11	4	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD12	4	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD13	4	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD21	4	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD22	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD23	4	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD11	13	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD12	13	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD13	13	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD21	13	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD22	13	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD23	13	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD11	14	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD12	14	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD13	14	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD21	14	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD22	14	0.14
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD23	14	0.14
(2,259)	1:B:670:TRP:H	1:B:667:ALA:HA	9	0.14
(2,259)	1:B:670:TRP:H	1:B:667:ALA:HA	10	0.14
(2,253)	1:B:669:LEU:H	1:B:666:TRP:HA	11	0.14
(2,245)	1:B:667:ALA:H	1:B:666:TRP:HD1	1	0.14
(2,242)	1:B:667:ALA:H	1:B:664:ASP:HA	3	0.14
(2,225)	1:B:664:ASP:H	1:B:663:LEU:H	10	0.14
(2,219)	1:B:663:LEU:H	1:B:664:ASP:H	10	0.14
(2,214)	1:B:661:LEU:HD11	1:B:662:GLU:HG2	7	0.14
(2,214)	1:B:661:LEU:HD11	1:B:662:GLU:HG3	7	0.14
(2,214)	1:B:661:LEU:HD12	1:B:662:GLU:HG2	7	0.14
(2,214)	1:B:661:LEU:HD12	1:B:662:GLU:HG3	7	0.14
(2,214)	1:B:661:LEU:HD13	1:B:662:GLU:HG2	7	0.14
(2,214)	1:B:661:LEU:HD13	1:B:662:GLU:HG3	7	0.14
(2,214)	1:B:661:LEU:HD21	1:B:662:GLU:HG2	7	0.14
(2,214)	1:B:661:LEU:HD21	1:B:662:GLU:HG3	7	0.14
(2,214)	1:B:661:LEU:HD22	1:B:662:GLU:HG2	7	0.14
(2,214)	1:B:661:LEU:HD22	1:B:662:GLU:HG3	7	0.14
(2,214)	1:B:661:LEU:HD23	1:B:662:GLU:HG2	7	0.14
(2,214)	1:B:661:LEU:HD23	1:B:662:GLU:HG3	7	0.14
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ1	4	0.14
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ2	4	0.14
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ3	4	0.14
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD2	1	0.14
(2,208)	1:B:839:ALA:H	1:B:808:LYS:HD3	1	0.14
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD11	3	0.14
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD12	3	0.14
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD13	3	0.14
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD11	3	0.14
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD12	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD13	3	0.14
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG2	10	0.14
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG3	10	0.14
(2,186)	1:A:808:LYS:H	1:A:838:ARG:HD2	8	0.14
(2,186)	1:A:808:LYS:H	1:A:838:ARG:HD3	8	0.14
(2,185)	1:A:808:LYS:H	1:A:838:ARG:HD2	8	0.14
(2,185)	1:A:808:LYS:H	1:A:838:ARG:HD3	8	0.14
(2,177)	1:A:803:TRP:HE1	1:B:764:SER:HG	10	0.14
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	1	0.14
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	1	0.14
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	1	0.14
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	1	0.14
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG12	9	0.14
(2,159)	1:A:794:LYS:H	1:A:847:ILE:HG13	9	0.14
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG12	9	0.14
(2,158)	1:A:794:LYS:H	1:A:847:ILE:HG13	9	0.14
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG12	1	0.14
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG13	1	0.14
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	4	0.14
(2,1487)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	4	0.14
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	4	0.14
(2,1487)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	4	0.14
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	4	0.14
(2,1487)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	4	0.14
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	4	0.14
(2,1487)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	4	0.14
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	13	0.14
(2,1485)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	13	0.14
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	13	0.14
(2,1485)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	13	0.14
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	13	0.14
(2,1485)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	13	0.14
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	13	0.14
(2,1485)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	13	0.14
(2,1475)	1:A:806:GLU:H	1:A:803:TRP:HB2	2	0.14
(2,1475)	1:A:806:GLU:H	1:A:803:TRP:HB3	2	0.14
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG12	6	0.14
(2,147)	1:A:782:VAL:H	1:B:746:ILE:HG13	6	0.14
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD11	2	0.14
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD12	2	0.14
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD13	2	0.14
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD11	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD12	3	0.14
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD13	3	0.14
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD11	13	0.14
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD12	13	0.14
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD13	13	0.14
(2,1457)	1:A:785:LEU:HD21	1:A:782:VAL:HA	7	0.14
(2,1457)	1:A:785:LEU:HD22	1:A:782:VAL:HA	7	0.14
(2,1457)	1:A:785:LEU:HD23	1:A:782:VAL:HA	7	0.14
(2,1451)	1:A:785:LEU:H	1:A:782:VAL:HA	1	0.14
(2,1444)	1:A:784:LEU:H	1:A:782:VAL:HA	7	0.14
(2,1443)	1:A:784:LEU:H	1:A:781:ILE:HA	3	0.14
(2,1443)	1:A:784:LEU:H	1:A:781:ILE:HA	10	0.14
(2,1431)	1:A:782:VAL:H	1:A:779:THR:HA	4	0.14
(2,1431)	1:A:782:VAL:H	1:A:779:THR:HA	10	0.14
(2,142)	1:A:781:ILE:H	1:B:746:ILE:HG12	9	0.14
(2,142)	1:A:781:ILE:H	1:B:746:ILE:HG13	9	0.14
(2,142)	1:A:781:ILE:H	1:B:746:ILE:HG12	13	0.14
(2,142)	1:A:781:ILE:H	1:B:746:ILE:HG13	13	0.14
(2,1414)	1:A:778:VAL:HG21	1:A:775:LEU:HA	1	0.14
(2,1414)	1:A:778:VAL:HG22	1:A:775:LEU:HA	1	0.14
(2,1414)	1:A:778:VAL:HG23	1:A:775:LEU:HA	1	0.14
(2,141)	1:B:771:LEU:H	1:A:806:GLU:HB2	15	0.14
(2,141)	1:B:771:LEU:H	1:A:806:GLU:HB3	15	0.14
(2,1395)	1:A:775:LEU:HD11	1:A:772:ARG:HA	8	0.14
(2,1395)	1:A:775:LEU:HD12	1:A:772:ARG:HA	8	0.14
(2,1395)	1:A:775:LEU:HD13	1:A:772:ARG:HA	8	0.14
(2,1395)	1:A:775:LEU:HD11	1:A:772:ARG:HA	15	0.14
(2,1395)	1:A:775:LEU:HD12	1:A:772:ARG:HA	15	0.14
(2,1395)	1:A:775:LEU:HD13	1:A:772:ARG:HA	15	0.14
(2,1373)	1:A:764:SER:H	1:A:771:LEU:HB2	3	0.14
(2,1373)	1:A:764:SER:H	1:A:771:LEU:HB3	3	0.14
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB1	6	0.14
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB2	6	0.14
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB3	6	0.14
(2,1352)	1:A:755:LEU:H	1:A:752:SER:HA	5	0.14
(2,1350)	1:A:754:ALA:HB1	1:A:758:ASP:H	6	0.14
(2,1350)	1:A:754:ALA:HB2	1:A:758:ASP:H	6	0.14
(2,1350)	1:A:754:ALA:HB3	1:A:758:ASP:H	6	0.14
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	3	0.14
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	3	0.14
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	3	0.14
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	3	0.14
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	3	0.14
(2,1323)	1:A:746:ILE:HG21	1:A:750:ASN:HD22	6	0.14
(2,1323)	1:A:746:ILE:HG22	1:A:750:ASN:HD22	6	0.14
(2,1323)	1:A:746:ILE:HG23	1:A:750:ASN:HD22	6	0.14
(2,1321)	1:A:746:ILE:HD11	1:A:743:ASP:HB2	4	0.14
(2,1321)	1:A:746:ILE:HD11	1:A:743:ASP:HB3	4	0.14
(2,1321)	1:A:746:ILE:HD12	1:A:743:ASP:HB2	4	0.14
(2,1321)	1:A:746:ILE:HD12	1:A:743:ASP:HB3	4	0.14
(2,1321)	1:A:746:ILE:HD13	1:A:743:ASP:HB2	4	0.14
(2,1321)	1:A:746:ILE:HD13	1:A:743:ASP:HB3	4	0.14
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD11	14	0.14
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD12	14	0.14
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD13	14	0.14
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD21	14	0.14
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD22	14	0.14
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD23	14	0.14
(2,1264)	1:A:707:ARG:H	1:A:704:LEU:HA	3	0.14
(2,1264)	1:A:707:ARG:H	1:A:704:LEU:HA	15	0.14
(2,126)	1:A:785:LEU:HD21	1:B:749:VAL:HB	15	0.14
(2,126)	1:A:785:LEU:HD22	1:B:749:VAL:HB	15	0.14
(2,126)	1:A:785:LEU:HD23	1:B:749:VAL:HB	15	0.14
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	12	0.14
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	12	0.14
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	12	0.14
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	12	0.14
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	12	0.14
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	12	0.14
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	13	0.14
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	13	0.14
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	13	0.14
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	13	0.14
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	13	0.14
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	13	0.14
(2,1245)	1:A:704:LEU:HD11	1:A:708:VAL:HG21	3	0.14
(2,1245)	1:A:704:LEU:HD11	1:A:708:VAL:HG22	3	0.14
(2,1245)	1:A:704:LEU:HD11	1:A:708:VAL:HG23	3	0.14
(2,1245)	1:A:704:LEU:HD12	1:A:708:VAL:HG21	3	0.14
(2,1245)	1:A:704:LEU:HD12	1:A:708:VAL:HG22	3	0.14
(2,1245)	1:A:704:LEU:HD12	1:A:708:VAL:HG23	3	0.14
(2,1245)	1:A:704:LEU:HD13	1:A:708:VAL:HG21	3	0.14
(2,1245)	1:A:704:LEU:HD13	1:A:708:VAL:HG22	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1245)	1:A:704:LEU:HD13	1:A:708:VAL:HG23	3	0.14
(2,1229)	1:A:702:LEU:HD21	1:A:706:ASN:HB2	4	0.14
(2,1229)	1:A:702:LEU:HD21	1:A:706:ASN:HB3	4	0.14
(2,1229)	1:A:702:LEU:HD22	1:A:706:ASN:HB2	4	0.14
(2,1229)	1:A:702:LEU:HD22	1:A:706:ASN:HB3	4	0.14
(2,1229)	1:A:702:LEU:HD23	1:A:706:ASN:HB2	4	0.14
(2,1229)	1:A:702:LEU:HD23	1:A:706:ASN:HB3	4	0.14
(2,1229)	1:A:702:LEU:HD21	1:A:706:ASN:HB2	8	0.14
(2,1229)	1:A:702:LEU:HD21	1:A:706:ASN:HB3	8	0.14
(2,1229)	1:A:702:LEU:HD22	1:A:706:ASN:HB2	8	0.14
(2,1229)	1:A:702:LEU:HD22	1:A:706:ASN:HB3	8	0.14
(2,1229)	1:A:702:LEU:HD23	1:A:706:ASN:HB2	8	0.14
(2,1229)	1:A:702:LEU:HD23	1:A:706:ASN:HB3	8	0.14
(2,1228)	1:A:702:LEU:HD11	1:A:699:PHE:HE1	7	0.14
(2,1228)	1:A:702:LEU:HD11	1:A:699:PHE:HE2	7	0.14
(2,1228)	1:A:702:LEU:HD12	1:A:699:PHE:HE1	7	0.14
(2,1228)	1:A:702:LEU:HD12	1:A:699:PHE:HE2	7	0.14
(2,1228)	1:A:702:LEU:HD13	1:A:699:PHE:HE1	7	0.14
(2,1228)	1:A:702:LEU:HD13	1:A:699:PHE:HE2	7	0.14
(2,1228)	1:A:702:LEU:HD11	1:A:699:PHE:HE1	9	0.14
(2,1228)	1:A:702:LEU:HD11	1:A:699:PHE:HE2	9	0.14
(2,1228)	1:A:702:LEU:HD12	1:A:699:PHE:HE1	9	0.14
(2,1228)	1:A:702:LEU:HD12	1:A:699:PHE:HE2	9	0.14
(2,1228)	1:A:702:LEU:HD13	1:A:699:PHE:HE1	9	0.14
(2,1228)	1:A:702:LEU:HD13	1:A:699:PHE:HE2	9	0.14
(2,1224)	1:A:702:LEU:H	1:A:699:PHE:HA	7	0.14
(2,1219)	1:A:701:VAL:H	1:A:698:VAL:HA	9	0.14
(2,1219)	1:A:701:VAL:H	1:A:698:VAL:HA	13	0.14
(2,1217)	1:A:700:ALA:HB1	1:A:697:ILE:HA	15	0.14
(2,1217)	1:A:700:ALA:HB2	1:A:697:ILE:HA	15	0.14
(2,1217)	1:A:700:ALA:HB3	1:A:697:ILE:HA	15	0.14
(2,1206)	1:A:698:VAL:HG11	1:A:695:LEU:HG	1	0.14
(2,1206)	1:A:698:VAL:HG12	1:A:695:LEU:HG	1	0.14
(2,1206)	1:A:698:VAL:HG13	1:A:695:LEU:HG	1	0.14
(2,1195)	1:A:695:LEU:HD21	1:A:698:VAL:HB	13	0.14
(2,1195)	1:A:695:LEU:HD22	1:A:698:VAL:HB	13	0.14
(2,1195)	1:A:695:LEU:HD23	1:A:698:VAL:HB	13	0.14
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	4	0.14
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	4	0.14
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	4	0.14
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	4	0.14
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	4	0.14
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	11	0.14
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	11	0.14
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	11	0.14
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	11	0.14
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	11	0.14
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	11	0.14
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	12	0.14
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	12	0.14
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	12	0.14
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	12	0.14
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	12	0.14
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	12	0.14
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	15	0.14
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	15	0.14
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	15	0.14
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	15	0.14
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	15	0.14
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	15	0.14
(2,1193)	1:A:695:LEU:HD11	1:A:691:SER:HB2	8	0.14
(2,1193)	1:A:695:LEU:HD11	1:A:691:SER:HB3	8	0.14
(2,1193)	1:A:695:LEU:HD12	1:A:691:SER:HB2	8	0.14
(2,1193)	1:A:695:LEU:HD12	1:A:691:SER:HB3	8	0.14
(2,1193)	1:A:695:LEU:HD13	1:A:691:SER:HB2	8	0.14
(2,1193)	1:A:695:LEU:HD13	1:A:691:SER:HB3	8	0.14
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB2	4	0.14
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB3	4	0.14
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB2	4	0.14
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB3	4	0.14
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB2	4	0.14
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB3	4	0.14
(2,1143)	1:A:682:ILE:HG21	1:A:679:LEU:H	12	0.14
(2,1143)	1:A:682:ILE:HG22	1:A:679:LEU:H	12	0.14
(2,1143)	1:A:682:ILE:HG23	1:A:679:LEU:H	12	0.14
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD11	8	0.14
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD12	8	0.14
(2,1134)	1:A:678:TRP:HE1	1:A:675:ILE:HD13	8	0.14
(2,1130)	1:A:676:THR:HG21	1:A:681:TYR:HH	4	0.14
(2,1130)	1:A:676:THR:HG22	1:A:681:TYR:HH	4	0.14
(2,1130)	1:A:676:THR:HG23	1:A:681:TYR:HH	4	0.14
(2,1109)	1:A:670:TRP:H	1:A:667:ALA:HA	6	0.14
(2,1108)	1:A:669:LEU:HD11	1:A:672:TRP:HZ3	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1108)	1:A:669:LEU:HD12	1:A:672:TRP:HZ3	5	0.14
(2,1108)	1:A:669:LEU:HD13	1:A:672:TRP:HZ3	5	0.14
(2,1108)	1:A:669:LEU:HD21	1:A:672:TRP:HZ3	5	0.14
(2,1108)	1:A:669:LEU:HD22	1:A:672:TRP:HZ3	5	0.14
(2,1108)	1:A:669:LEU:HD23	1:A:672:TRP:HZ3	5	0.14
(2,1108)	1:A:669:LEU:HD11	1:A:672:TRP:HZ3	7	0.14
(2,1108)	1:A:669:LEU:HD12	1:A:672:TRP:HZ3	7	0.14
(2,1108)	1:A:669:LEU:HD13	1:A:672:TRP:HZ3	7	0.14
(2,1108)	1:A:669:LEU:HD21	1:A:672:TRP:HZ3	7	0.14
(2,1108)	1:A:669:LEU:HD22	1:A:672:TRP:HZ3	7	0.14
(2,1108)	1:A:669:LEU:HD23	1:A:672:TRP:HZ3	7	0.14
(2,1095)	1:A:667:ALA:H	1:A:666:TRP:HD1	13	0.14
(2,1092)	1:A:667:ALA:H	1:A:664:ASP:HA	12	0.14
(2,1091)	1:A:666:TRP:HE1	1:A:662:GLU:H	14	0.14
(2,1091)	1:A:666:TRP:HE1	1:A:662:GLU:H	15	0.14
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD2	13	0.14
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD3	13	0.14
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD2	13	0.14
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD3	13	0.14
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD2	13	0.14
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD3	13	0.14
(2,1079)	1:A:665:LYS:H	1:A:664:ASP:HA	3	0.14
(2,1079)	1:A:665:LYS:H	1:A:664:ASP:HA	13	0.14
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD1	4	0.14
(2,1062)	1:A:770:ARG:HH11	1:A:773:ASP:OD2	4	0.14
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD1	4	0.14
(2,1062)	1:A:770:ARG:HH12	1:A:773:ASP:OD2	4	0.14
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD1	4	0.14
(2,1062)	1:A:770:ARG:HH21	1:A:773:ASP:OD2	4	0.14
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD1	4	0.14
(2,1062)	1:A:770:ARG:HH22	1:A:773:ASP:OD2	4	0.14
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD1	13	0.14
(2,1060)	1:A:744:ARG:HH11	1:A:741:ASP:OD2	13	0.14
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD1	13	0.14
(2,1060)	1:A:744:ARG:HH12	1:A:741:ASP:OD2	13	0.14
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD1	13	0.14
(2,1060)	1:A:744:ARG:HH21	1:A:741:ASP:OD2	13	0.14
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD1	13	0.14
(2,1060)	1:A:744:ARG:HH22	1:A:741:ASP:OD2	13	0.14
(2,1050)	1:A:806:GLU:H	1:A:803:TRP:HB2	2	0.14
(2,1050)	1:A:806:GLU:H	1:A:803:TRP:HB3	2	0.14
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD2	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,105)	1:A:763:LEU:H	1:B:742:ARG:HD3	1	0.14
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD11	2	0.14
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD12	2	0.14
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD13	2	0.14
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD11	3	0.14
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD12	3	0.14
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD13	3	0.14
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD11	13	0.14
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD12	13	0.14
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD13	13	0.14
(2,1032)	1:A:785:LEU:HD21	1:A:782:VAL:HA	7	0.14
(2,1032)	1:A:785:LEU:HD22	1:A:782:VAL:HA	7	0.14
(2,1032)	1:A:785:LEU:HD23	1:A:782:VAL:HA	7	0.14
(2,1026)	1:A:785:LEU:H	1:A:782:VAL:HA	1	0.14
(2,1019)	1:A:784:LEU:H	1:A:782:VAL:HA	7	0.14
(2,1018)	1:A:784:LEU:H	1:A:781:ILE:HA	3	0.14
(2,1018)	1:A:784:LEU:H	1:A:781:ILE:HA	10	0.14
(2,1006)	1:A:782:VAL:H	1:A:779:THR:HA	4	0.14
(2,1006)	1:A:782:VAL:H	1:A:779:THR:HA	10	0.14
(1,95)	1:B:794:LYS:O	1:B:798:ASN:H	3	0.14
(1,91)	1:B:792:ALA:O	1:B:796:TRP:H	3	0.14
(1,90)	1:B:791:GLU:O	1:B:795:TYR:N	10	0.14
(1,9)	1:B:794:LYS:O	1:B:798:ASN:H	3	0.14
(1,89)	1:B:791:GLU:O	1:B:795:TYR:H	2	0.14
(1,85)	1:B:850:GLY:O	1:B:854:ILE:H	15	0.14
(1,83)	1:B:849:GLN:O	1:B:853:ARG:H	11	0.14
(1,75)	1:B:837:SER:O	1:B:841:ARG:H	10	0.14
(1,73)	1:B:836:ALA:O	1:B:840:ILE:H	2	0.14
(1,73)	1:B:836:ALA:O	1:B:840:ILE:H	4	0.14
(1,69)	1:B:834:GLN:O	1:B:838:ARG:H	8	0.14
(1,61)	1:B:830:ILE:O	1:B:834:GLN:H	9	0.14
(1,5)	1:B:792:ALA:O	1:B:796:TRP:H	3	0.14
(1,47)	1:B:813:SER:O	1:B:817:ALA:H	12	0.14
(1,41)	1:B:810:SER:O	1:B:814:LEU:H	14	0.14
(1,4)	1:B:791:GLU:O	1:B:795:TYR:N	10	0.14
(1,3)	1:B:791:GLU:O	1:B:795:TYR:H	2	0.14
(1,257)	1:B:850:GLY:O	1:B:854:ILE:H	15	0.14
(1,255)	1:B:849:GLN:O	1:B:853:ARG:H	11	0.14
(1,247)	1:B:837:SER:O	1:B:841:ARG:H	10	0.14
(1,245)	1:B:836:ALA:O	1:B:840:ILE:H	2	0.14
(1,245)	1:B:836:ALA:O	1:B:840:ILE:H	4	0.14
(1,241)	1:B:834:GLN:O	1:B:838:ARG:H	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:B:830:ILE:O	1:B:834:GLN:H	9	0.14
(1,23)	1:B:801:GLN:O	1:B:805:GLN:H	5	0.14
(1,219)	1:B:813:SER:O	1:B:817:ALA:H	12	0.14
(1,213)	1:B:810:SER:O	1:B:814:LEU:H	14	0.14
(1,195)	1:B:801:GLN:O	1:B:805:GLN:H	5	0.14
(1,191)	1:B:799:LEU:O	1:B:803:TRP:H	11	0.14
(1,191)	1:B:799:LEU:O	1:B:803:TRP:H	12	0.14
(1,19)	1:B:799:LEU:O	1:B:803:TRP:H	11	0.14
(1,19)	1:B:799:LEU:O	1:B:803:TRP:H	12	0.14
(1,189)	1:B:798:ASN:O	1:B:802:TYR:H	11	0.14
(1,189)	1:B:798:ASN:O	1:B:802:TYR:H	13	0.14
(1,181)	1:B:794:LYS:O	1:B:798:ASN:H	3	0.14
(1,177)	1:B:792:ALA:O	1:B:796:TRP:H	3	0.14
(1,176)	1:B:791:GLU:O	1:B:795:TYR:N	10	0.14
(1,175)	1:B:791:GLU:O	1:B:795:TYR:H	2	0.14
(1,171)	1:B:850:GLY:O	1:B:854:ILE:H	15	0.14
(1,17)	1:B:798:ASN:O	1:B:802:TYR:H	11	0.14
(1,17)	1:B:798:ASN:O	1:B:802:TYR:H	13	0.14
(1,169)	1:B:849:GLN:O	1:B:853:ARG:H	11	0.14
(1,161)	1:B:837:SER:O	1:B:841:ARG:H	10	0.14
(1,159)	1:B:836:ALA:O	1:B:840:ILE:H	2	0.14
(1,159)	1:B:836:ALA:O	1:B:840:ILE:H	4	0.14
(1,155)	1:B:834:GLN:O	1:B:838:ARG:H	8	0.14
(1,147)	1:B:830:ILE:O	1:B:834:GLN:H	9	0.14
(1,133)	1:B:813:SER:O	1:B:817:ALA:H	12	0.14
(1,127)	1:B:810:SER:O	1:B:814:LEU:H	14	0.14
(1,109)	1:B:801:GLN:O	1:B:805:GLN:H	5	0.14
(1,105)	1:B:799:LEU:O	1:B:803:TRP:H	11	0.14
(1,105)	1:B:799:LEU:O	1:B:803:TRP:H	12	0.14
(1,103)	1:B:798:ASN:O	1:B:802:TYR:H	11	0.14
(1,103)	1:B:798:ASN:O	1:B:802:TYR:H	13	0.14
(2,990)	1:A:779:THR:H	1:A:776:LEU:HA	3	0.13
(2,99)	1:A:758:ASP:H	1:B:715:LEU:HD21	4	0.13
(2,99)	1:A:758:ASP:H	1:B:715:LEU:HD22	4	0.13
(2,99)	1:A:758:ASP:H	1:B:715:LEU:HD23	4	0.13
(2,983)	1:A:777:ILE:HG21	1:A:780:ARG:HD2	1	0.13
(2,983)	1:A:777:ILE:HG21	1:A:780:ARG:HD3	1	0.13
(2,983)	1:A:777:ILE:HG22	1:A:780:ARG:HD2	1	0.13
(2,983)	1:A:777:ILE:HG22	1:A:780:ARG:HD3	1	0.13
(2,983)	1:A:777:ILE:HG23	1:A:780:ARG:HD2	1	0.13
(2,983)	1:A:777:ILE:HG23	1:A:780:ARG:HD3	1	0.13
(2,977)	1:A:777:ILE:H	1:A:774:LEU:HA	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,972)	1:A:776:LEU:H	1:A:775:LEU:HA	10	0.13
(2,951)	1:A:771:LEU:HD11	1:A:768:TYR:HE1	5	0.13
(2,951)	1:A:771:LEU:HD11	1:A:768:TYR:HE2	5	0.13
(2,951)	1:A:771:LEU:HD12	1:A:768:TYR:HE1	5	0.13
(2,951)	1:A:771:LEU:HD12	1:A:768:TYR:HE2	5	0.13
(2,951)	1:A:771:LEU:HD13	1:A:768:TYR:HE1	5	0.13
(2,951)	1:A:771:LEU:HD13	1:A:768:TYR:HE2	5	0.13
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	3	0.13
(2,945)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	3	0.13
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	3	0.13
(2,945)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	3	0.13
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	3	0.13
(2,945)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	3	0.13
(2,939)	1:A:760:LEU:HD11	1:A:756:ILE:HG12	12	0.13
(2,939)	1:A:760:LEU:HD11	1:A:756:ILE:HG13	12	0.13
(2,939)	1:A:760:LEU:HD12	1:A:756:ILE:HG12	12	0.13
(2,939)	1:A:760:LEU:HD12	1:A:756:ILE:HG13	12	0.13
(2,939)	1:A:760:LEU:HD13	1:A:756:ILE:HG12	12	0.13
(2,939)	1:A:760:LEU:HD13	1:A:756:ILE:HG13	12	0.13
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB1	1	0.13
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB2	1	0.13
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB3	1	0.13
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB1	12	0.13
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB2	12	0.13
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB3	12	0.13
(2,932)	1:A:755:LEU:HD21	1:A:759:ASP:HB3	12	0.13
(2,932)	1:A:755:LEU:HD22	1:A:759:ASP:HB3	12	0.13
(2,932)	1:A:755:LEU:HD23	1:A:759:ASP:HB3	12	0.13
(2,927)	1:A:755:LEU:H	1:A:752:SER:HA	13	0.13
(2,925)	1:A:754:ALA:HB1	1:A:758:ASP:H	1	0.13
(2,925)	1:A:754:ALA:HB2	1:A:758:ASP:H	1	0.13
(2,925)	1:A:754:ALA:HB3	1:A:758:ASP:H	1	0.13
(2,925)	1:A:754:ALA:HB1	1:A:758:ASP:H	12	0.13
(2,925)	1:A:754:ALA:HB2	1:A:758:ASP:H	12	0.13
(2,925)	1:A:754:ALA:HB3	1:A:758:ASP:H	12	0.13
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	12	0.13
(2,917)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	12	0.13
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	12	0.13
(2,917)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	12	0.13
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	12	0.13
(2,917)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	12	0.13
(2,916)	1:A:753:LEU:HD11	1:A:757:TRP:HB2	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,916)	1:A:753:LEU:HD11	1:A:757:TRP:HB3	15	0.13
(2,916)	1:A:753:LEU:HD12	1:A:757:TRP:HB2	15	0.13
(2,916)	1:A:753:LEU:HD12	1:A:757:TRP:HB3	15	0.13
(2,916)	1:A:753:LEU:HD13	1:A:757:TRP:HB2	15	0.13
(2,916)	1:A:753:LEU:HD13	1:A:757:TRP:HB3	15	0.13
(2,907)	1:A:749:VAL:H	1:A:746:ILE:HA	6	0.13
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB2	3	0.13
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB3	3	0.13
(2,899)	1:A:747:ARG:H	1:A:744:ARG:HA	8	0.13
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB2	1	0.13
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB3	1	0.13
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB2	1	0.13
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB3	1	0.13
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB2	1	0.13
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB3	1	0.13
(2,845)	1:A:707:ARG:H	1:A:707:ARG:HG2	1	0.13
(2,845)	1:A:707:ARG:H	1:A:707:ARG:HG3	1	0.13
(2,845)	1:A:707:ARG:H	1:A:707:ARG:HG2	13	0.13
(2,845)	1:A:707:ARG:H	1:A:707:ARG:HG3	13	0.13
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD2	10	0.13
(2,84)	1:A:709:ARG:H	1:B:714:PRO:HD3	10	0.13
(2,828)	1:A:705:VAL:HG11	1:A:709:ARG:HD2	13	0.13
(2,828)	1:A:705:VAL:HG11	1:A:709:ARG:HD3	13	0.13
(2,828)	1:A:705:VAL:HG12	1:A:709:ARG:HD2	13	0.13
(2,828)	1:A:705:VAL:HG12	1:A:709:ARG:HD3	13	0.13
(2,828)	1:A:705:VAL:HG13	1:A:709:ARG:HD2	13	0.13
(2,828)	1:A:705:VAL:HG13	1:A:709:ARG:HD3	13	0.13
(2,821)	1:A:705:VAL:H	1:A:702:LEU:HA	2	0.13
(2,810)	1:A:704:LEU:H	1:A:701:VAL:HA	3	0.13
(2,803)	1:A:702:LEU:HD11	1:A:699:PHE:HE1	8	0.13
(2,803)	1:A:702:LEU:HD11	1:A:699:PHE:HE2	8	0.13
(2,803)	1:A:702:LEU:HD12	1:A:699:PHE:HE1	8	0.13
(2,803)	1:A:702:LEU:HD12	1:A:699:PHE:HE2	8	0.13
(2,803)	1:A:702:LEU:HD13	1:A:699:PHE:HE1	8	0.13
(2,803)	1:A:702:LEU:HD13	1:A:699:PHE:HE2	8	0.13
(2,797)	1:A:701:VAL:HG11	1:A:698:VAL:HA	2	0.13
(2,797)	1:A:701:VAL:HG12	1:A:698:VAL:HA	2	0.13
(2,797)	1:A:701:VAL:HG13	1:A:698:VAL:HA	2	0.13
(2,794)	1:A:701:VAL:H	1:A:698:VAL:HA	12	0.13
(2,782)	1:A:698:VAL:HG11	1:A:699:PHE:HD1	5	0.13
(2,782)	1:A:698:VAL:HG11	1:A:699:PHE:HD2	5	0.13
(2,782)	1:A:698:VAL:HG12	1:A:699:PHE:HD1	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,782)	1:A:698:VAL:HG12	1:A:699:PHE:HD2	5	0.13
(2,782)	1:A:698:VAL:HG13	1:A:699:PHE:HD1	5	0.13
(2,782)	1:A:698:VAL:HG13	1:A:699:PHE:HD2	5	0.13
(2,780)	1:A:698:VAL:HG11	1:A:695:LEU:HA	4	0.13
(2,780)	1:A:698:VAL:HG12	1:A:695:LEU:HA	4	0.13
(2,780)	1:A:698:VAL:HG13	1:A:695:LEU:HA	4	0.13
(2,780)	1:A:698:VAL:HG11	1:A:695:LEU:HA	10	0.13
(2,780)	1:A:698:VAL:HG12	1:A:695:LEU:HA	10	0.13
(2,780)	1:A:698:VAL:HG13	1:A:695:LEU:HA	10	0.13
(2,770)	1:A:695:LEU:HD21	1:A:698:VAL:HB	3	0.13
(2,770)	1:A:695:LEU:HD22	1:A:698:VAL:HB	3	0.13
(2,770)	1:A:695:LEU:HD23	1:A:698:VAL:HB	3	0.13
(2,768)	1:A:695:LEU:HD11	1:A:691:SER:HB2	13	0.13
(2,768)	1:A:695:LEU:HD11	1:A:691:SER:HB3	13	0.13
(2,768)	1:A:695:LEU:HD12	1:A:691:SER:HB2	13	0.13
(2,768)	1:A:695:LEU:HD12	1:A:691:SER:HB3	13	0.13
(2,768)	1:A:695:LEU:HD13	1:A:691:SER:HB2	13	0.13
(2,768)	1:A:695:LEU:HD13	1:A:691:SER:HB3	13	0.13
(2,761)	1:A:693:ILE:HD11	1:A:697:ILE:H	3	0.13
(2,761)	1:A:693:ILE:HD12	1:A:697:ILE:H	3	0.13
(2,761)	1:A:693:ILE:HD13	1:A:697:ILE:H	3	0.13
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE1	10	0.13
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE2	10	0.13
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE1	10	0.13
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE2	10	0.13
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE1	10	0.13
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE2	10	0.13
(2,747)	1:A:687:ILE:HG21	1:A:691:SER:HG	11	0.13
(2,747)	1:A:687:ILE:HG22	1:A:691:SER:HG	11	0.13
(2,747)	1:A:687:ILE:HG23	1:A:691:SER:HG	11	0.13
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	5	0.13
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	5	0.13
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	5	0.13
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	5	0.13
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	5	0.13
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	5	0.13
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD11	12	0.13
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD12	12	0.13
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD13	12	0.13
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD21	12	0.13
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD22	12	0.13
(2,710)	1:A:678:TRP:HE1	1:A:679:LEU:HD23	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,705)	1:A:676:THR:HG21	1:A:681:TYR:HH	7	0.13
(2,705)	1:A:676:THR:HG22	1:A:681:TYR:HH	7	0.13
(2,705)	1:A:676:THR:HG23	1:A:681:TYR:HH	7	0.13
(2,701)	1:A:676:THR:HG21	1:A:666:TRP:HZ3	12	0.13
(2,701)	1:A:676:THR:HG22	1:A:666:TRP:HZ3	12	0.13
(2,701)	1:A:676:THR:HG23	1:A:666:TRP:HZ3	12	0.13
(2,684)	1:A:670:TRP:H	1:A:667:ALA:HA	13	0.13
(2,683)	1:A:669:LEU:HD11	1:A:672:TRP:HZ3	14	0.13
(2,683)	1:A:669:LEU:HD12	1:A:672:TRP:HZ3	14	0.13
(2,683)	1:A:669:LEU:HD13	1:A:672:TRP:HZ3	14	0.13
(2,683)	1:A:669:LEU:HD21	1:A:672:TRP:HZ3	14	0.13
(2,683)	1:A:669:LEU:HD22	1:A:672:TRP:HZ3	14	0.13
(2,683)	1:A:669:LEU:HD23	1:A:672:TRP:HZ3	14	0.13
(2,670)	1:A:667:ALA:H	1:A:666:TRP:HD1	3	0.13
(2,666)	1:A:666:TRP:HE1	1:A:662:GLU:H	12	0.13
(2,654)	1:A:665:LYS:H	1:A:664:ASP:HA	9	0.13
(2,653)	1:A:665:LYS:H	1:A:662:GLU:HA	1	0.13
(2,653)	1:A:665:LYS:H	1:A:662:GLU:HA	12	0.13
(2,639)	1:A:661:LEU:HD11	1:A:662:GLU:HG2	5	0.13
(2,639)	1:A:661:LEU:HD11	1:A:662:GLU:HG3	5	0.13
(2,639)	1:A:661:LEU:HD12	1:A:662:GLU:HG2	5	0.13
(2,639)	1:A:661:LEU:HD12	1:A:662:GLU:HG3	5	0.13
(2,639)	1:A:661:LEU:HD13	1:A:662:GLU:HG2	5	0.13
(2,639)	1:A:661:LEU:HD13	1:A:662:GLU:HG3	5	0.13
(2,639)	1:A:661:LEU:HD21	1:A:662:GLU:HG2	5	0.13
(2,639)	1:A:661:LEU:HD21	1:A:662:GLU:HG3	5	0.13
(2,639)	1:A:661:LEU:HD22	1:A:662:GLU:HG2	5	0.13
(2,639)	1:A:661:LEU:HD22	1:A:662:GLU:HG3	5	0.13
(2,639)	1:A:661:LEU:HD23	1:A:662:GLU:HG2	5	0.13
(2,639)	1:A:661:LEU:HD23	1:A:662:GLU:HG3	5	0.13
(2,639)	1:A:661:LEU:HD11	1:A:662:GLU:HG2	15	0.13
(2,639)	1:A:661:LEU:HD11	1:A:662:GLU:HG3	15	0.13
(2,639)	1:A:661:LEU:HD12	1:A:662:GLU:HG2	15	0.13
(2,639)	1:A:661:LEU:HD12	1:A:662:GLU:HG3	15	0.13
(2,639)	1:A:661:LEU:HD13	1:A:662:GLU:HG2	15	0.13
(2,639)	1:A:661:LEU:HD13	1:A:662:GLU:HG3	15	0.13
(2,639)	1:A:661:LEU:HD21	1:A:662:GLU:HG2	15	0.13
(2,639)	1:A:661:LEU:HD21	1:A:662:GLU:HG3	15	0.13
(2,639)	1:A:661:LEU:HD22	1:A:662:GLU:HG2	15	0.13
(2,639)	1:A:661:LEU:HD22	1:A:662:GLU:HG3	15	0.13
(2,639)	1:A:661:LEU:HD23	1:A:662:GLU:HG2	15	0.13
(2,639)	1:A:661:LEU:HD23	1:A:662:GLU:HG3	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD2	7	0.13
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD3	7	0.13
(2,630)	1:B:835:GLY:H	1:B:834:GLN:HE21	14	0.13
(2,630)	1:B:835:GLY:H	1:B:834:GLN:HE22	14	0.13
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD11	4	0.13
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD12	4	0.13
(2,627)	1:B:819:ALA:H	1:B:820:ILE:HD13	4	0.13
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB2	5	0.13
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB3	5	0.13
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB2	12	0.13
(2,625)	1:B:806:GLU:H	1:B:803:TRP:HB3	12	0.13
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD11	8	0.13
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD12	8	0.13
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD13	8	0.13
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD21	8	0.13
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD22	8	0.13
(2,624)	1:B:803:TRP:HE1	1:B:800:LEU:HD23	8	0.13
(2,618)	1:B:797:TRP:H	1:B:796:TRP:HD1	15	0.13
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD21	13	0.13
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD22	13	0.13
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD23	13	0.13
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD11	6	0.13
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD12	6	0.13
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD13	6	0.13
(2,615)	1:B:796:TRP:HE1	1:B:796:TRP:H	6	0.13
(2,615)	1:B:796:TRP:HE1	1:B:796:TRP:H	14	0.13
(2,601)	1:B:785:LEU:H	1:B:782:VAL:HA	4	0.13
(2,60)	1:A:700:ALA:HB1	1:B:699:PHE:HD1	8	0.13
(2,60)	1:A:700:ALA:HB1	1:B:699:PHE:HD2	8	0.13
(2,60)	1:A:700:ALA:HB2	1:B:699:PHE:HD1	8	0.13
(2,60)	1:A:700:ALA:HB2	1:B:699:PHE:HD2	8	0.13
(2,60)	1:A:700:ALA:HB3	1:B:699:PHE:HD1	8	0.13
(2,60)	1:A:700:ALA:HB3	1:B:699:PHE:HD2	8	0.13
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD2	2	0.13
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD3	2	0.13
(2,581)	1:B:782:VAL:H	1:B:779:THR:HA	4	0.13
(2,576)	1:B:781:ILE:H	1:B:780:ARG:HA	1	0.13
(2,565)	1:B:779:THR:H	1:B:776:LEU:HA	2	0.13
(2,558)	1:B:777:ILE:HG21	1:B:780:ARG:HD2	14	0.13
(2,558)	1:B:777:ILE:HG21	1:B:780:ARG:HD3	14	0.13
(2,558)	1:B:777:ILE:HG22	1:B:780:ARG:HD2	14	0.13
(2,558)	1:B:777:ILE:HG22	1:B:780:ARG:HD3	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,558)	1:B:777:ILE:HG23	1:B:780:ARG:HD2	14	0.13
(2,558)	1:B:777:ILE:HG23	1:B:780:ARG:HD3	14	0.13
(2,545)	1:B:775:LEU:HD11	1:B:772:ARG:HA	14	0.13
(2,545)	1:B:775:LEU:HD12	1:B:772:ARG:HA	14	0.13
(2,545)	1:B:775:LEU:HD13	1:B:772:ARG:HA	14	0.13
(2,541)	1:B:775:LEU:H	1:B:774:LEU:HA	3	0.13
(2,530)	1:B:773:ASP:H	1:B:770:ARG:HA	11	0.13
(2,522)	1:B:764:SER:H	1:B:761:ARG:HA	12	0.13
(2,507)	1:B:755:LEU:HD21	1:B:759:ASP:HB3	4	0.13
(2,507)	1:B:755:LEU:HD22	1:B:759:ASP:HB3	4	0.13
(2,507)	1:B:755:LEU:HD23	1:B:759:ASP:HB3	4	0.13
(2,5)	1:A:663:LEU:H	1:A:661:LEU:HB2	4	0.13
(2,5)	1:A:663:LEU:H	1:A:661:LEU:HB3	4	0.13
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB2	7	0.13
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB3	7	0.13
(2,473)	1:B:746:ILE:HG21	1:B:750:ASN:HD22	13	0.13
(2,473)	1:B:746:ILE:HG22	1:B:750:ASN:HD22	13	0.13
(2,473)	1:B:746:ILE:HG23	1:B:750:ASN:HD22	13	0.13
(2,471)	1:B:746:ILE:HD11	1:B:743:ASP:HB2	11	0.13
(2,471)	1:B:746:ILE:HD11	1:B:743:ASP:HB3	11	0.13
(2,471)	1:B:746:ILE:HD12	1:B:743:ASP:HB2	11	0.13
(2,471)	1:B:746:ILE:HD12	1:B:743:ASP:HB3	11	0.13
(2,471)	1:B:746:ILE:HD13	1:B:743:ASP:HB2	11	0.13
(2,471)	1:B:746:ILE:HD13	1:B:743:ASP:HB3	11	0.13
(2,465)	1:B:746:ILE:H	1:B:743:ASP:HB2	15	0.13
(2,465)	1:B:746:ILE:H	1:B:743:ASP:HB3	15	0.13
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB2	1	0.13
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB3	1	0.13
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB2	13	0.13
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB3	13	0.13
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB2	3	0.13
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB3	3	0.13
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB2	3	0.13
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB3	3	0.13
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB2	3	0.13
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB3	3	0.13
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB2	6	0.13
(2,406)	1:B:705:VAL:HG21	1:B:706:ASN:HB3	6	0.13
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB2	6	0.13
(2,406)	1:B:705:VAL:HG22	1:B:706:ASN:HB3	6	0.13
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB2	6	0.13
(2,406)	1:B:705:VAL:HG23	1:B:706:ASN:HB3	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,390)	1:B:704:LEU:H	1:B:704:LEU:HB3	10	0.13
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD1	14	0.13
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD2	14	0.13
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD1	14	0.13
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD2	14	0.13
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD1	14	0.13
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD2	14	0.13
(2,37)	1:B:692:LEU:HD21	1:A:694:GLY:H	8	0.13
(2,37)	1:B:692:LEU:HD22	1:A:694:GLY:H	8	0.13
(2,37)	1:B:692:LEU:HD23	1:A:694:GLY:H	8	0.13
(2,37)	1:B:692:LEU:HD21	1:A:694:GLY:H	9	0.13
(2,37)	1:B:692:LEU:HD22	1:A:694:GLY:H	9	0.13
(2,37)	1:B:692:LEU:HD23	1:A:694:GLY:H	9	0.13
(2,37)	1:B:692:LEU:HD21	1:A:694:GLY:H	14	0.13
(2,37)	1:B:692:LEU:HD22	1:A:694:GLY:H	14	0.13
(2,37)	1:B:692:LEU:HD23	1:A:694:GLY:H	14	0.13
(2,358)	1:B:698:VAL:HG11	1:B:702:LEU:HB2	14	0.13
(2,358)	1:B:698:VAL:HG11	1:B:702:LEU:HB3	14	0.13
(2,358)	1:B:698:VAL:HG12	1:B:702:LEU:HB2	14	0.13
(2,358)	1:B:698:VAL:HG12	1:B:702:LEU:HB3	14	0.13
(2,358)	1:B:698:VAL:HG13	1:B:702:LEU:HB2	14	0.13
(2,358)	1:B:698:VAL:HG13	1:B:702:LEU:HB3	14	0.13
(2,340)	1:B:693:ILE:HG21	1:B:696:ARG:HG2	13	0.13
(2,340)	1:B:693:ILE:HG21	1:B:696:ARG:HG3	13	0.13
(2,340)	1:B:693:ILE:HG22	1:B:696:ARG:HG2	13	0.13
(2,340)	1:B:693:ILE:HG22	1:B:696:ARG:HG3	13	0.13
(2,340)	1:B:693:ILE:HG23	1:B:696:ARG:HG2	13	0.13
(2,340)	1:B:693:ILE:HG23	1:B:696:ARG:HG3	13	0.13
(2,338)	1:B:693:ILE:HG21	1:B:693:ILE:H	10	0.13
(2,338)	1:B:693:ILE:HG22	1:B:693:ILE:H	10	0.13
(2,338)	1:B:693:ILE:HG23	1:B:693:ILE:H	10	0.13
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG21	2	0.13
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG22	2	0.13
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG23	2	0.13
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG21	2	0.13
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG22	2	0.13
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG23	2	0.13
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG21	2	0.13
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG22	2	0.13
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG23	2	0.13
(2,305)	1:B:684:ILE:HG21	1:B:685:PHE:HD1	1	0.13
(2,305)	1:B:684:ILE:HG21	1:B:685:PHE:HD2	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,305)	1:B:684:ILE:HG22	1:B:685:PHE:HD1	1	0.13
(2,305)	1:B:684:ILE:HG22	1:B:685:PHE:HD2	1	0.13
(2,305)	1:B:684:ILE:HG23	1:B:685:PHE:HD1	1	0.13
(2,305)	1:B:684:ILE:HG23	1:B:685:PHE:HD2	1	0.13
(2,305)	1:B:684:ILE:HG21	1:B:685:PHE:HD1	6	0.13
(2,305)	1:B:684:ILE:HG21	1:B:685:PHE:HD2	6	0.13
(2,305)	1:B:684:ILE:HG22	1:B:685:PHE:HD1	6	0.13
(2,305)	1:B:684:ILE:HG22	1:B:685:PHE:HD2	6	0.13
(2,305)	1:B:684:ILE:HG23	1:B:685:PHE:HD1	6	0.13
(2,305)	1:B:684:ILE:HG23	1:B:685:PHE:HD2	6	0.13
(2,305)	1:B:684:ILE:HG21	1:B:685:PHE:HD1	11	0.13
(2,305)	1:B:684:ILE:HG21	1:B:685:PHE:HD2	11	0.13
(2,305)	1:B:684:ILE:HG22	1:B:685:PHE:HD1	11	0.13
(2,305)	1:B:684:ILE:HG22	1:B:685:PHE:HD2	11	0.13
(2,305)	1:B:684:ILE:HG23	1:B:685:PHE:HD1	11	0.13
(2,305)	1:B:684:ILE:HG23	1:B:685:PHE:HD2	11	0.13
(2,304)	1:B:684:ILE:HG21	1:B:685:PHE:HB2	9	0.13
(2,304)	1:B:684:ILE:HG21	1:B:685:PHE:HB3	9	0.13
(2,304)	1:B:684:ILE:HG22	1:B:685:PHE:HB2	9	0.13
(2,304)	1:B:684:ILE:HG22	1:B:685:PHE:HB3	9	0.13
(2,304)	1:B:684:ILE:HG23	1:B:685:PHE:HB2	9	0.13
(2,304)	1:B:684:ILE:HG23	1:B:685:PHE:HB3	9	0.13
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD11	8	0.13
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD12	8	0.13
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD13	8	0.13
(2,288)	1:B:679:LEU:HD11	1:B:678:TRP:HH2	3	0.13
(2,288)	1:B:679:LEU:HD12	1:B:678:TRP:HH2	3	0.13
(2,288)	1:B:679:LEU:HD13	1:B:678:TRP:HH2	3	0.13
(2,288)	1:B:679:LEU:HD21	1:B:678:TRP:HH2	3	0.13
(2,288)	1:B:679:LEU:HD22	1:B:678:TRP:HH2	3	0.13
(2,288)	1:B:679:LEU:HD23	1:B:678:TRP:HH2	3	0.13
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD11	6	0.13
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD12	6	0.13
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD13	6	0.13
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD21	6	0.13
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD22	6	0.13
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD23	6	0.13
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD11	13	0.13
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD12	13	0.13
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD13	13	0.13
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD21	13	0.13
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD22	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,285)	1:B:678:TRP:HE1	1:B:679:LEU:HD23	13	0.13
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD11	14	0.13
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD12	14	0.13
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD13	14	0.13
(2,277)	1:B:676:THR:HG21	1:B:669:LEU:HA	6	0.13
(2,277)	1:B:676:THR:HG22	1:B:669:LEU:HA	6	0.13
(2,277)	1:B:676:THR:HG23	1:B:669:LEU:HA	6	0.13
(2,276)	1:B:676:THR:HG21	1:B:666:TRP:HZ3	7	0.13
(2,276)	1:B:676:THR:HG22	1:B:666:TRP:HZ3	7	0.13
(2,276)	1:B:676:THR:HG23	1:B:666:TRP:HZ3	7	0.13
(2,272)	1:B:674:ASP:H	1:B:677:ASN:H	2	0.13
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD11	2	0.13
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD12	2	0.13
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD13	2	0.13
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD21	2	0.13
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD22	2	0.13
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD23	2	0.13
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD11	1	0.13
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD12	1	0.13
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD13	1	0.13
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD21	1	0.13
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD22	1	0.13
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD23	1	0.13
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD11	6	0.13
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD12	6	0.13
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD13	6	0.13
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD21	6	0.13
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD22	6	0.13
(2,264)	1:B:670:TRP:HE1	1:B:669:LEU:HD23	6	0.13
(2,253)	1:B:669:LEU:H	1:B:666:TRP:HA	10	0.13
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD11	7	0.13
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD12	7	0.13
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD13	7	0.13
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD21	7	0.13
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD22	7	0.13
(2,248)	1:B:667:ALA:HB1	1:B:663:LEU:HD23	7	0.13
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD11	7	0.13
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD12	7	0.13
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD13	7	0.13
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD21	7	0.13
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD22	7	0.13
(2,248)	1:B:667:ALA:HB2	1:B:663:LEU:HD23	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD11	7	0.13
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD12	7	0.13
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD13	7	0.13
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD21	7	0.13
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD22	7	0.13
(2,248)	1:B:667:ALA:HB3	1:B:663:LEU:HD23	7	0.13
(2,245)	1:B:667:ALA:H	1:B:666:TRP:HD1	3	0.13
(2,242)	1:B:667:ALA:H	1:B:664:ASP:HA	4	0.13
(2,225)	1:B:664:ASP:H	1:B:663:LEU:H	7	0.13
(2,22)	1:B:678:TRP:HE1	1:A:687:ILE:HD11	8	0.13
(2,22)	1:B:678:TRP:HE1	1:A:687:ILE:HD12	8	0.13
(2,22)	1:B:678:TRP:HE1	1:A:687:ILE:HD13	8	0.13
(2,219)	1:B:663:LEU:H	1:B:664:ASP:H	7	0.13
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ1	7	0.13
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ2	7	0.13
(2,211)	1:B:839:ALA:H	1:B:808:LYS:HZ3	7	0.13
(2,207)	1:A:831:GLU:H	1:A:816:ASN:HD21	9	0.13
(2,207)	1:A:831:GLU:H	1:A:816:ASN:HD22	9	0.13
(2,206)	1:A:831:GLU:H	1:A:816:ASN:HD21	9	0.13
(2,206)	1:A:831:GLU:H	1:A:816:ASN:HD22	9	0.13
(2,204)	1:A:827:ASP:H	1:A:820:ILE:HG12	10	0.13
(2,204)	1:A:827:ASP:H	1:A:820:ILE:HG13	10	0.13
(2,203)	1:A:827:ASP:H	1:A:820:ILE:HG12	10	0.13
(2,203)	1:A:827:ASP:H	1:A:820:ILE:HG13	10	0.13
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD11	14	0.13
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD12	14	0.13
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD13	14	0.13
(2,169)	1:B:797:TRP:HE1	1:B:848:ARG:HB2	8	0.13
(2,169)	1:B:797:TRP:HE1	1:B:848:ARG:HB3	8	0.13
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG2	8	0.13
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG3	8	0.13
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD21	8	0.13
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD22	8	0.13
(2,1467)	1:A:796:TRP:HE1	1:A:799:LEU:HD23	8	0.13
(2,1465)	1:A:796:TRP:HE1	1:A:796:TRP:H	5	0.13
(2,1436)	1:A:782:VAL:HG21	1:A:779:THR:HA	11	0.13
(2,1436)	1:A:782:VAL:HG22	1:A:779:THR:HA	11	0.13
(2,1436)	1:A:782:VAL:HG23	1:A:779:THR:HA	11	0.13
(2,1431)	1:A:782:VAL:H	1:A:779:THR:HA	8	0.13
(2,1426)	1:A:781:ILE:H	1:A:780:ARG:HA	3	0.13
(2,1426)	1:A:781:ILE:H	1:A:780:ARG:HA	9	0.13
(2,1415)	1:A:779:THR:H	1:A:776:LEU:HA	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,141)	1:B:771:LEU:H	1:A:806:GLU:HB2	13	0.13
(2,141)	1:B:771:LEU:H	1:A:806:GLU:HB3	13	0.13
(2,1408)	1:A:777:ILE:HG21	1:A:780:ARG:HD2	1	0.13
(2,1408)	1:A:777:ILE:HG21	1:A:780:ARG:HD3	1	0.13
(2,1408)	1:A:777:ILE:HG22	1:A:780:ARG:HD2	1	0.13
(2,1408)	1:A:777:ILE:HG22	1:A:780:ARG:HD3	1	0.13
(2,1408)	1:A:777:ILE:HG23	1:A:780:ARG:HD2	1	0.13
(2,1408)	1:A:777:ILE:HG23	1:A:780:ARG:HD3	1	0.13
(2,1402)	1:A:777:ILE:H	1:A:774:LEU:HA	13	0.13
(2,1397)	1:A:776:LEU:H	1:A:775:LEU:HA	10	0.13
(2,1376)	1:A:771:LEU:HD11	1:A:768:TYR:HE1	5	0.13
(2,1376)	1:A:771:LEU:HD11	1:A:768:TYR:HE2	5	0.13
(2,1376)	1:A:771:LEU:HD12	1:A:768:TYR:HE1	5	0.13
(2,1376)	1:A:771:LEU:HD12	1:A:768:TYR:HE2	5	0.13
(2,1376)	1:A:771:LEU:HD13	1:A:768:TYR:HE1	5	0.13
(2,1376)	1:A:771:LEU:HD13	1:A:768:TYR:HE2	5	0.13
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE1	3	0.13
(2,1370)	1:A:763:LEU:HD21	1:A:768:TYR:HE2	3	0.13
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE1	3	0.13
(2,1370)	1:A:763:LEU:HD22	1:A:768:TYR:HE2	3	0.13
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE1	3	0.13
(2,1370)	1:A:763:LEU:HD23	1:A:768:TYR:HE2	3	0.13
(2,1364)	1:A:760:LEU:HD11	1:A:756:ILE:HG12	12	0.13
(2,1364)	1:A:760:LEU:HD11	1:A:756:ILE:HG13	12	0.13
(2,1364)	1:A:760:LEU:HD12	1:A:756:ILE:HG12	12	0.13
(2,1364)	1:A:760:LEU:HD12	1:A:756:ILE:HG13	12	0.13
(2,1364)	1:A:760:LEU:HD13	1:A:756:ILE:HG12	12	0.13
(2,1364)	1:A:760:LEU:HD13	1:A:756:ILE:HG13	12	0.13
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB1	1	0.13
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB2	1	0.13
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB3	1	0.13
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB1	12	0.13
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB2	12	0.13
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB3	12	0.13
(2,1357)	1:A:755:LEU:HD21	1:A:759:ASP:HB3	12	0.13
(2,1357)	1:A:755:LEU:HD22	1:A:759:ASP:HB3	12	0.13
(2,1357)	1:A:755:LEU:HD23	1:A:759:ASP:HB3	12	0.13
(2,1352)	1:A:755:LEU:H	1:A:752:SER:HA	13	0.13
(2,1350)	1:A:754:ALA:HB1	1:A:758:ASP:H	1	0.13
(2,1350)	1:A:754:ALA:HB2	1:A:758:ASP:H	1	0.13
(2,1350)	1:A:754:ALA:HB3	1:A:758:ASP:H	1	0.13
(2,1350)	1:A:754:ALA:HB1	1:A:758:ASP:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1350)	1:A:754:ALA:HB2	1:A:758:ASP:H	12	0.13
(2,1350)	1:A:754:ALA:HB3	1:A:758:ASP:H	12	0.13
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB2	12	0.13
(2,1342)	1:A:753:LEU:HD21	1:A:750:ASN:HB3	12	0.13
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB2	12	0.13
(2,1342)	1:A:753:LEU:HD22	1:A:750:ASN:HB3	12	0.13
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB2	12	0.13
(2,1342)	1:A:753:LEU:HD23	1:A:750:ASN:HB3	12	0.13
(2,1341)	1:A:753:LEU:HD11	1:A:757:TRP:HB2	15	0.13
(2,1341)	1:A:753:LEU:HD11	1:A:757:TRP:HB3	15	0.13
(2,1341)	1:A:753:LEU:HD12	1:A:757:TRP:HB2	15	0.13
(2,1341)	1:A:753:LEU:HD12	1:A:757:TRP:HB3	15	0.13
(2,1341)	1:A:753:LEU:HD13	1:A:757:TRP:HB2	15	0.13
(2,1341)	1:A:753:LEU:HD13	1:A:757:TRP:HB3	15	0.13
(2,1332)	1:A:749:VAL:H	1:A:746:ILE:HA	6	0.13
(2,1324)	1:A:747:ARG:H	1:A:744:ARG:HA	8	0.13
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB2	1	0.13
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB3	1	0.13
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB2	1	0.13
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB3	1	0.13
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB2	1	0.13
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB3	1	0.13
(2,1270)	1:A:707:ARG:H	1:A:707:ARG:HG2	1	0.13
(2,1270)	1:A:707:ARG:H	1:A:707:ARG:HG3	1	0.13
(2,1270)	1:A:707:ARG:H	1:A:707:ARG:HG2	13	0.13
(2,1270)	1:A:707:ARG:H	1:A:707:ARG:HG3	13	0.13
(2,1253)	1:A:705:VAL:HG11	1:A:709:ARG:HD2	13	0.13
(2,1253)	1:A:705:VAL:HG11	1:A:709:ARG:HD3	13	0.13
(2,1253)	1:A:705:VAL:HG12	1:A:709:ARG:HD2	13	0.13
(2,1253)	1:A:705:VAL:HG12	1:A:709:ARG:HD3	13	0.13
(2,1253)	1:A:705:VAL:HG13	1:A:709:ARG:HD2	13	0.13
(2,1253)	1:A:705:VAL:HG13	1:A:709:ARG:HD3	13	0.13
(2,1246)	1:A:705:VAL:H	1:A:702:LEU:HA	2	0.13
(2,1235)	1:A:704:LEU:H	1:A:701:VAL:HA	3	0.13
(2,1228)	1:A:702:LEU:HD11	1:A:699:PHE:HE1	8	0.13
(2,1228)	1:A:702:LEU:HD11	1:A:699:PHE:HE2	8	0.13
(2,1228)	1:A:702:LEU:HD12	1:A:699:PHE:HE1	8	0.13
(2,1228)	1:A:702:LEU:HD12	1:A:699:PHE:HE2	8	0.13
(2,1228)	1:A:702:LEU:HD13	1:A:699:PHE:HE1	8	0.13
(2,1228)	1:A:702:LEU:HD13	1:A:699:PHE:HE2	8	0.13
(2,1222)	1:A:701:VAL:HG11	1:A:698:VAL:HA	2	0.13
(2,1222)	1:A:701:VAL:HG12	1:A:698:VAL:HA	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1222)	1:A:701:VAL:HG13	1:A:698:VAL:HA	2	0.13
(2,1219)	1:A:701:VAL:H	1:A:698:VAL:HA	12	0.13
(2,1207)	1:A:698:VAL:HG11	1:A:699:PHE:HD1	5	0.13
(2,1207)	1:A:698:VAL:HG11	1:A:699:PHE:HD2	5	0.13
(2,1207)	1:A:698:VAL:HG12	1:A:699:PHE:HD1	5	0.13
(2,1207)	1:A:698:VAL:HG12	1:A:699:PHE:HD2	5	0.13
(2,1207)	1:A:698:VAL:HG13	1:A:699:PHE:HD1	5	0.13
(2,1207)	1:A:698:VAL:HG13	1:A:699:PHE:HD2	5	0.13
(2,1205)	1:A:698:VAL:HG11	1:A:695:LEU:HA	4	0.13
(2,1205)	1:A:698:VAL:HG12	1:A:695:LEU:HA	4	0.13
(2,1205)	1:A:698:VAL:HG13	1:A:695:LEU:HA	4	0.13
(2,1205)	1:A:698:VAL:HG11	1:A:695:LEU:HA	10	0.13
(2,1205)	1:A:698:VAL:HG12	1:A:695:LEU:HA	10	0.13
(2,1205)	1:A:698:VAL:HG13	1:A:695:LEU:HA	10	0.13
(2,1195)	1:A:695:LEU:HD21	1:A:698:VAL:HB	3	0.13
(2,1195)	1:A:695:LEU:HD22	1:A:698:VAL:HB	3	0.13
(2,1195)	1:A:695:LEU:HD23	1:A:698:VAL:HB	3	0.13
(2,1193)	1:A:695:LEU:HD11	1:A:691:SER:HB2	13	0.13
(2,1193)	1:A:695:LEU:HD11	1:A:691:SER:HB3	13	0.13
(2,1193)	1:A:695:LEU:HD12	1:A:691:SER:HB2	13	0.13
(2,1193)	1:A:695:LEU:HD12	1:A:691:SER:HB3	13	0.13
(2,1193)	1:A:695:LEU:HD13	1:A:691:SER:HB2	13	0.13
(2,1193)	1:A:695:LEU:HD13	1:A:691:SER:HB3	13	0.13
(2,1186)	1:A:693:ILE:HD11	1:A:697:ILE:H	3	0.13
(2,1186)	1:A:693:ILE:HD12	1:A:697:ILE:H	3	0.13
(2,1186)	1:A:693:ILE:HD13	1:A:697:ILE:H	3	0.13
(2,1172)	1:A:687:ILE:HG21	1:A:691:SER:HG	11	0.13
(2,1172)	1:A:687:ILE:HG22	1:A:691:SER:HG	11	0.13
(2,1172)	1:A:687:ILE:HG23	1:A:691:SER:HG	11	0.13
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	5	0.13
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	5	0.13
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	5	0.13
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	5	0.13
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	5	0.13
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	5	0.13
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD11	12	0.13
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD12	12	0.13
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD13	12	0.13
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD21	12	0.13
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD22	12	0.13
(2,1135)	1:A:678:TRP:HE1	1:A:679:LEU:HD23	12	0.13
(2,1130)	1:A:676:THR:HG21	1:A:681:TYR:HH	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1130)	1:A:676:THR:HG22	1:A:681:TYR:HH	7	0.13
(2,1130)	1:A:676:THR:HG23	1:A:681:TYR:HH	7	0.13
(2,1126)	1:A:676:THR:HG21	1:A:666:TRP:HZ3	12	0.13
(2,1126)	1:A:676:THR:HG22	1:A:666:TRP:HZ3	12	0.13
(2,1126)	1:A:676:THR:HG23	1:A:666:TRP:HZ3	12	0.13
(2,1109)	1:A:670:TRP:H	1:A:667:ALA:HA	13	0.13
(2,1108)	1:A:669:LEU:HD11	1:A:672:TRP:HZ3	14	0.13
(2,1108)	1:A:669:LEU:HD12	1:A:672:TRP:HZ3	14	0.13
(2,1108)	1:A:669:LEU:HD13	1:A:672:TRP:HZ3	14	0.13
(2,1108)	1:A:669:LEU:HD21	1:A:672:TRP:HZ3	14	0.13
(2,1108)	1:A:669:LEU:HD22	1:A:672:TRP:HZ3	14	0.13
(2,1108)	1:A:669:LEU:HD23	1:A:672:TRP:HZ3	14	0.13
(2,1095)	1:A:667:ALA:H	1:A:666:TRP:HD1	3	0.13
(2,1091)	1:A:666:TRP:HE1	1:A:662:GLU:H	12	0.13
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD2	3	0.13
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD3	3	0.13
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD2	3	0.13
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD3	3	0.13
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD2	3	0.13
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD3	3	0.13
(2,1079)	1:A:665:LYS:H	1:A:664:ASP:HA	9	0.13
(2,1078)	1:A:665:LYS:H	1:A:662:GLU:HA	1	0.13
(2,1078)	1:A:665:LYS:H	1:A:662:GLU:HA	12	0.13
(2,1064)	1:A:661:LEU:HD11	1:A:662:GLU:HG2	5	0.13
(2,1064)	1:A:661:LEU:HD11	1:A:662:GLU:HG3	5	0.13
(2,1064)	1:A:661:LEU:HD12	1:A:662:GLU:HG2	5	0.13
(2,1064)	1:A:661:LEU:HD12	1:A:662:GLU:HG3	5	0.13
(2,1064)	1:A:661:LEU:HD13	1:A:662:GLU:HG2	5	0.13
(2,1064)	1:A:661:LEU:HD13	1:A:662:GLU:HG3	5	0.13
(2,1064)	1:A:661:LEU:HD21	1:A:662:GLU:HG2	5	0.13
(2,1064)	1:A:661:LEU:HD21	1:A:662:GLU:HG3	5	0.13
(2,1064)	1:A:661:LEU:HD22	1:A:662:GLU:HG2	5	0.13
(2,1064)	1:A:661:LEU:HD22	1:A:662:GLU:HG3	5	0.13
(2,1064)	1:A:661:LEU:HD23	1:A:662:GLU:HG2	5	0.13
(2,1064)	1:A:661:LEU:HD23	1:A:662:GLU:HG3	5	0.13
(2,1064)	1:A:661:LEU:HD11	1:A:662:GLU:HG2	15	0.13
(2,1064)	1:A:661:LEU:HD11	1:A:662:GLU:HG3	15	0.13
(2,1064)	1:A:661:LEU:HD12	1:A:662:GLU:HG2	15	0.13
(2,1064)	1:A:661:LEU:HD12	1:A:662:GLU:HG3	15	0.13
(2,1064)	1:A:661:LEU:HD13	1:A:662:GLU:HG2	15	0.13
(2,1064)	1:A:661:LEU:HD13	1:A:662:GLU:HG3	15	0.13
(2,1064)	1:A:661:LEU:HD21	1:A:662:GLU:HG2	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1064)	1:A:661:LEU:HD21	1:A:662:GLU:HG3	15	0.13
(2,1064)	1:A:661:LEU:HD22	1:A:662:GLU:HG2	15	0.13
(2,1064)	1:A:661:LEU:HD22	1:A:662:GLU:HG3	15	0.13
(2,1064)	1:A:661:LEU:HD23	1:A:662:GLU:HG2	15	0.13
(2,1064)	1:A:661:LEU:HD23	1:A:662:GLU:HG3	15	0.13
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG2	8	0.13
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG3	8	0.13
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD21	8	0.13
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD22	8	0.13
(2,1042)	1:A:796:TRP:HE1	1:A:799:LEU:HD23	8	0.13
(2,1040)	1:A:796:TRP:HE1	1:A:796:TRP:H	5	0.13
(2,102)	1:A:759:ASP:H	1:B:709:ARG:HD2	14	0.13
(2,102)	1:A:759:ASP:H	1:B:709:ARG:HD3	14	0.13
(2,1011)	1:A:782:VAL:HG21	1:A:779:THR:HA	11	0.13
(2,1011)	1:A:782:VAL:HG22	1:A:779:THR:HA	11	0.13
(2,1011)	1:A:782:VAL:HG23	1:A:779:THR:HA	11	0.13
(2,1006)	1:A:782:VAL:H	1:A:779:THR:HA	8	0.13
(2,1001)	1:A:781:ILE:H	1:A:780:ARG:HA	3	0.13
(2,1001)	1:A:781:ILE:H	1:A:780:ARG:HA	9	0.13
(1,98)	1:B:795:TYR:O	1:B:799:LEU:N	13	0.13
(1,96)	1:B:794:LYS:O	1:B:798:ASN:N	5	0.13
(1,96)	1:B:794:LYS:O	1:B:798:ASN:N	15	0.13
(1,93)	1:B:793:LEU:O	1:B:797:TRP:H	10	0.13
(1,89)	1:B:791:GLU:O	1:B:795:TYR:H	3	0.13
(1,85)	1:B:850:GLY:O	1:B:854:ILE:H	3	0.13
(1,75)	1:B:837:SER:O	1:B:841:ARG:H	2	0.13
(1,7)	1:B:793:LEU:O	1:B:797:TRP:H	10	0.13
(1,3)	1:B:791:GLU:O	1:B:795:TYR:H	3	0.13
(1,27)	1:B:803:TRP:O	1:B:807:LEU:H	4	0.13
(1,257)	1:B:850:GLY:O	1:B:854:ILE:H	3	0.13
(1,25)	1:B:802:TYR:O	1:B:806:GLU:H	2	0.13
(1,25)	1:B:802:TYR:O	1:B:806:GLU:H	4	0.13
(1,25)	1:B:802:TYR:O	1:B:806:GLU:H	7	0.13
(1,25)	1:B:802:TYR:O	1:B:806:GLU:H	15	0.13
(1,247)	1:B:837:SER:O	1:B:841:ARG:H	2	0.13
(1,23)	1:B:801:GLN:O	1:B:805:GLN:H	7	0.13
(1,23)	1:B:801:GLN:O	1:B:805:GLN:H	10	0.13
(1,20)	1:B:799:LEU:O	1:B:803:TRP:N	3	0.13
(1,199)	1:B:803:TRP:O	1:B:807:LEU:H	4	0.13
(1,197)	1:B:802:TYR:O	1:B:806:GLU:H	2	0.13
(1,197)	1:B:802:TYR:O	1:B:806:GLU:H	4	0.13
(1,197)	1:B:802:TYR:O	1:B:806:GLU:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	1:B:802:TYR:O	1:B:806:GLU:H	15	0.13
(1,195)	1:B:801:GLN:O	1:B:805:GLN:H	7	0.13
(1,195)	1:B:801:GLN:O	1:B:805:GLN:H	10	0.13
(1,192)	1:B:799:LEU:O	1:B:803:TRP:N	3	0.13
(1,191)	1:B:799:LEU:O	1:B:803:TRP:H	5	0.13
(1,19)	1:B:799:LEU:O	1:B:803:TRP:H	5	0.13
(1,184)	1:B:795:TYR:O	1:B:799:LEU:N	13	0.13
(1,182)	1:B:794:LYS:O	1:B:798:ASN:N	5	0.13
(1,182)	1:B:794:LYS:O	1:B:798:ASN:N	15	0.13
(1,179)	1:B:793:LEU:O	1:B:797:TRP:H	10	0.13
(1,175)	1:B:791:GLU:O	1:B:795:TYR:H	3	0.13
(1,171)	1:B:850:GLY:O	1:B:854:ILE:H	3	0.13
(1,161)	1:B:837:SER:O	1:B:841:ARG:H	2	0.13
(1,12)	1:B:795:TYR:O	1:B:799:LEU:N	13	0.13
(1,113)	1:B:803:TRP:O	1:B:807:LEU:H	4	0.13
(1,111)	1:B:802:TYR:O	1:B:806:GLU:H	2	0.13
(1,111)	1:B:802:TYR:O	1:B:806:GLU:H	4	0.13
(1,111)	1:B:802:TYR:O	1:B:806:GLU:H	7	0.13
(1,111)	1:B:802:TYR:O	1:B:806:GLU:H	15	0.13
(1,109)	1:B:801:GLN:O	1:B:805:GLN:H	7	0.13
(1,109)	1:B:801:GLN:O	1:B:805:GLN:H	10	0.13
(1,106)	1:B:799:LEU:O	1:B:803:TRP:N	3	0.13
(1,105)	1:B:799:LEU:O	1:B:803:TRP:H	5	0.13
(1,10)	1:B:794:LYS:O	1:B:798:ASN:N	5	0.13
(1,10)	1:B:794:LYS:O	1:B:798:ASN:N	15	0.13
(2,976)	1:A:776:LEU:HD11	1:A:773:ASP:HB2	15	0.12
(2,976)	1:A:776:LEU:HD11	1:A:773:ASP:HB3	15	0.12
(2,976)	1:A:776:LEU:HD12	1:A:773:ASP:HB2	15	0.12
(2,976)	1:A:776:LEU:HD12	1:A:773:ASP:HB3	15	0.12
(2,976)	1:A:776:LEU:HD13	1:A:773:ASP:HB2	15	0.12
(2,976)	1:A:776:LEU:HD13	1:A:773:ASP:HB3	15	0.12
(2,951)	1:A:771:LEU:HD11	1:A:768:TYR:HE1	15	0.12
(2,951)	1:A:771:LEU:HD11	1:A:768:TYR:HE2	15	0.12
(2,951)	1:A:771:LEU:HD12	1:A:768:TYR:HE1	15	0.12
(2,951)	1:A:771:LEU:HD12	1:A:768:TYR:HE2	15	0.12
(2,951)	1:A:771:LEU:HD13	1:A:768:TYR:HE1	15	0.12
(2,951)	1:A:771:LEU:HD13	1:A:768:TYR:HE2	15	0.12
(2,946)	1:A:763:LEU:HD21	1:A:771:LEU:HB2	9	0.12
(2,946)	1:A:763:LEU:HD21	1:A:771:LEU:HB3	9	0.12
(2,946)	1:A:763:LEU:HD22	1:A:771:LEU:HB2	9	0.12
(2,946)	1:A:763:LEU:HD22	1:A:771:LEU:HB3	9	0.12
(2,946)	1:A:763:LEU:HD23	1:A:771:LEU:HB2	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,946)	1:A:763:LEU:HD23	1:A:771:LEU:HB3	9	0.12
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB1	11	0.12
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB2	11	0.12
(2,934)	1:A:758:ASP:H	1:A:754:ALA:HB3	11	0.12
(2,927)	1:A:755:LEU:H	1:A:752:SER:HA	8	0.12
(2,926)	1:A:755:LEU:H	1:A:751:GLY:HA2	14	0.12
(2,926)	1:A:755:LEU:H	1:A:751:GLY:HA3	14	0.12
(2,925)	1:A:754:ALA:HB1	1:A:758:ASP:H	11	0.12
(2,925)	1:A:754:ALA:HB2	1:A:758:ASP:H	11	0.12
(2,925)	1:A:754:ALA:HB3	1:A:758:ASP:H	11	0.12
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	9	0.12
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	9	0.12
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	9	0.12
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	9	0.12
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	9	0.12
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	9	0.12
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB2	14	0.12
(2,918)	1:A:754:ALA:H	1:A:750:ASN:HB3	14	0.12
(2,904)	1:A:748:LEU:H	1:A:745:SER:HA	10	0.12
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB2	9	0.12
(2,9)	1:A:664:ASP:H	1:B:660:LEU:HB3	9	0.12
(2,890)	1:A:746:ILE:H	1:A:743:ASP:HB2	8	0.12
(2,890)	1:A:746:ILE:H	1:A:743:ASP:HB3	8	0.12
(2,854)	1:A:708:VAL:HG21	1:A:707:ARG:HD2	6	0.12
(2,854)	1:A:708:VAL:HG21	1:A:707:ARG:HD3	6	0.12
(2,854)	1:A:708:VAL:HG22	1:A:707:ARG:HD2	6	0.12
(2,854)	1:A:708:VAL:HG22	1:A:707:ARG:HD3	6	0.12
(2,854)	1:A:708:VAL:HG23	1:A:707:ARG:HD2	6	0.12
(2,854)	1:A:708:VAL:HG23	1:A:707:ARG:HD3	6	0.12
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD11	2	0.12
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD12	2	0.12
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD13	2	0.12
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD21	2	0.12
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD22	2	0.12
(2,847)	1:A:707:ARG:HE	1:A:704:LEU:HD23	2	0.12
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	2	0.12
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	2	0.12
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	2	0.12
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	2	0.12
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	2	0.12
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	2	0.12
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,831)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	14	0.12
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	14	0.12
(2,831)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	14	0.12
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	14	0.12
(2,831)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	14	0.12
(2,830)	1:A:705:VAL:HG21	1:A:702:LEU:HG	10	0.12
(2,830)	1:A:705:VAL:HG22	1:A:702:LEU:HG	10	0.12
(2,830)	1:A:705:VAL:HG23	1:A:702:LEU:HG	10	0.12
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	2	0.12
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	2	0.12
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	2	0.12
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	2	0.12
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	2	0.12
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	2	0.12
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	7	0.12
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	7	0.12
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	7	0.12
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	7	0.12
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	7	0.12
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	7	0.12
(2,780)	1:A:698:VAL:HG11	1:A:695:LEU:HA	11	0.12
(2,780)	1:A:698:VAL:HG12	1:A:695:LEU:HA	11	0.12
(2,780)	1:A:698:VAL:HG13	1:A:695:LEU:HA	11	0.12
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB1	11	0.12
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB2	11	0.12
(2,779)	1:A:697:ILE:HG21	1:A:700:ALA:HB3	11	0.12
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB1	11	0.12
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB2	11	0.12
(2,779)	1:A:697:ILE:HG22	1:A:700:ALA:HB3	11	0.12
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB1	11	0.12
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB2	11	0.12
(2,779)	1:A:697:ILE:HG23	1:A:700:ALA:HB3	11	0.12
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	14	0.12
(2,769)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	14	0.12
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	14	0.12
(2,769)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	14	0.12
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	14	0.12
(2,769)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	14	0.12
(2,768)	1:A:695:LEU:HD11	1:A:691:SER:HB2	6	0.12
(2,768)	1:A:695:LEU:HD11	1:A:691:SER:HB3	6	0.12
(2,768)	1:A:695:LEU:HD12	1:A:691:SER:HB2	6	0.12
(2,768)	1:A:695:LEU:HD12	1:A:691:SER:HB3	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,768)	1:A:695:LEU:HD13	1:A:691:SER:HB2	6	0.12
(2,768)	1:A:695:LEU:HD13	1:A:691:SER:HB3	6	0.12
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	8	0.12
(2,730)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	8	0.12
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	8	0.12
(2,730)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	8	0.12
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	8	0.12
(2,730)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	8	0.12
(2,718)	1:A:682:ILE:HG21	1:A:679:LEU:H	8	0.12
(2,718)	1:A:682:ILE:HG22	1:A:679:LEU:H	8	0.12
(2,718)	1:A:682:ILE:HG23	1:A:679:LEU:H	8	0.12
(2,715)	1:A:680:TRP:HE1	1:A:684:ILE:HD11	15	0.12
(2,715)	1:A:680:TRP:HE1	1:A:684:ILE:HD12	15	0.12
(2,715)	1:A:680:TRP:HE1	1:A:684:ILE:HD13	15	0.12
(2,711)	1:A:678:TRP:HE1	1:A:682:ILE:H	12	0.12
(2,701)	1:A:676:THR:HG21	1:A:666:TRP:HZ3	6	0.12
(2,701)	1:A:676:THR:HG22	1:A:666:TRP:HZ3	6	0.12
(2,701)	1:A:676:THR:HG23	1:A:666:TRP:HZ3	6	0.12
(2,693)	1:A:672:TRP:H	1:A:673:PHE:H	15	0.12
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD11	6	0.12
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD12	6	0.12
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD13	6	0.12
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD21	6	0.12
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD22	6	0.12
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD23	6	0.12
(2,683)	1:A:669:LEU:HD11	1:A:672:TRP:HZ3	10	0.12
(2,683)	1:A:669:LEU:HD12	1:A:672:TRP:HZ3	10	0.12
(2,683)	1:A:669:LEU:HD13	1:A:672:TRP:HZ3	10	0.12
(2,683)	1:A:669:LEU:HD21	1:A:672:TRP:HZ3	10	0.12
(2,683)	1:A:669:LEU:HD22	1:A:672:TRP:HZ3	10	0.12
(2,683)	1:A:669:LEU:HD23	1:A:672:TRP:HZ3	10	0.12
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD11	9	0.12
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD12	9	0.12
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD13	9	0.12
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD21	9	0.12
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD22	9	0.12
(2,673)	1:A:667:ALA:HB1	1:A:663:LEU:HD23	9	0.12
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD11	9	0.12
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD12	9	0.12
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD13	9	0.12
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD21	9	0.12
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD22	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,673)	1:A:667:ALA:HB2	1:A:663:LEU:HD23	9	0.12
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD11	9	0.12
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD12	9	0.12
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD13	9	0.12
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD21	9	0.12
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD22	9	0.12
(2,673)	1:A:667:ALA:HB3	1:A:663:LEU:HD23	9	0.12
(2,672)	1:A:667:ALA:HB1	1:A:664:ASP:HA	3	0.12
(2,672)	1:A:667:ALA:HB2	1:A:664:ASP:HA	3	0.12
(2,672)	1:A:667:ALA:HB3	1:A:664:ASP:HA	3	0.12
(2,672)	1:A:667:ALA:HB1	1:A:664:ASP:HA	13	0.12
(2,672)	1:A:667:ALA:HB2	1:A:664:ASP:HA	13	0.12
(2,672)	1:A:667:ALA:HB3	1:A:664:ASP:HA	13	0.12
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD2	3	0.12
(2,631)	1:B:839:ALA:H	1:B:838:ARG:HD3	3	0.12
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB2	5	0.12
(2,62)	1:A:700:ALA:HB1	1:A:702:LEU:HB3	5	0.12
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB2	5	0.12
(2,62)	1:A:700:ALA:HB2	1:A:702:LEU:HB3	5	0.12
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB2	5	0.12
(2,62)	1:A:700:ALA:HB3	1:A:702:LEU:HB3	5	0.12
(2,615)	1:B:796:TRP:HE1	1:B:796:TRP:H	1	0.12
(2,608)	1:B:786:GLY:H	1:B:782:VAL:HA	14	0.12
(2,601)	1:B:785:LEU:H	1:B:782:VAL:HA	9	0.12
(2,60)	1:A:700:ALA:HB1	1:B:699:PHE:HD1	6	0.12
(2,60)	1:A:700:ALA:HB1	1:B:699:PHE:HD2	6	0.12
(2,60)	1:A:700:ALA:HB2	1:B:699:PHE:HD1	6	0.12
(2,60)	1:A:700:ALA:HB2	1:B:699:PHE:HD2	6	0.12
(2,60)	1:A:700:ALA:HB3	1:B:699:PHE:HD1	6	0.12
(2,60)	1:A:700:ALA:HB3	1:B:699:PHE:HD2	6	0.12
(2,60)	1:A:700:ALA:HB1	1:B:699:PHE:HD1	15	0.12
(2,60)	1:A:700:ALA:HB1	1:B:699:PHE:HD2	15	0.12
(2,60)	1:A:700:ALA:HB2	1:B:699:PHE:HD1	15	0.12
(2,60)	1:A:700:ALA:HB2	1:B:699:PHE:HD2	15	0.12
(2,60)	1:A:700:ALA:HB3	1:B:699:PHE:HD1	15	0.12
(2,60)	1:A:700:ALA:HB3	1:B:699:PHE:HD2	15	0.12
(2,599)	1:B:784:LEU:HD11	1:B:787:ARG:HD2	9	0.12
(2,599)	1:B:784:LEU:HD11	1:B:787:ARG:HD3	9	0.12
(2,599)	1:B:784:LEU:HD12	1:B:787:ARG:HD2	9	0.12
(2,599)	1:B:784:LEU:HD12	1:B:787:ARG:HD3	9	0.12
(2,599)	1:B:784:LEU:HD13	1:B:787:ARG:HD2	9	0.12
(2,599)	1:B:784:LEU:HD13	1:B:787:ARG:HD3	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,593)	1:B:784:LEU:H	1:B:781:ILE:HA	9	0.12
(2,593)	1:B:784:LEU:H	1:B:781:ILE:HA	10	0.12
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD2	4	0.12
(2,588)	1:B:783:GLU:H	1:B:780:ARG:HD3	4	0.12
(2,587)	1:B:783:GLU:H	1:B:780:ARG:HA	2	0.12
(2,587)	1:B:783:GLU:H	1:B:780:ARG:HA	14	0.12
(2,581)	1:B:782:VAL:H	1:B:779:THR:HA	11	0.12
(2,565)	1:B:779:THR:H	1:B:776:LEU:HA	11	0.12
(2,541)	1:B:775:LEU:H	1:B:774:LEU:HA	15	0.12
(2,531)	1:B:773:ASP:H	1:B:770:ARG:HD2	9	0.12
(2,531)	1:B:773:ASP:H	1:B:770:ARG:HD3	9	0.12
(2,528)	1:B:772:ARG:H	1:B:771:LEU:H	11	0.12
(2,524)	1:B:771:LEU:H	1:B:772:ARG:H	11	0.12
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE1	8	0.12
(2,520)	1:B:763:LEU:HD21	1:B:768:TYR:HE2	8	0.12
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE1	8	0.12
(2,520)	1:B:763:LEU:HD22	1:B:768:TYR:HE2	8	0.12
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE1	8	0.12
(2,520)	1:B:763:LEU:HD23	1:B:768:TYR:HE2	8	0.12
(2,519)	1:B:763:LEU:HD11	1:B:764:SER:HG	10	0.12
(2,519)	1:B:763:LEU:HD12	1:B:764:SER:HG	10	0.12
(2,519)	1:B:763:LEU:HD13	1:B:764:SER:HG	10	0.12
(2,499)	1:B:754:ALA:HB1	1:B:753:LEU:HD21	10	0.12
(2,499)	1:B:754:ALA:HB1	1:B:753:LEU:HD22	10	0.12
(2,499)	1:B:754:ALA:HB1	1:B:753:LEU:HD23	10	0.12
(2,499)	1:B:754:ALA:HB2	1:B:753:LEU:HD21	10	0.12
(2,499)	1:B:754:ALA:HB2	1:B:753:LEU:HD22	10	0.12
(2,499)	1:B:754:ALA:HB2	1:B:753:LEU:HD23	10	0.12
(2,499)	1:B:754:ALA:HB3	1:B:753:LEU:HD21	10	0.12
(2,499)	1:B:754:ALA:HB3	1:B:753:LEU:HD22	10	0.12
(2,499)	1:B:754:ALA:HB3	1:B:753:LEU:HD23	10	0.12
(2,485)	1:B:753:LEU:H	1:B:750:ASN:HA	12	0.12
(2,48)	1:A:693:ILE:HD11	1:B:696:ARG:HH21	11	0.12
(2,48)	1:A:693:ILE:HD11	1:B:696:ARG:HH22	11	0.12
(2,48)	1:A:693:ILE:HD12	1:B:696:ARG:HH21	11	0.12
(2,48)	1:A:693:ILE:HD12	1:B:696:ARG:HH22	11	0.12
(2,48)	1:A:693:ILE:HD13	1:B:696:ARG:HH21	11	0.12
(2,48)	1:A:693:ILE:HD13	1:B:696:ARG:HH22	11	0.12
(2,473)	1:B:746:ILE:HG21	1:B:750:ASN:HD22	7	0.12
(2,473)	1:B:746:ILE:HG22	1:B:750:ASN:HD22	7	0.12
(2,473)	1:B:746:ILE:HG23	1:B:750:ASN:HD22	7	0.12
(2,465)	1:B:746:ILE:H	1:B:743:ASP:HB2	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,465)	1:B:746:ILE:H	1:B:743:ASP:HB3	8	0.12
(2,439)	1:B:710:GLN:H	1:B:708:VAL:HA	4	0.12
(2,407)	1:B:706:ASN:H	1:B:703:SER:HA	13	0.12
(2,403)	1:B:705:VAL:HG11	1:B:709:ARG:HD2	3	0.12
(2,403)	1:B:705:VAL:HG11	1:B:709:ARG:HD3	3	0.12
(2,403)	1:B:705:VAL:HG12	1:B:709:ARG:HD2	3	0.12
(2,403)	1:B:705:VAL:HG12	1:B:709:ARG:HD3	3	0.12
(2,403)	1:B:705:VAL:HG13	1:B:709:ARG:HD2	3	0.12
(2,403)	1:B:705:VAL:HG13	1:B:709:ARG:HD3	3	0.12
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD1	11	0.12
(2,377)	1:B:702:LEU:HD11	1:B:699:PHE:HD2	11	0.12
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD1	11	0.12
(2,377)	1:B:702:LEU:HD12	1:B:699:PHE:HD2	11	0.12
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD1	11	0.12
(2,377)	1:B:702:LEU:HD13	1:B:699:PHE:HD2	11	0.12
(2,358)	1:B:698:VAL:HG11	1:B:702:LEU:HB2	1	0.12
(2,358)	1:B:698:VAL:HG11	1:B:702:LEU:HB3	1	0.12
(2,358)	1:B:698:VAL:HG12	1:B:702:LEU:HB2	1	0.12
(2,358)	1:B:698:VAL:HG12	1:B:702:LEU:HB3	1	0.12
(2,358)	1:B:698:VAL:HG13	1:B:702:LEU:HB2	1	0.12
(2,358)	1:B:698:VAL:HG13	1:B:702:LEU:HB3	1	0.12
(2,357)	1:B:698:VAL:HG11	1:B:699:PHE:HD1	12	0.12
(2,357)	1:B:698:VAL:HG11	1:B:699:PHE:HD2	12	0.12
(2,357)	1:B:698:VAL:HG12	1:B:699:PHE:HD1	12	0.12
(2,357)	1:B:698:VAL:HG12	1:B:699:PHE:HD2	12	0.12
(2,357)	1:B:698:VAL:HG13	1:B:699:PHE:HD1	12	0.12
(2,357)	1:B:698:VAL:HG13	1:B:699:PHE:HD2	12	0.12
(2,356)	1:B:698:VAL:HG11	1:B:695:LEU:HG	2	0.12
(2,356)	1:B:698:VAL:HG12	1:B:695:LEU:HG	2	0.12
(2,356)	1:B:698:VAL:HG13	1:B:695:LEU:HG	2	0.12
(2,356)	1:B:698:VAL:HG11	1:B:695:LEU:HG	13	0.12
(2,356)	1:B:698:VAL:HG12	1:B:695:LEU:HG	13	0.12
(2,356)	1:B:698:VAL:HG13	1:B:695:LEU:HG	13	0.12
(2,352)	1:B:697:ILE:HG21	1:B:694:GLY:HA2	14	0.12
(2,352)	1:B:697:ILE:HG21	1:B:694:GLY:HA3	14	0.12
(2,352)	1:B:697:ILE:HG22	1:B:694:GLY:HA2	14	0.12
(2,352)	1:B:697:ILE:HG22	1:B:694:GLY:HA3	14	0.12
(2,352)	1:B:697:ILE:HG23	1:B:694:GLY:HA2	14	0.12
(2,352)	1:B:697:ILE:HG23	1:B:694:GLY:HA3	14	0.12
(2,340)	1:B:693:ILE:HG21	1:B:696:ARG:HG2	3	0.12
(2,340)	1:B:693:ILE:HG21	1:B:696:ARG:HG3	3	0.12
(2,340)	1:B:693:ILE:HG22	1:B:696:ARG:HG2	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,340)	1:B:693:ILE:HG22	1:B:696:ARG:HG3	3	0.12
(2,340)	1:B:693:ILE:HG23	1:B:696:ARG:HG2	3	0.12
(2,340)	1:B:693:ILE:HG23	1:B:696:ARG:HG3	3	0.12
(2,336)	1:B:693:ILE:HD11	1:B:697:ILE:H	12	0.12
(2,336)	1:B:693:ILE:HD12	1:B:697:ILE:H	12	0.12
(2,336)	1:B:693:ILE:HD13	1:B:697:ILE:H	12	0.12
(2,330)	1:B:692:LEU:HD11	1:B:689:VAL:HA	3	0.12
(2,330)	1:B:692:LEU:HD12	1:B:689:VAL:HA	3	0.12
(2,330)	1:B:692:LEU:HD13	1:B:689:VAL:HA	3	0.12
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG21	5	0.12
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG22	5	0.12
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG23	5	0.12
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG21	5	0.12
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG22	5	0.12
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG23	5	0.12
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG21	5	0.12
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG22	5	0.12
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG23	5	0.12
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG21	13	0.12
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG22	13	0.12
(2,33)	1:A:687:ILE:HG21	1:B:689:VAL:HG23	13	0.12
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG21	13	0.12
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG22	13	0.12
(2,33)	1:A:687:ILE:HG22	1:B:689:VAL:HG23	13	0.12
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG21	13	0.12
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG22	13	0.12
(2,33)	1:A:687:ILE:HG23	1:B:689:VAL:HG23	13	0.12
(2,327)	1:B:689:VAL:HG21	1:B:685:PHE:HE1	14	0.12
(2,327)	1:B:689:VAL:HG21	1:B:685:PHE:HE2	14	0.12
(2,327)	1:B:689:VAL:HG22	1:B:685:PHE:HE1	14	0.12
(2,327)	1:B:689:VAL:HG22	1:B:685:PHE:HE2	14	0.12
(2,327)	1:B:689:VAL:HG23	1:B:685:PHE:HE1	14	0.12
(2,327)	1:B:689:VAL:HG23	1:B:685:PHE:HE2	14	0.12
(2,324)	1:B:688:ILE:HG21	1:B:692:LEU:HG	4	0.12
(2,324)	1:B:688:ILE:HG22	1:B:692:LEU:HG	4	0.12
(2,324)	1:B:688:ILE:HG23	1:B:692:LEU:HG	4	0.12
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD11	15	0.12
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD12	15	0.12
(2,30)	1:A:687:ILE:H	1:B:686:ILE:HD13	15	0.12
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB2	8	0.12
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB3	8	0.12
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB2	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB3	8	0.12
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB2	8	0.12
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB3	8	0.12
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB2	11	0.12
(2,297)	1:B:682:ILE:HD11	1:B:685:PHE:HB3	11	0.12
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB2	11	0.12
(2,297)	1:B:682:ILE:HD12	1:B:685:PHE:HB3	11	0.12
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB2	11	0.12
(2,297)	1:B:682:ILE:HD13	1:B:685:PHE:HB3	11	0.12
(2,296)	1:B:682:ILE:HD11	1:B:681:TYR:H	7	0.12
(2,296)	1:B:682:ILE:HD12	1:B:681:TYR:H	7	0.12
(2,296)	1:B:682:ILE:HD13	1:B:681:TYR:H	7	0.12
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD11	13	0.12
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD12	13	0.12
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD13	13	0.12
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD11	12	0.12
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD12	12	0.12
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD13	12	0.12
(2,280)	1:B:676:THR:HG21	1:B:681:TYR:HH	4	0.12
(2,280)	1:B:676:THR:HG22	1:B:681:TYR:HH	4	0.12
(2,280)	1:B:676:THR:HG23	1:B:681:TYR:HH	4	0.12
(2,276)	1:B:676:THR:HG21	1:B:666:TRP:HZ3	1	0.12
(2,276)	1:B:676:THR:HG22	1:B:666:TRP:HZ3	1	0.12
(2,276)	1:B:676:THR:HG23	1:B:666:TRP:HZ3	1	0.12
(2,276)	1:B:676:THR:HG21	1:B:666:TRP:HZ3	5	0.12
(2,276)	1:B:676:THR:HG22	1:B:666:TRP:HZ3	5	0.12
(2,276)	1:B:676:THR:HG23	1:B:666:TRP:HZ3	5	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD11	3	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD12	3	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD13	3	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD21	3	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD22	3	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD23	3	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD11	4	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD12	4	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD13	4	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD21	4	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD22	4	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD23	4	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD11	6	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD12	6	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD13	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD21	6	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD22	6	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD23	6	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD11	14	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD12	14	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD13	14	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD21	14	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD22	14	0.12
(2,269)	1:B:672:TRP:HE1	1:B:669:LEU:HD23	14	0.12
(2,268)	1:B:672:TRP:H	1:B:673:PHE:H	1	0.12
(2,259)	1:B:670:TRP:H	1:B:667:ALA:HA	13	0.12
(2,242)	1:B:667:ALA:H	1:B:664:ASP:HA	11	0.12
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG12	12	0.12
(2,202)	1:B:827:ASP:H	1:B:820:ILE:HG13	12	0.12
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD11	8	0.12
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD12	8	0.12
(2,198)	1:A:826:THR:H	1:A:820:ILE:HD13	8	0.12
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD11	8	0.12
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD12	8	0.12
(2,197)	1:A:826:THR:H	1:A:820:ILE:HD13	8	0.12
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD11	7	0.12
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD12	7	0.12
(2,196)	1:B:826:THR:H	1:B:820:ILE:HD13	7	0.12
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG2	14	0.12
(2,190)	1:B:816:ASN:H	1:B:831:GLU:HG3	14	0.12
(2,19)	1:B:678:TRP:HE1	1:A:683:ARG:HE	11	0.12
(2,186)	1:A:808:LYS:H	1:A:838:ARG:HD2	2	0.12
(2,186)	1:A:808:LYS:H	1:A:838:ARG:HD3	2	0.12
(2,186)	1:A:808:LYS:H	1:A:838:ARG:HD2	10	0.12
(2,186)	1:A:808:LYS:H	1:A:838:ARG:HD3	10	0.12
(2,185)	1:A:808:LYS:H	1:A:838:ARG:HD2	2	0.12
(2,185)	1:A:808:LYS:H	1:A:838:ARG:HD3	2	0.12
(2,185)	1:A:808:LYS:H	1:A:838:ARG:HD2	10	0.12
(2,185)	1:A:808:LYS:H	1:A:838:ARG:HD3	10	0.12
(2,183)	1:A:806:GLU:H	1:B:772:ARG:HE	3	0.12
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG12	15	0.12
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG13	15	0.12
(2,153)	1:A:792:ALA:H	1:B:752:SER:HB2	10	0.12
(2,153)	1:A:792:ALA:H	1:B:752:SER:HB3	10	0.12
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG11	1	0.12
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG12	1	0.12
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG13	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG21	1	0.12
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG22	1	0.12
(2,1478)	1:A:826:THR:H	1:A:822:VAL:HG23	1	0.12
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD11	6	0.12
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD12	6	0.12
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD13	6	0.12
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD11	11	0.12
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD12	11	0.12
(2,1466)	1:A:796:TRP:HE1	1:A:799:LEU:HD13	11	0.12
(2,1465)	1:A:796:TRP:HE1	1:A:796:TRP:H	8	0.12
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD11	5	0.12
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD12	5	0.12
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD13	5	0.12
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD21	5	0.12
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD22	5	0.12
(2,1463)	1:A:790:TRP:HE1	1:A:793:LEU:HD23	5	0.12
(2,1439)	1:A:783:GLU:H	1:A:782:VAL:HA	14	0.12
(2,1437)	1:A:783:GLU:H	1:A:780:ARG:HA	2	0.12
(2,1426)	1:A:781:ILE:H	1:A:780:ARG:HA	1	0.12
(2,1401)	1:A:776:LEU:HD11	1:A:773:ASP:HB2	15	0.12
(2,1401)	1:A:776:LEU:HD11	1:A:773:ASP:HB3	15	0.12
(2,1401)	1:A:776:LEU:HD12	1:A:773:ASP:HB2	15	0.12
(2,1401)	1:A:776:LEU:HD12	1:A:773:ASP:HB3	15	0.12
(2,1401)	1:A:776:LEU:HD13	1:A:773:ASP:HB2	15	0.12
(2,1401)	1:A:776:LEU:HD13	1:A:773:ASP:HB3	15	0.12
(2,1376)	1:A:771:LEU:HD11	1:A:768:TYR:HE1	15	0.12
(2,1376)	1:A:771:LEU:HD11	1:A:768:TYR:HE2	15	0.12
(2,1376)	1:A:771:LEU:HD12	1:A:768:TYR:HE1	15	0.12
(2,1376)	1:A:771:LEU:HD12	1:A:768:TYR:HE2	15	0.12
(2,1376)	1:A:771:LEU:HD13	1:A:768:TYR:HE1	15	0.12
(2,1376)	1:A:771:LEU:HD13	1:A:768:TYR:HE2	15	0.12
(2,1371)	1:A:763:LEU:HD21	1:A:771:LEU:HB2	9	0.12
(2,1371)	1:A:763:LEU:HD21	1:A:771:LEU:HB3	9	0.12
(2,1371)	1:A:763:LEU:HD22	1:A:771:LEU:HB2	9	0.12
(2,1371)	1:A:763:LEU:HD22	1:A:771:LEU:HB3	9	0.12
(2,1371)	1:A:763:LEU:HD23	1:A:771:LEU:HB2	9	0.12
(2,1371)	1:A:763:LEU:HD23	1:A:771:LEU:HB3	9	0.12
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB1	11	0.12
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB2	11	0.12
(2,1359)	1:A:758:ASP:H	1:A:754:ALA:HB3	11	0.12
(2,1352)	1:A:755:LEU:H	1:A:752:SER:HA	8	0.12
(2,1351)	1:A:755:LEU:H	1:A:751:GLY:HA2	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1351)	1:A:755:LEU:H	1:A:751:GLY:HA3	14	0.12
(2,1350)	1:A:754:ALA:HB1	1:A:758:ASP:H	11	0.12
(2,1350)	1:A:754:ALA:HB2	1:A:758:ASP:H	11	0.12
(2,1350)	1:A:754:ALA:HB3	1:A:758:ASP:H	11	0.12
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	9	0.12
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	9	0.12
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	9	0.12
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	9	0.12
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	9	0.12
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	9	0.12
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB2	14	0.12
(2,1343)	1:A:754:ALA:H	1:A:750:ASN:HB3	14	0.12
(2,1329)	1:A:748:LEU:H	1:A:745:SER:HA	10	0.12
(2,1315)	1:A:746:ILE:H	1:A:743:ASP:HB2	8	0.12
(2,1315)	1:A:746:ILE:H	1:A:743:ASP:HB3	8	0.12
(2,13)	1:B:666:TRP:HE1	1:A:666:TRP:HD1	11	0.12
(2,1279)	1:A:708:VAL:HG21	1:A:707:ARG:HD2	6	0.12
(2,1279)	1:A:708:VAL:HG21	1:A:707:ARG:HD3	6	0.12
(2,1279)	1:A:708:VAL:HG22	1:A:707:ARG:HD2	6	0.12
(2,1279)	1:A:708:VAL:HG22	1:A:707:ARG:HD3	6	0.12
(2,1279)	1:A:708:VAL:HG23	1:A:707:ARG:HD2	6	0.12
(2,1279)	1:A:708:VAL:HG23	1:A:707:ARG:HD3	6	0.12
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD11	2	0.12
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD12	2	0.12
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD13	2	0.12
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD21	2	0.12
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD22	2	0.12
(2,1272)	1:A:707:ARG:HE	1:A:704:LEU:HD23	2	0.12
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	2	0.12
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	2	0.12
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	2	0.12
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	2	0.12
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	2	0.12
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	2	0.12
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB2	14	0.12
(2,1256)	1:A:705:VAL:HG21	1:A:706:ASN:HB3	14	0.12
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB2	14	0.12
(2,1256)	1:A:705:VAL:HG22	1:A:706:ASN:HB3	14	0.12
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB2	14	0.12
(2,1256)	1:A:705:VAL:HG23	1:A:706:ASN:HB3	14	0.12
(2,1255)	1:A:705:VAL:HG21	1:A:702:LEU:HG	10	0.12
(2,1255)	1:A:705:VAL:HG22	1:A:702:LEU:HG	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1255)	1:A:705:VAL:HG23	1:A:702:LEU:HG	10	0.12
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	2	0.12
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	2	0.12
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	2	0.12
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	2	0.12
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	2	0.12
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	2	0.12
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	7	0.12
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	7	0.12
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	7	0.12
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	7	0.12
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	7	0.12
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	7	0.12
(2,1205)	1:A:698:VAL:HG11	1:A:695:LEU:HA	11	0.12
(2,1205)	1:A:698:VAL:HG12	1:A:695:LEU:HA	11	0.12
(2,1205)	1:A:698:VAL:HG13	1:A:695:LEU:HA	11	0.12
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB1	11	0.12
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB2	11	0.12
(2,1204)	1:A:697:ILE:HG21	1:A:700:ALA:HB3	11	0.12
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB1	11	0.12
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB2	11	0.12
(2,1204)	1:A:697:ILE:HG22	1:A:700:ALA:HB3	11	0.12
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB1	11	0.12
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB2	11	0.12
(2,1204)	1:A:697:ILE:HG23	1:A:700:ALA:HB3	11	0.12
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD2	14	0.12
(2,1194)	1:A:695:LEU:HD21	1:A:696:ARG:HD3	14	0.12
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD2	14	0.12
(2,1194)	1:A:695:LEU:HD22	1:A:696:ARG:HD3	14	0.12
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD2	14	0.12
(2,1194)	1:A:695:LEU:HD23	1:A:696:ARG:HD3	14	0.12
(2,1193)	1:A:695:LEU:HD11	1:A:691:SER:HB2	6	0.12
(2,1193)	1:A:695:LEU:HD11	1:A:691:SER:HB3	6	0.12
(2,1193)	1:A:695:LEU:HD12	1:A:691:SER:HB2	6	0.12
(2,1193)	1:A:695:LEU:HD12	1:A:691:SER:HB3	6	0.12
(2,1193)	1:A:695:LEU:HD13	1:A:691:SER:HB2	6	0.12
(2,1193)	1:A:695:LEU:HD13	1:A:691:SER:HB3	6	0.12
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD1	8	0.12
(2,1155)	1:A:684:ILE:HG21	1:A:685:PHE:HD2	8	0.12
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD1	8	0.12
(2,1155)	1:A:684:ILE:HG22	1:A:685:PHE:HD2	8	0.12
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD1	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1155)	1:A:684:ILE:HG23	1:A:685:PHE:HD2	8	0.12
(2,1143)	1:A:682:ILE:HG21	1:A:679:LEU:H	8	0.12
(2,1143)	1:A:682:ILE:HG22	1:A:679:LEU:H	8	0.12
(2,1143)	1:A:682:ILE:HG23	1:A:679:LEU:H	8	0.12
(2,1140)	1:A:680:TRP:HE1	1:A:684:ILE:HD11	15	0.12
(2,1140)	1:A:680:TRP:HE1	1:A:684:ILE:HD12	15	0.12
(2,1140)	1:A:680:TRP:HE1	1:A:684:ILE:HD13	15	0.12
(2,1136)	1:A:678:TRP:HE1	1:A:682:ILE:H	12	0.12
(2,1126)	1:A:676:THR:HG21	1:A:666:TRP:HZ3	6	0.12
(2,1126)	1:A:676:THR:HG22	1:A:666:TRP:HZ3	6	0.12
(2,1126)	1:A:676:THR:HG23	1:A:666:TRP:HZ3	6	0.12
(2,1118)	1:A:672:TRP:H	1:A:673:PHE:H	15	0.12
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD11	6	0.12
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD12	6	0.12
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD13	6	0.12
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD21	6	0.12
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD22	6	0.12
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD23	6	0.12
(2,1108)	1:A:669:LEU:HD11	1:A:672:TRP:HZ3	10	0.12
(2,1108)	1:A:669:LEU:HD12	1:A:672:TRP:HZ3	10	0.12
(2,1108)	1:A:669:LEU:HD13	1:A:672:TRP:HZ3	10	0.12
(2,1108)	1:A:669:LEU:HD21	1:A:672:TRP:HZ3	10	0.12
(2,1108)	1:A:669:LEU:HD22	1:A:672:TRP:HZ3	10	0.12
(2,1108)	1:A:669:LEU:HD23	1:A:672:TRP:HZ3	10	0.12
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD11	9	0.12
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD12	9	0.12
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD13	9	0.12
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD21	9	0.12
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD22	9	0.12
(2,1098)	1:A:667:ALA:HB1	1:A:663:LEU:HD23	9	0.12
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD11	9	0.12
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD12	9	0.12
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD13	9	0.12
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD21	9	0.12
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD22	9	0.12
(2,1098)	1:A:667:ALA:HB2	1:A:663:LEU:HD23	9	0.12
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD11	9	0.12
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD12	9	0.12
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD13	9	0.12
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD21	9	0.12
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD22	9	0.12
(2,1098)	1:A:667:ALA:HB3	1:A:663:LEU:HD23	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1097)	1:A:667:ALA:HB1	1:A:664:ASP:HA	3	0.12
(2,1097)	1:A:667:ALA:HB2	1:A:664:ASP:HA	3	0.12
(2,1097)	1:A:667:ALA:HB3	1:A:664:ASP:HA	3	0.12
(2,1097)	1:A:667:ALA:HB1	1:A:664:ASP:HA	13	0.12
(2,1097)	1:A:667:ALA:HB2	1:A:664:ASP:HA	13	0.12
(2,1097)	1:A:667:ALA:HB3	1:A:664:ASP:HA	13	0.12
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD2	5	0.12
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD3	5	0.12
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD2	5	0.12
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD3	5	0.12
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD2	5	0.12
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD3	5	0.12
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG11	1	0.12
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG12	1	0.12
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG13	1	0.12
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG21	1	0.12
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG22	1	0.12
(2,1053)	1:A:826:THR:H	1:A:822:VAL:HG23	1	0.12
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD11	6	0.12
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD12	6	0.12
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD13	6	0.12
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD11	11	0.12
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD12	11	0.12
(2,1041)	1:A:796:TRP:HE1	1:A:799:LEU:HD13	11	0.12
(2,1040)	1:A:796:TRP:HE1	1:A:796:TRP:H	8	0.12
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD11	5	0.12
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD12	5	0.12
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD13	5	0.12
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD21	5	0.12
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD22	5	0.12
(2,1038)	1:A:790:TRP:HE1	1:A:793:LEU:HD23	5	0.12
(2,1014)	1:A:783:GLU:H	1:A:782:VAL:HA	14	0.12
(2,1012)	1:A:783:GLU:H	1:A:780:ARG:HA	2	0.12
(2,1001)	1:A:781:ILE:H	1:A:780:ARG:HA	1	0.12
(1,98)	1:B:795:TYR:O	1:B:799:LEU:N	5	0.12
(1,91)	1:B:792:ALA:O	1:B:796:TRP:H	1	0.12
(1,91)	1:B:792:ALA:O	1:B:796:TRP:H	4	0.12
(1,85)	1:B:850:GLY:O	1:B:854:ILE:H	8	0.12
(1,85)	1:B:850:GLY:O	1:B:854:ILE:H	11	0.12
(1,77)	1:B:846:ARG:O	1:B:850:GLY:H	10	0.12
(1,71)	1:B:835:GLY:O	1:B:839:ALA:H	11	0.12
(1,67)	1:B:833:VAL:O	1:B:837:SER:H	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,61)	1:B:830:ILE:O	1:B:834:GLN:H	2	0.12
(1,61)	1:B:830:ILE:O	1:B:834:GLN:H	5	0.12
(1,56)	1:B:827:ASP:O	1:B:831:GLU:N	6	0.12
(1,53)	1:B:826:THR:O	1:B:830:ILE:H	15	0.12
(1,5)	1:B:792:ALA:O	1:B:796:TRP:H	1	0.12
(1,5)	1:B:792:ALA:O	1:B:796:TRP:H	4	0.12
(1,47)	1:B:813:SER:O	1:B:817:ALA:H	7	0.12
(1,41)	1:B:810:SER:O	1:B:814:LEU:H	8	0.12
(1,257)	1:B:850:GLY:O	1:B:854:ILE:H	8	0.12
(1,257)	1:B:850:GLY:O	1:B:854:ILE:H	11	0.12
(1,249)	1:B:846:ARG:O	1:B:850:GLY:H	10	0.12
(1,243)	1:B:835:GLY:O	1:B:839:ALA:H	11	0.12
(1,239)	1:B:833:VAL:O	1:B:837:SER:H	5	0.12
(1,233)	1:B:830:ILE:O	1:B:834:GLN:H	2	0.12
(1,233)	1:B:830:ILE:O	1:B:834:GLN:H	5	0.12
(1,23)	1:B:801:GLN:O	1:B:805:GLN:H	1	0.12
(1,23)	1:B:801:GLN:O	1:B:805:GLN:H	2	0.12
(1,228)	1:B:827:ASP:O	1:B:831:GLU:N	6	0.12
(1,225)	1:B:826:THR:O	1:B:830:ILE:H	15	0.12
(1,219)	1:B:813:SER:O	1:B:817:ALA:H	7	0.12
(1,213)	1:B:810:SER:O	1:B:814:LEU:H	8	0.12
(1,20)	1:B:799:LEU:O	1:B:803:TRP:N	6	0.12
(1,20)	1:B:799:LEU:O	1:B:803:TRP:N	7	0.12
(1,195)	1:B:801:GLN:O	1:B:805:GLN:H	1	0.12
(1,195)	1:B:801:GLN:O	1:B:805:GLN:H	2	0.12
(1,192)	1:B:799:LEU:O	1:B:803:TRP:N	6	0.12
(1,192)	1:B:799:LEU:O	1:B:803:TRP:N	7	0.12
(1,189)	1:B:798:ASN:O	1:B:802:TYR:H	10	0.12
(1,187)	1:B:797:TRP:O	1:B:801:GLN:H	9	0.12
(1,187)	1:B:797:TRP:O	1:B:801:GLN:H	13	0.12
(1,184)	1:B:795:TYR:O	1:B:799:LEU:N	5	0.12
(1,177)	1:B:792:ALA:O	1:B:796:TRP:H	1	0.12
(1,177)	1:B:792:ALA:O	1:B:796:TRP:H	4	0.12
(1,171)	1:B:850:GLY:O	1:B:854:ILE:H	8	0.12
(1,171)	1:B:850:GLY:O	1:B:854:ILE:H	11	0.12
(1,17)	1:B:798:ASN:O	1:B:802:TYR:H	10	0.12
(1,163)	1:B:846:ARG:O	1:B:850:GLY:H	10	0.12
(1,157)	1:B:835:GLY:O	1:B:839:ALA:H	11	0.12
(1,153)	1:B:833:VAL:O	1:B:837:SER:H	5	0.12
(1,15)	1:B:797:TRP:O	1:B:801:GLN:H	9	0.12
(1,15)	1:B:797:TRP:O	1:B:801:GLN:H	13	0.12
(1,147)	1:B:830:ILE:O	1:B:834:GLN:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:B:830:ILE:O	1:B:834:GLN:H	5	0.12
(1,142)	1:B:827:ASP:O	1:B:831:GLU:N	6	0.12
(1,139)	1:B:826:THR:O	1:B:830:ILE:H	15	0.12
(1,133)	1:B:813:SER:O	1:B:817:ALA:H	7	0.12
(1,127)	1:B:810:SER:O	1:B:814:LEU:H	8	0.12
(1,12)	1:B:795:TYR:O	1:B:799:LEU:N	5	0.12
(1,109)	1:B:801:GLN:O	1:B:805:GLN:H	1	0.12
(1,109)	1:B:801:GLN:O	1:B:805:GLN:H	2	0.12
(1,106)	1:B:799:LEU:O	1:B:803:TRP:N	6	0.12
(1,106)	1:B:799:LEU:O	1:B:803:TRP:N	7	0.12
(1,103)	1:B:798:ASN:O	1:B:802:TYR:H	10	0.12
(1,101)	1:B:797:TRP:O	1:B:801:GLN:H	9	0.12
(1,101)	1:B:797:TRP:O	1:B:801:GLN:H	13	0.12
(2,966)	1:A:775:LEU:H	1:A:774:LEU:HA	7	0.11
(2,96)	1:A:755:LEU:HD11	1:B:710:GLN:HE21	5	0.11
(2,96)	1:A:755:LEU:HD11	1:B:710:GLN:HE22	5	0.11
(2,96)	1:A:755:LEU:HD12	1:B:710:GLN:HE21	5	0.11
(2,96)	1:A:755:LEU:HD12	1:B:710:GLN:HE22	5	0.11
(2,96)	1:A:755:LEU:HD13	1:B:710:GLN:HE21	5	0.11
(2,96)	1:A:755:LEU:HD13	1:B:710:GLN:HE22	5	0.11
(2,96)	1:A:755:LEU:HD11	1:B:710:GLN:HE21	10	0.11
(2,96)	1:A:755:LEU:HD11	1:B:710:GLN:HE22	10	0.11
(2,96)	1:A:755:LEU:HD12	1:B:710:GLN:HE21	10	0.11
(2,96)	1:A:755:LEU:HD12	1:B:710:GLN:HE22	10	0.11
(2,96)	1:A:755:LEU:HD13	1:B:710:GLN:HE21	10	0.11
(2,96)	1:A:755:LEU:HD13	1:B:710:GLN:HE22	10	0.11
(2,939)	1:A:760:LEU:HD11	1:A:756:ILE:HG12	2	0.11
(2,939)	1:A:760:LEU:HD11	1:A:756:ILE:HG13	2	0.11
(2,939)	1:A:760:LEU:HD12	1:A:756:ILE:HG12	2	0.11
(2,939)	1:A:760:LEU:HD12	1:A:756:ILE:HG13	2	0.11
(2,939)	1:A:760:LEU:HD13	1:A:756:ILE:HG12	2	0.11
(2,939)	1:A:760:LEU:HD13	1:A:756:ILE:HG13	2	0.11
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	6	0.11
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	6	0.11
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	6	0.11
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	6	0.11
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	6	0.11
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	6	0.11
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	10	0.11
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	10	0.11
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	10	0.11
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	10	0.11
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	10	0.11
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	13	0.11
(2,923)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	13	0.11
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	13	0.11
(2,923)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	13	0.11
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	13	0.11
(2,923)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	13	0.11
(2,904)	1:A:748:LEU:H	1:A:745:SER:HA	4	0.11
(2,904)	1:A:748:LEU:H	1:A:745:SER:HA	11	0.11
(2,897)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	2	0.11
(2,897)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	2	0.11
(2,897)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	2	0.11
(2,897)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	9	0.11
(2,897)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	9	0.11
(2,897)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	9	0.11
(2,869)	1:A:710:GLN:H	1:A:710:GLN:HB3	11	0.11
(2,865)	1:A:710:GLN:H	1:A:709:ARG:HA	13	0.11
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB2	14	0.11
(2,855)	1:A:708:VAL:HG21	1:A:745:SER:HB3	14	0.11
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB2	14	0.11
(2,855)	1:A:708:VAL:HG22	1:A:745:SER:HB3	14	0.11
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB2	14	0.11
(2,855)	1:A:708:VAL:HG23	1:A:745:SER:HB3	14	0.11
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD2	5	0.11
(2,846)	1:A:707:ARG:H	1:A:707:ARG:HD3	5	0.11
(2,839)	1:A:707:ARG:H	1:A:704:LEU:HA	10	0.11
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB2	13	0.11
(2,838)	1:A:707:ARG:H	1:A:703:SER:HB3	13	0.11
(2,821)	1:A:705:VAL:H	1:A:702:LEU:HA	4	0.11
(2,821)	1:A:705:VAL:H	1:A:702:LEU:HA	13	0.11
(2,821)	1:A:705:VAL:H	1:A:702:LEU:HA	14	0.11
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	10	0.11
(2,818)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	10	0.11
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	10	0.11
(2,818)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	10	0.11
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	10	0.11
(2,818)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	10	0.11
(2,799)	1:A:702:LEU:H	1:A:699:PHE:HA	11	0.11
(2,798)	1:A:701:VAL:HG21	1:A:698:VAL:HA	15	0.11
(2,798)	1:A:701:VAL:HG22	1:A:698:VAL:HA	15	0.11
(2,798)	1:A:701:VAL:HG23	1:A:698:VAL:HA	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,781)	1:A:698:VAL:HG11	1:A:695:LEU:HG	7	0.11
(2,781)	1:A:698:VAL:HG12	1:A:695:LEU:HG	7	0.11
(2,781)	1:A:698:VAL:HG13	1:A:695:LEU:HG	7	0.11
(2,777)	1:A:697:ILE:HG21	1:A:694:GLY:HA2	7	0.11
(2,777)	1:A:697:ILE:HG21	1:A:694:GLY:HA3	7	0.11
(2,777)	1:A:697:ILE:HG22	1:A:694:GLY:HA2	7	0.11
(2,777)	1:A:697:ILE:HG22	1:A:694:GLY:HA3	7	0.11
(2,777)	1:A:697:ILE:HG23	1:A:694:GLY:HA2	7	0.11
(2,777)	1:A:697:ILE:HG23	1:A:694:GLY:HA3	7	0.11
(2,770)	1:A:695:LEU:HD21	1:A:698:VAL:HB	6	0.11
(2,770)	1:A:695:LEU:HD22	1:A:698:VAL:HB	6	0.11
(2,770)	1:A:695:LEU:HD23	1:A:698:VAL:HB	6	0.11
(2,763)	1:A:693:ILE:HG21	1:A:693:ILE:H	13	0.11
(2,763)	1:A:693:ILE:HG22	1:A:693:ILE:H	13	0.11
(2,763)	1:A:693:ILE:HG23	1:A:693:ILE:H	13	0.11
(2,758)	1:A:692:LEU:HD11	1:A:696:ARG:HH11	13	0.11
(2,758)	1:A:692:LEU:HD11	1:A:696:ARG:HH12	13	0.11
(2,758)	1:A:692:LEU:HD11	1:A:696:ARG:HH21	13	0.11
(2,758)	1:A:692:LEU:HD11	1:A:696:ARG:HH22	13	0.11
(2,758)	1:A:692:LEU:HD12	1:A:696:ARG:HH11	13	0.11
(2,758)	1:A:692:LEU:HD12	1:A:696:ARG:HH12	13	0.11
(2,758)	1:A:692:LEU:HD12	1:A:696:ARG:HH21	13	0.11
(2,758)	1:A:692:LEU:HD12	1:A:696:ARG:HH22	13	0.11
(2,758)	1:A:692:LEU:HD13	1:A:696:ARG:HH11	13	0.11
(2,758)	1:A:692:LEU:HD13	1:A:696:ARG:HH12	13	0.11
(2,758)	1:A:692:LEU:HD13	1:A:696:ARG:HH21	13	0.11
(2,758)	1:A:692:LEU:HD13	1:A:696:ARG:HH22	13	0.11
(2,757)	1:A:692:LEU:HD11	1:A:691:SER:HB2	8	0.11
(2,757)	1:A:692:LEU:HD11	1:A:691:SER:HB3	8	0.11
(2,757)	1:A:692:LEU:HD12	1:A:691:SER:HB2	8	0.11
(2,757)	1:A:692:LEU:HD12	1:A:691:SER:HB3	8	0.11
(2,757)	1:A:692:LEU:HD13	1:A:691:SER:HB2	8	0.11
(2,757)	1:A:692:LEU:HD13	1:A:691:SER:HB3	8	0.11
(2,755)	1:A:692:LEU:HD11	1:A:689:VAL:HA	11	0.11
(2,755)	1:A:692:LEU:HD12	1:A:689:VAL:HA	11	0.11
(2,755)	1:A:692:LEU:HD13	1:A:689:VAL:HA	11	0.11
(2,752)	1:A:689:VAL:HG21	1:A:685:PHE:HE1	6	0.11
(2,752)	1:A:689:VAL:HG21	1:A:685:PHE:HE2	6	0.11
(2,752)	1:A:689:VAL:HG22	1:A:685:PHE:HE1	6	0.11
(2,752)	1:A:689:VAL:HG22	1:A:685:PHE:HE2	6	0.11
(2,752)	1:A:689:VAL:HG23	1:A:685:PHE:HE1	6	0.11
(2,752)	1:A:689:VAL:HG23	1:A:685:PHE:HE2	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE1	14	0.11
(2,75)	1:A:708:VAL:HG21	1:B:712:TYR:HE2	14	0.11
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE1	14	0.11
(2,75)	1:A:708:VAL:HG22	1:B:712:TYR:HE2	14	0.11
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE1	14	0.11
(2,75)	1:A:708:VAL:HG23	1:B:712:TYR:HE2	14	0.11
(2,748)	1:A:688:ILE:HD11	1:A:684:ILE:HD11	14	0.11
(2,748)	1:A:688:ILE:HD11	1:A:684:ILE:HD12	14	0.11
(2,748)	1:A:688:ILE:HD11	1:A:684:ILE:HD13	14	0.11
(2,748)	1:A:688:ILE:HD12	1:A:684:ILE:HD11	14	0.11
(2,748)	1:A:688:ILE:HD12	1:A:684:ILE:HD12	14	0.11
(2,748)	1:A:688:ILE:HD12	1:A:684:ILE:HD13	14	0.11
(2,748)	1:A:688:ILE:HD13	1:A:684:ILE:HD11	14	0.11
(2,748)	1:A:688:ILE:HD13	1:A:684:ILE:HD12	14	0.11
(2,748)	1:A:688:ILE:HD13	1:A:684:ILE:HD13	14	0.11
(2,743)	1:A:686:ILE:HD11	1:A:685:PHE:H	13	0.11
(2,743)	1:A:686:ILE:HD12	1:A:685:PHE:H	13	0.11
(2,743)	1:A:686:ILE:HD13	1:A:685:PHE:H	13	0.11
(2,742)	1:A:686:ILE:HD11	1:A:683:ARG:HA	13	0.11
(2,742)	1:A:686:ILE:HD12	1:A:683:ARG:HA	13	0.11
(2,742)	1:A:686:ILE:HD13	1:A:683:ARG:HA	13	0.11
(2,726)	1:A:684:ILE:HD11	1:A:681:TYR:HA	15	0.11
(2,726)	1:A:684:ILE:HD12	1:A:681:TYR:HA	15	0.11
(2,726)	1:A:684:ILE:HD13	1:A:681:TYR:HA	15	0.11
(2,722)	1:A:682:ILE:HD11	1:A:685:PHE:HB2	5	0.11
(2,722)	1:A:682:ILE:HD11	1:A:685:PHE:HB3	5	0.11
(2,722)	1:A:682:ILE:HD12	1:A:685:PHE:HB2	5	0.11
(2,722)	1:A:682:ILE:HD12	1:A:685:PHE:HB3	5	0.11
(2,722)	1:A:682:ILE:HD13	1:A:685:PHE:HB2	5	0.11
(2,722)	1:A:682:ILE:HD13	1:A:685:PHE:HB3	5	0.11
(2,722)	1:A:682:ILE:HD11	1:A:685:PHE:HB2	10	0.11
(2,722)	1:A:682:ILE:HD11	1:A:685:PHE:HB3	10	0.11
(2,722)	1:A:682:ILE:HD12	1:A:685:PHE:HB2	10	0.11
(2,722)	1:A:682:ILE:HD12	1:A:685:PHE:HB3	10	0.11
(2,722)	1:A:682:ILE:HD13	1:A:685:PHE:HB2	10	0.11
(2,722)	1:A:682:ILE:HD13	1:A:685:PHE:HB3	10	0.11
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB2	8	0.11
(2,72)	1:A:708:VAL:HG21	1:B:712:TYR:HB3	8	0.11
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB2	8	0.11
(2,72)	1:A:708:VAL:HG22	1:B:712:TYR:HB3	8	0.11
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB2	8	0.11
(2,72)	1:A:708:VAL:HG23	1:B:712:TYR:HB3	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,717)	1:A:681:TYR:H	1:A:682:ILE:H	9	0.11
(2,717)	1:A:681:TYR:H	1:A:682:ILE:H	11	0.11
(2,714)	1:A:680:TRP:HE1	1:A:683:ARG:HH21	2	0.11
(2,714)	1:A:680:TRP:HE1	1:A:683:ARG:HH22	2	0.11
(2,713)	1:A:679:LEU:HD11	1:A:678:TRP:HH2	10	0.11
(2,713)	1:A:679:LEU:HD12	1:A:678:TRP:HH2	10	0.11
(2,713)	1:A:679:LEU:HD13	1:A:678:TRP:HH2	10	0.11
(2,713)	1:A:679:LEU:HD21	1:A:678:TRP:HH2	10	0.11
(2,713)	1:A:679:LEU:HD22	1:A:678:TRP:HH2	10	0.11
(2,713)	1:A:679:LEU:HD23	1:A:678:TRP:HH2	10	0.11
(2,711)	1:A:678:TRP:HE1	1:A:682:ILE:H	1	0.11
(2,694)	1:A:672:TRP:HE1	1:A:669:LEU:HD11	15	0.11
(2,694)	1:A:672:TRP:HE1	1:A:669:LEU:HD12	15	0.11
(2,694)	1:A:672:TRP:HE1	1:A:669:LEU:HD13	15	0.11
(2,694)	1:A:672:TRP:HE1	1:A:669:LEU:HD21	15	0.11
(2,694)	1:A:672:TRP:HE1	1:A:669:LEU:HD22	15	0.11
(2,694)	1:A:672:TRP:HE1	1:A:669:LEU:HD23	15	0.11
(2,69)	1:A:704:LEU:HD21	1:B:706:ASN:HB2	13	0.11
(2,69)	1:A:704:LEU:HD21	1:B:706:ASN:HB3	13	0.11
(2,69)	1:A:704:LEU:HD22	1:B:706:ASN:HB2	13	0.11
(2,69)	1:A:704:LEU:HD22	1:B:706:ASN:HB3	13	0.11
(2,69)	1:A:704:LEU:HD23	1:B:706:ASN:HB2	13	0.11
(2,69)	1:A:704:LEU:HD23	1:B:706:ASN:HB3	13	0.11
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD11	12	0.11
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD12	12	0.11
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD13	12	0.11
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD21	12	0.11
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD22	12	0.11
(2,689)	1:A:670:TRP:HE1	1:A:669:LEU:HD23	12	0.11
(2,688)	1:A:670:TRP:HE1	1:A:667:ALA:HB1	10	0.11
(2,688)	1:A:670:TRP:HE1	1:A:667:ALA:HB2	10	0.11
(2,688)	1:A:670:TRP:HE1	1:A:667:ALA:HB3	10	0.11
(2,683)	1:A:669:LEU:HD11	1:A:672:TRP:HZ3	1	0.11
(2,683)	1:A:669:LEU:HD12	1:A:672:TRP:HZ3	1	0.11
(2,683)	1:A:669:LEU:HD13	1:A:672:TRP:HZ3	1	0.11
(2,683)	1:A:669:LEU:HD21	1:A:672:TRP:HZ3	1	0.11
(2,683)	1:A:669:LEU:HD22	1:A:672:TRP:HZ3	1	0.11
(2,683)	1:A:669:LEU:HD23	1:A:672:TRP:HZ3	1	0.11
(2,683)	1:A:669:LEU:HD11	1:A:672:TRP:HZ3	8	0.11
(2,683)	1:A:669:LEU:HD12	1:A:672:TRP:HZ3	8	0.11
(2,683)	1:A:669:LEU:HD13	1:A:672:TRP:HZ3	8	0.11
(2,683)	1:A:669:LEU:HD21	1:A:672:TRP:HZ3	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,683)	1:A:669:LEU:HD22	1:A:672:TRP:HZ3	8	0.11
(2,683)	1:A:669:LEU:HD23	1:A:672:TRP:HZ3	8	0.11
(2,672)	1:A:667:ALA:HB1	1:A:664:ASP:HA	14	0.11
(2,672)	1:A:667:ALA:HB2	1:A:664:ASP:HA	14	0.11
(2,672)	1:A:667:ALA:HB3	1:A:664:ASP:HA	14	0.11
(2,672)	1:A:667:ALA:HB1	1:A:664:ASP:HA	15	0.11
(2,672)	1:A:667:ALA:HB2	1:A:664:ASP:HA	15	0.11
(2,672)	1:A:667:ALA:HB3	1:A:664:ASP:HA	15	0.11
(2,667)	1:A:667:ALA:H	1:A:664:ASP:HA	10	0.11
(2,666)	1:A:666:TRP:HE1	1:A:662:GLU:H	5	0.11
(2,653)	1:A:665:LYS:H	1:A:662:GLU:HA	7	0.11
(2,649)	1:A:664:ASP:H	1:A:663:LEU:HA	1	0.11
(2,649)	1:A:664:ASP:H	1:A:663:LEU:HA	6	0.11
(2,649)	1:A:664:ASP:H	1:A:663:LEU:HA	7	0.11
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG11	6	0.11
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG12	6	0.11
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG13	6	0.11
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG21	6	0.11
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG22	6	0.11
(2,628)	1:B:826:THR:H	1:B:822:VAL:HG23	6	0.11
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD21	14	0.11
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD22	14	0.11
(2,617)	1:B:796:TRP:HE1	1:B:799:LEU:HD23	14	0.11
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD11	1	0.11
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD12	1	0.11
(2,616)	1:B:796:TRP:HE1	1:B:799:LEU:HD13	1	0.11
(2,600)	1:B:784:LEU:HD21	1:B:781:ILE:HA	9	0.11
(2,600)	1:B:784:LEU:HD22	1:B:781:ILE:HA	9	0.11
(2,600)	1:B:784:LEU:HD23	1:B:781:ILE:HA	9	0.11
(2,589)	1:B:783:GLU:H	1:B:782:VAL:HA	13	0.11
(2,586)	1:B:782:VAL:HG21	1:B:779:THR:HA	1	0.11
(2,586)	1:B:782:VAL:HG22	1:B:779:THR:HA	1	0.11
(2,586)	1:B:782:VAL:HG23	1:B:779:THR:HA	1	0.11
(2,586)	1:B:782:VAL:HG21	1:B:779:THR:HA	10	0.11
(2,586)	1:B:782:VAL:HG22	1:B:779:THR:HA	10	0.11
(2,586)	1:B:782:VAL:HG23	1:B:779:THR:HA	10	0.11
(2,580)	1:B:781:ILE:HG21	1:B:778:VAL:HA	2	0.11
(2,580)	1:B:781:ILE:HG22	1:B:778:VAL:HA	2	0.11
(2,580)	1:B:781:ILE:HG23	1:B:778:VAL:HA	2	0.11
(2,576)	1:B:781:ILE:H	1:B:780:ARG:HA	3	0.11
(2,576)	1:B:781:ILE:H	1:B:780:ARG:HA	8	0.11
(2,576)	1:B:781:ILE:H	1:B:780:ARG:HA	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,576)	1:B:781:ILE:H	1:B:780:ARG:HA	14	0.11
(2,564)	1:B:778:VAL:HG21	1:B:775:LEU:HA	13	0.11
(2,564)	1:B:778:VAL:HG22	1:B:775:LEU:HA	13	0.11
(2,564)	1:B:778:VAL:HG23	1:B:775:LEU:HA	13	0.11
(2,558)	1:B:777:ILE:HG21	1:B:780:ARG:HD2	15	0.11
(2,558)	1:B:777:ILE:HG21	1:B:780:ARG:HD3	15	0.11
(2,558)	1:B:777:ILE:HG22	1:B:780:ARG:HD2	15	0.11
(2,558)	1:B:777:ILE:HG22	1:B:780:ARG:HD3	15	0.11
(2,558)	1:B:777:ILE:HG23	1:B:780:ARG:HD2	15	0.11
(2,558)	1:B:777:ILE:HG23	1:B:780:ARG:HD3	15	0.11
(2,551)	1:B:776:LEU:HD11	1:B:773:ASP:HB2	9	0.11
(2,551)	1:B:776:LEU:HD11	1:B:773:ASP:HB3	9	0.11
(2,551)	1:B:776:LEU:HD12	1:B:773:ASP:HB2	9	0.11
(2,551)	1:B:776:LEU:HD12	1:B:773:ASP:HB3	9	0.11
(2,551)	1:B:776:LEU:HD13	1:B:773:ASP:HB2	9	0.11
(2,551)	1:B:776:LEU:HD13	1:B:773:ASP:HB3	9	0.11
(2,545)	1:B:775:LEU:HD11	1:B:772:ARG:HA	11	0.11
(2,545)	1:B:775:LEU:HD12	1:B:772:ARG:HA	11	0.11
(2,545)	1:B:775:LEU:HD13	1:B:772:ARG:HA	11	0.11
(2,526)	1:B:771:LEU:HD11	1:B:768:TYR:HE1	5	0.11
(2,526)	1:B:771:LEU:HD11	1:B:768:TYR:HE2	5	0.11
(2,526)	1:B:771:LEU:HD12	1:B:768:TYR:HE1	5	0.11
(2,526)	1:B:771:LEU:HD12	1:B:768:TYR:HE2	5	0.11
(2,526)	1:B:771:LEU:HD13	1:B:768:TYR:HE1	5	0.11
(2,526)	1:B:771:LEU:HD13	1:B:768:TYR:HE2	5	0.11
(2,518)	1:B:763:LEU:HD11	1:B:759:ASP:HA	9	0.11
(2,518)	1:B:763:LEU:HD12	1:B:759:ASP:HA	9	0.11
(2,518)	1:B:763:LEU:HD13	1:B:759:ASP:HA	9	0.11
(2,506)	1:B:755:LEU:H	1:B:756:ILE:H	12	0.11
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB2	12	0.11
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB3	12	0.11
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB2	13	0.11
(2,493)	1:B:754:ALA:H	1:B:750:ASN:HB3	13	0.11
(2,483)	1:B:749:VAL:H	1:B:748:LEU:HA	12	0.11
(2,479)	1:B:748:LEU:H	1:B:745:SER:HA	14	0.11
(2,465)	1:B:746:ILE:H	1:B:743:ASP:HB2	5	0.11
(2,465)	1:B:746:ILE:H	1:B:743:ASP:HB3	5	0.11
(2,43)	1:B:693:ILE:H	1:A:693:ILE:HD11	4	0.11
(2,43)	1:B:693:ILE:H	1:A:693:ILE:HD12	4	0.11
(2,43)	1:B:693:ILE:H	1:A:693:ILE:HD13	4	0.11
(2,43)	1:B:693:ILE:H	1:A:693:ILE:HD11	10	0.11
(2,43)	1:B:693:ILE:H	1:A:693:ILE:HD12	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,43)	1:B:693:ILE:H	1:A:693:ILE:HD13	10	0.11
(2,429)	1:B:708:VAL:HG21	1:B:707:ARG:HD2	8	0.11
(2,429)	1:B:708:VAL:HG21	1:B:707:ARG:HD3	8	0.11
(2,429)	1:B:708:VAL:HG22	1:B:707:ARG:HD2	8	0.11
(2,429)	1:B:708:VAL:HG22	1:B:707:ARG:HD3	8	0.11
(2,429)	1:B:708:VAL:HG23	1:B:707:ARG:HD2	8	0.11
(2,429)	1:B:708:VAL:HG23	1:B:707:ARG:HD3	8	0.11
(2,421)	1:B:707:ARG:H	1:B:707:ARG:HD2	13	0.11
(2,421)	1:B:707:ARG:H	1:B:707:ARG:HD3	13	0.11
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB2	14	0.11
(2,413)	1:B:707:ARG:H	1:B:703:SER:HB3	14	0.11
(2,405)	1:B:705:VAL:HG21	1:B:702:LEU:HG	6	0.11
(2,405)	1:B:705:VAL:HG22	1:B:702:LEU:HG	6	0.11
(2,405)	1:B:705:VAL:HG23	1:B:702:LEU:HG	6	0.11
(2,405)	1:B:705:VAL:HG21	1:B:702:LEU:HG	7	0.11
(2,405)	1:B:705:VAL:HG22	1:B:702:LEU:HG	7	0.11
(2,405)	1:B:705:VAL:HG23	1:B:702:LEU:HG	7	0.11
(2,390)	1:B:704:LEU:H	1:B:704:LEU:HB3	12	0.11
(2,37)	1:B:692:LEU:HD21	1:A:694:GLY:H	2	0.11
(2,37)	1:B:692:LEU:HD22	1:A:694:GLY:H	2	0.11
(2,37)	1:B:692:LEU:HD23	1:A:694:GLY:H	2	0.11
(2,37)	1:B:692:LEU:HD21	1:A:694:GLY:H	5	0.11
(2,37)	1:B:692:LEU:HD22	1:A:694:GLY:H	5	0.11
(2,37)	1:B:692:LEU:HD23	1:A:694:GLY:H	5	0.11
(2,367)	1:B:700:ALA:HB1	1:B:697:ILE:HA	14	0.11
(2,367)	1:B:700:ALA:HB2	1:B:697:ILE:HA	14	0.11
(2,367)	1:B:700:ALA:HB3	1:B:697:ILE:HA	14	0.11
(2,356)	1:B:698:VAL:HG11	1:B:695:LEU:HG	5	0.11
(2,356)	1:B:698:VAL:HG12	1:B:695:LEU:HG	5	0.11
(2,356)	1:B:698:VAL:HG13	1:B:695:LEU:HG	5	0.11
(2,355)	1:B:698:VAL:HG11	1:B:695:LEU:HA	2	0.11
(2,355)	1:B:698:VAL:HG12	1:B:695:LEU:HA	2	0.11
(2,355)	1:B:698:VAL:HG13	1:B:695:LEU:HA	2	0.11
(2,352)	1:B:697:ILE:HG21	1:B:694:GLY:HA2	7	0.11
(2,352)	1:B:697:ILE:HG21	1:B:694:GLY:HA3	7	0.11
(2,352)	1:B:697:ILE:HG22	1:B:694:GLY:HA2	7	0.11
(2,352)	1:B:697:ILE:HG22	1:B:694:GLY:HA3	7	0.11
(2,352)	1:B:697:ILE:HG23	1:B:694:GLY:HA2	7	0.11
(2,352)	1:B:697:ILE:HG23	1:B:694:GLY:HA3	7	0.11
(2,336)	1:B:693:ILE:HD11	1:B:697:ILE:H	13	0.11
(2,336)	1:B:693:ILE:HD12	1:B:697:ILE:H	13	0.11
(2,336)	1:B:693:ILE:HD13	1:B:697:ILE:H	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,330)	1:B:692:LEU:HD11	1:B:689:VAL:HA	10	0.11
(2,330)	1:B:692:LEU:HD12	1:B:689:VAL:HA	10	0.11
(2,330)	1:B:692:LEU:HD13	1:B:689:VAL:HA	10	0.11
(2,324)	1:B:688:ILE:HG21	1:B:692:LEU:HG	13	0.11
(2,324)	1:B:688:ILE:HG22	1:B:692:LEU:HG	13	0.11
(2,324)	1:B:688:ILE:HG23	1:B:692:LEU:HG	13	0.11
(2,304)	1:B:684:ILE:HG21	1:B:685:PHE:HB2	7	0.11
(2,304)	1:B:684:ILE:HG21	1:B:685:PHE:HB3	7	0.11
(2,304)	1:B:684:ILE:HG22	1:B:685:PHE:HB2	7	0.11
(2,304)	1:B:684:ILE:HG22	1:B:685:PHE:HB3	7	0.11
(2,304)	1:B:684:ILE:HG23	1:B:685:PHE:HB2	7	0.11
(2,304)	1:B:684:ILE:HG23	1:B:685:PHE:HB3	7	0.11
(2,301)	1:B:684:ILE:HD11	1:B:681:TYR:HA	10	0.11
(2,301)	1:B:684:ILE:HD12	1:B:681:TYR:HA	10	0.11
(2,301)	1:B:684:ILE:HD13	1:B:681:TYR:HA	10	0.11
(2,296)	1:B:682:ILE:HD11	1:B:681:TYR:H	4	0.11
(2,296)	1:B:682:ILE:HD12	1:B:681:TYR:H	4	0.11
(2,296)	1:B:682:ILE:HD13	1:B:681:TYR:H	4	0.11
(2,292)	1:B:681:TYR:H	1:B:682:ILE:H	9	0.11
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD11	1	0.11
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD12	1	0.11
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD13	1	0.11
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD11	15	0.11
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD12	15	0.11
(2,290)	1:B:680:TRP:HE1	1:B:684:ILE:HD13	15	0.11
(2,286)	1:B:678:TRP:HE1	1:B:682:ILE:H	4	0.11
(2,286)	1:B:678:TRP:HE1	1:B:682:ILE:H	15	0.11
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD11	8	0.11
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD12	8	0.11
(2,284)	1:B:678:TRP:HE1	1:B:675:ILE:HD13	8	0.11
(2,276)	1:B:676:THR:HG21	1:B:666:TRP:HZ3	14	0.11
(2,276)	1:B:676:THR:HG22	1:B:666:TRP:HZ3	14	0.11
(2,276)	1:B:676:THR:HG23	1:B:666:TRP:HZ3	14	0.11
(2,268)	1:B:672:TRP:H	1:B:673:PHE:H	11	0.11
(2,268)	1:B:672:TRP:H	1:B:673:PHE:H	15	0.11
(2,263)	1:B:670:TRP:HE1	1:B:667:ALA:HB1	7	0.11
(2,263)	1:B:670:TRP:HE1	1:B:667:ALA:HB2	7	0.11
(2,263)	1:B:670:TRP:HE1	1:B:667:ALA:HB3	7	0.11
(2,245)	1:B:667:ALA:H	1:B:666:TRP:HD1	8	0.11
(2,243)	1:B:667:ALA:H	1:B:666:TRP:HA	9	0.11
(2,242)	1:B:667:ALA:H	1:B:664:ASP:HA	8	0.11
(2,234)	1:B:666:TRP:H	1:B:663:LEU:HA	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,233)	1:B:665:LYS:H	1:B:666:TRP:HD1	2	0.11
(2,228)	1:B:665:LYS:H	1:B:662:GLU:HA	12	0.11
(2,205)	1:B:831:GLU:H	1:B:816:ASN:HD21	13	0.11
(2,205)	1:B:831:GLU:H	1:B:816:ASN:HD22	13	0.11
(2,192)	1:A:816:ASN:H	1:A:831:GLU:HG2	6	0.11
(2,192)	1:A:816:ASN:H	1:A:831:GLU:HG3	6	0.11
(2,191)	1:A:816:ASN:H	1:A:831:GLU:HG2	6	0.11
(2,191)	1:A:816:ASN:H	1:A:831:GLU:HG3	6	0.11
(2,177)	1:A:803:TRP:HE1	1:B:764:SER:HG	11	0.11
(2,177)	1:A:803:TRP:HE1	1:B:764:SER:HG	12	0.11
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	15	0.11
(2,171)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	15	0.11
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB2	15	0.11
(2,170)	1:A:797:TRP:HE1	1:A:848:ARG:HB3	15	0.11
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG12	6	0.11
(2,157)	1:B:794:LYS:H	1:B:847:ILE:HG13	6	0.11
(2,1482)	1:A:852:GLU:H	1:A:848:ARG:HG2	13	0.11
(2,1482)	1:A:852:GLU:H	1:A:848:ARG:HG3	13	0.11
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD2	10	0.11
(2,1481)	1:A:839:ALA:H	1:A:838:ARG:HD3	10	0.11
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG2	14	0.11
(2,1479)	1:A:835:GLY:H	1:A:834:GLN:HG3	14	0.11
(2,1475)	1:A:806:GLU:H	1:A:803:TRP:HB2	3	0.11
(2,1475)	1:A:806:GLU:H	1:A:803:TRP:HB3	3	0.11
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	11	0.11
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	11	0.11
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	11	0.11
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	11	0.11
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	11	0.11
(2,1474)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	11	0.11
(2,1436)	1:A:782:VAL:HG21	1:A:779:THR:HA	13	0.11
(2,1436)	1:A:782:VAL:HG22	1:A:779:THR:HA	13	0.11
(2,1436)	1:A:782:VAL:HG23	1:A:779:THR:HA	13	0.11
(2,141)	1:B:771:LEU:H	1:A:806:GLU:HB2	4	0.11
(2,141)	1:B:771:LEU:H	1:A:806:GLU:HB3	4	0.11
(2,1391)	1:A:775:LEU:H	1:A:774:LEU:HA	7	0.11
(2,1364)	1:A:760:LEU:HD11	1:A:756:ILE:HG12	2	0.11
(2,1364)	1:A:760:LEU:HD11	1:A:756:ILE:HG13	2	0.11
(2,1364)	1:A:760:LEU:HD12	1:A:756:ILE:HG12	2	0.11
(2,1364)	1:A:760:LEU:HD12	1:A:756:ILE:HG13	2	0.11
(2,1364)	1:A:760:LEU:HD13	1:A:756:ILE:HG12	2	0.11
(2,1364)	1:A:760:LEU:HD13	1:A:756:ILE:HG13	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	6	0.11
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	6	0.11
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	6	0.11
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	6	0.11
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	6	0.11
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	6	0.11
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	10	0.11
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	10	0.11
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	10	0.11
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	10	0.11
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	10	0.11
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	10	0.11
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA2	13	0.11
(2,1348)	1:A:754:ALA:HB1	1:A:751:GLY:HA3	13	0.11
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA2	13	0.11
(2,1348)	1:A:754:ALA:HB2	1:A:751:GLY:HA3	13	0.11
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA2	13	0.11
(2,1348)	1:A:754:ALA:HB3	1:A:751:GLY:HA3	13	0.11
(2,1329)	1:A:748:LEU:H	1:A:745:SER:HA	4	0.11
(2,1329)	1:A:748:LEU:H	1:A:745:SER:HA	11	0.11
(2,1322)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	2	0.11
(2,1322)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	2	0.11
(2,1322)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	2	0.11
(2,1322)	1:A:746:ILE:HG21	1:A:750:ASN:HD21	9	0.11
(2,1322)	1:A:746:ILE:HG22	1:A:750:ASN:HD21	9	0.11
(2,1322)	1:A:746:ILE:HG23	1:A:750:ASN:HD21	9	0.11
(2,1294)	1:A:710:GLN:H	1:A:710:GLN:HB3	11	0.11
(2,1290)	1:A:710:GLN:H	1:A:709:ARG:HA	13	0.11
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB2	14	0.11
(2,1280)	1:A:708:VAL:HG21	1:A:745:SER:HB3	14	0.11
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB2	14	0.11
(2,1280)	1:A:708:VAL:HG22	1:A:745:SER:HB3	14	0.11
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB2	14	0.11
(2,1280)	1:A:708:VAL:HG23	1:A:745:SER:HB3	14	0.11
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD2	5	0.11
(2,1271)	1:A:707:ARG:H	1:A:707:ARG:HD3	5	0.11
(2,1264)	1:A:707:ARG:H	1:A:704:LEU:HA	10	0.11
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB2	13	0.11
(2,1263)	1:A:707:ARG:H	1:A:703:SER:HB3	13	0.11
(2,126)	1:A:785:LEU:HD21	1:B:749:VAL:HB	6	0.11
(2,126)	1:A:785:LEU:HD22	1:B:749:VAL:HB	6	0.11
(2,126)	1:A:785:LEU:HD23	1:B:749:VAL:HB	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1246)	1:A:705:VAL:H	1:A:702:LEU:HA	4	0.11
(2,1246)	1:A:705:VAL:H	1:A:702:LEU:HA	13	0.11
(2,1246)	1:A:705:VAL:H	1:A:702:LEU:HA	14	0.11
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD2	10	0.11
(2,1243)	1:A:704:LEU:HD11	1:A:707:ARG:HD3	10	0.11
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD2	10	0.11
(2,1243)	1:A:704:LEU:HD12	1:A:707:ARG:HD3	10	0.11
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD2	10	0.11
(2,1243)	1:A:704:LEU:HD13	1:A:707:ARG:HD3	10	0.11
(2,1224)	1:A:702:LEU:H	1:A:699:PHE:HA	11	0.11
(2,1223)	1:A:701:VAL:HG21	1:A:698:VAL:HA	15	0.11
(2,1223)	1:A:701:VAL:HG22	1:A:698:VAL:HA	15	0.11
(2,1223)	1:A:701:VAL:HG23	1:A:698:VAL:HA	15	0.11
(2,1206)	1:A:698:VAL:HG11	1:A:695:LEU:HG	7	0.11
(2,1206)	1:A:698:VAL:HG12	1:A:695:LEU:HG	7	0.11
(2,1206)	1:A:698:VAL:HG13	1:A:695:LEU:HG	7	0.11
(2,1202)	1:A:697:ILE:HG21	1:A:694:GLY:HA2	7	0.11
(2,1202)	1:A:697:ILE:HG21	1:A:694:GLY:HA3	7	0.11
(2,1202)	1:A:697:ILE:HG22	1:A:694:GLY:HA2	7	0.11
(2,1202)	1:A:697:ILE:HG22	1:A:694:GLY:HA3	7	0.11
(2,1202)	1:A:697:ILE:HG23	1:A:694:GLY:HA2	7	0.11
(2,1202)	1:A:697:ILE:HG23	1:A:694:GLY:HA3	7	0.11
(2,1195)	1:A:695:LEU:HD21	1:A:698:VAL:HB	6	0.11
(2,1195)	1:A:695:LEU:HD22	1:A:698:VAL:HB	6	0.11
(2,1195)	1:A:695:LEU:HD23	1:A:698:VAL:HB	6	0.11
(2,1188)	1:A:693:ILE:HG21	1:A:693:ILE:H	13	0.11
(2,1188)	1:A:693:ILE:HG22	1:A:693:ILE:H	13	0.11
(2,1188)	1:A:693:ILE:HG23	1:A:693:ILE:H	13	0.11
(2,1183)	1:A:692:LEU:HD11	1:A:696:ARG:HH11	13	0.11
(2,1183)	1:A:692:LEU:HD11	1:A:696:ARG:HH12	13	0.11
(2,1183)	1:A:692:LEU:HD11	1:A:696:ARG:HH21	13	0.11
(2,1183)	1:A:692:LEU:HD11	1:A:696:ARG:HH22	13	0.11
(2,1183)	1:A:692:LEU:HD12	1:A:696:ARG:HH11	13	0.11
(2,1183)	1:A:692:LEU:HD12	1:A:696:ARG:HH12	13	0.11
(2,1183)	1:A:692:LEU:HD12	1:A:696:ARG:HH21	13	0.11
(2,1183)	1:A:692:LEU:HD12	1:A:696:ARG:HH22	13	0.11
(2,1183)	1:A:692:LEU:HD13	1:A:696:ARG:HH11	13	0.11
(2,1183)	1:A:692:LEU:HD13	1:A:696:ARG:HH12	13	0.11
(2,1183)	1:A:692:LEU:HD13	1:A:696:ARG:HH21	13	0.11
(2,1183)	1:A:692:LEU:HD13	1:A:696:ARG:HH22	13	0.11
(2,1182)	1:A:692:LEU:HD11	1:A:691:SER:HB2	8	0.11
(2,1182)	1:A:692:LEU:HD11	1:A:691:SER:HB3	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1182)	1:A:692:LEU:HD12	1:A:691:SER:HB2	8	0.11
(2,1182)	1:A:692:LEU:HD12	1:A:691:SER:HB3	8	0.11
(2,1182)	1:A:692:LEU:HD13	1:A:691:SER:HB2	8	0.11
(2,1182)	1:A:692:LEU:HD13	1:A:691:SER:HB3	8	0.11
(2,1180)	1:A:692:LEU:HD11	1:A:689:VAL:HA	11	0.11
(2,1180)	1:A:692:LEU:HD12	1:A:689:VAL:HA	11	0.11
(2,1180)	1:A:692:LEU:HD13	1:A:689:VAL:HA	11	0.11
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB2	1	0.11
(2,118)	1:B:785:LEU:HD21	1:A:716:SER:HB3	1	0.11
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB2	1	0.11
(2,118)	1:B:785:LEU:HD22	1:A:716:SER:HB3	1	0.11
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB2	1	0.11
(2,118)	1:B:785:LEU:HD23	1:A:716:SER:HB3	1	0.11
(2,1177)	1:A:689:VAL:HG21	1:A:685:PHE:HE1	6	0.11
(2,1177)	1:A:689:VAL:HG21	1:A:685:PHE:HE2	6	0.11
(2,1177)	1:A:689:VAL:HG22	1:A:685:PHE:HE1	6	0.11
(2,1177)	1:A:689:VAL:HG22	1:A:685:PHE:HE2	6	0.11
(2,1177)	1:A:689:VAL:HG23	1:A:685:PHE:HE1	6	0.11
(2,1177)	1:A:689:VAL:HG23	1:A:685:PHE:HE2	6	0.11
(2,1173)	1:A:688:ILE:HD11	1:A:684:ILE:HD11	14	0.11
(2,1173)	1:A:688:ILE:HD11	1:A:684:ILE:HD12	14	0.11
(2,1173)	1:A:688:ILE:HD11	1:A:684:ILE:HD13	14	0.11
(2,1173)	1:A:688:ILE:HD12	1:A:684:ILE:HD11	14	0.11
(2,1173)	1:A:688:ILE:HD12	1:A:684:ILE:HD12	14	0.11
(2,1173)	1:A:688:ILE:HD12	1:A:684:ILE:HD13	14	0.11
(2,1173)	1:A:688:ILE:HD13	1:A:684:ILE:HD11	14	0.11
(2,1173)	1:A:688:ILE:HD13	1:A:684:ILE:HD12	14	0.11
(2,1173)	1:A:688:ILE:HD13	1:A:684:ILE:HD13	14	0.11
(2,1168)	1:A:686:ILE:HD11	1:A:685:PHE:H	13	0.11
(2,1168)	1:A:686:ILE:HD12	1:A:685:PHE:H	13	0.11
(2,1168)	1:A:686:ILE:HD13	1:A:685:PHE:H	13	0.11
(2,1167)	1:A:686:ILE:HD11	1:A:683:ARG:HA	13	0.11
(2,1167)	1:A:686:ILE:HD12	1:A:683:ARG:HA	13	0.11
(2,1167)	1:A:686:ILE:HD13	1:A:683:ARG:HA	13	0.11
(2,1151)	1:A:684:ILE:HD11	1:A:681:TYR:HA	15	0.11
(2,1151)	1:A:684:ILE:HD12	1:A:681:TYR:HA	15	0.11
(2,1151)	1:A:684:ILE:HD13	1:A:681:TYR:HA	15	0.11
(2,1147)	1:A:682:ILE:HD11	1:A:685:PHE:HB2	5	0.11
(2,1147)	1:A:682:ILE:HD11	1:A:685:PHE:HB3	5	0.11
(2,1147)	1:A:682:ILE:HD12	1:A:685:PHE:HB2	5	0.11
(2,1147)	1:A:682:ILE:HD12	1:A:685:PHE:HB3	5	0.11
(2,1147)	1:A:682:ILE:HD13	1:A:685:PHE:HB2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1147)	1:A:682:ILE:HD13	1:A:685:PHE:HB3	5	0.11
(2,1147)	1:A:682:ILE:HD11	1:A:685:PHE:HB2	10	0.11
(2,1147)	1:A:682:ILE:HD11	1:A:685:PHE:HB3	10	0.11
(2,1147)	1:A:682:ILE:HD12	1:A:685:PHE:HB2	10	0.11
(2,1147)	1:A:682:ILE:HD12	1:A:685:PHE:HB3	10	0.11
(2,1147)	1:A:682:ILE:HD13	1:A:685:PHE:HB2	10	0.11
(2,1147)	1:A:682:ILE:HD13	1:A:685:PHE:HB3	10	0.11
(2,1142)	1:A:681:TYR:H	1:A:682:ILE:H	9	0.11
(2,1142)	1:A:681:TYR:H	1:A:682:ILE:H	11	0.11
(2,1139)	1:A:680:TRP:HE1	1:A:683:ARG:HH21	2	0.11
(2,1139)	1:A:680:TRP:HE1	1:A:683:ARG:HH22	2	0.11
(2,1138)	1:A:679:LEU:HD11	1:A:678:TRP:HH2	10	0.11
(2,1138)	1:A:679:LEU:HD12	1:A:678:TRP:HH2	10	0.11
(2,1138)	1:A:679:LEU:HD13	1:A:678:TRP:HH2	10	0.11
(2,1138)	1:A:679:LEU:HD21	1:A:678:TRP:HH2	10	0.11
(2,1138)	1:A:679:LEU:HD22	1:A:678:TRP:HH2	10	0.11
(2,1138)	1:A:679:LEU:HD23	1:A:678:TRP:HH2	10	0.11
(2,1136)	1:A:678:TRP:HE1	1:A:682:ILE:H	1	0.11
(2,1119)	1:A:672:TRP:HE1	1:A:669:LEU:HD11	15	0.11
(2,1119)	1:A:672:TRP:HE1	1:A:669:LEU:HD12	15	0.11
(2,1119)	1:A:672:TRP:HE1	1:A:669:LEU:HD13	15	0.11
(2,1119)	1:A:672:TRP:HE1	1:A:669:LEU:HD21	15	0.11
(2,1119)	1:A:672:TRP:HE1	1:A:669:LEU:HD22	15	0.11
(2,1119)	1:A:672:TRP:HE1	1:A:669:LEU:HD23	15	0.11
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD11	12	0.11
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD12	12	0.11
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD13	12	0.11
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD21	12	0.11
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD22	12	0.11
(2,1114)	1:A:670:TRP:HE1	1:A:669:LEU:HD23	12	0.11
(2,1113)	1:A:670:TRP:HE1	1:A:667:ALA:HB1	10	0.11
(2,1113)	1:A:670:TRP:HE1	1:A:667:ALA:HB2	10	0.11
(2,1113)	1:A:670:TRP:HE1	1:A:667:ALA:HB3	10	0.11
(2,1108)	1:A:669:LEU:HD11	1:A:672:TRP:HZ3	1	0.11
(2,1108)	1:A:669:LEU:HD12	1:A:672:TRP:HZ3	1	0.11
(2,1108)	1:A:669:LEU:HD13	1:A:672:TRP:HZ3	1	0.11
(2,1108)	1:A:669:LEU:HD21	1:A:672:TRP:HZ3	1	0.11
(2,1108)	1:A:669:LEU:HD22	1:A:672:TRP:HZ3	1	0.11
(2,1108)	1:A:669:LEU:HD23	1:A:672:TRP:HZ3	1	0.11
(2,1108)	1:A:669:LEU:HD11	1:A:672:TRP:HZ3	8	0.11
(2,1108)	1:A:669:LEU:HD12	1:A:672:TRP:HZ3	8	0.11
(2,1108)	1:A:669:LEU:HD13	1:A:672:TRP:HZ3	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1108)	1:A:669:LEU:HD21	1:A:672:TRP:HZ3	8	0.11
(2,1108)	1:A:669:LEU:HD22	1:A:672:TRP:HZ3	8	0.11
(2,1108)	1:A:669:LEU:HD23	1:A:672:TRP:HZ3	8	0.11
(2,1097)	1:A:667:ALA:HB1	1:A:664:ASP:HA	14	0.11
(2,1097)	1:A:667:ALA:HB2	1:A:664:ASP:HA	14	0.11
(2,1097)	1:A:667:ALA:HB3	1:A:664:ASP:HA	14	0.11
(2,1097)	1:A:667:ALA:HB1	1:A:664:ASP:HA	15	0.11
(2,1097)	1:A:667:ALA:HB2	1:A:664:ASP:HA	15	0.11
(2,1097)	1:A:667:ALA:HB3	1:A:664:ASP:HA	15	0.11
(2,1092)	1:A:667:ALA:H	1:A:664:ASP:HA	10	0.11
(2,1091)	1:A:666:TRP:HE1	1:A:662:GLU:H	5	0.11
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD2	2	0.11
(2,108)	1:A:777:ILE:HD11	1:B:742:ARG:HD3	2	0.11
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD2	2	0.11
(2,108)	1:A:777:ILE:HD12	1:B:742:ARG:HD3	2	0.11
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD2	2	0.11
(2,108)	1:A:777:ILE:HD13	1:B:742:ARG:HD3	2	0.11
(2,1078)	1:A:665:LYS:H	1:A:662:GLU:HA	7	0.11
(2,1074)	1:A:664:ASP:H	1:A:663:LEU:HA	1	0.11
(2,1074)	1:A:664:ASP:H	1:A:663:LEU:HA	6	0.11
(2,1074)	1:A:664:ASP:H	1:A:663:LEU:HA	7	0.11
(2,1057)	1:A:852:GLU:H	1:A:848:ARG:HG2	13	0.11
(2,1057)	1:A:852:GLU:H	1:A:848:ARG:HG3	13	0.11
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD2	10	0.11
(2,1056)	1:A:839:ALA:H	1:A:838:ARG:HD3	10	0.11
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG2	14	0.11
(2,1054)	1:A:835:GLY:H	1:A:834:GLN:HG3	14	0.11
(2,1050)	1:A:806:GLU:H	1:A:803:TRP:HB2	3	0.11
(2,1050)	1:A:806:GLU:H	1:A:803:TRP:HB3	3	0.11
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD11	11	0.11
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD12	11	0.11
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD13	11	0.11
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD21	11	0.11
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD22	11	0.11
(2,1049)	1:A:803:TRP:HE1	1:A:800:LEU:HD23	11	0.11
(2,1011)	1:A:782:VAL:HG21	1:A:779:THR:HA	13	0.11
(2,1011)	1:A:782:VAL:HG22	1:A:779:THR:HA	13	0.11
(2,1011)	1:A:782:VAL:HG23	1:A:779:THR:HA	13	0.11
(1,98)	1:B:795:TYR:O	1:B:799:LEU:N	12	0.11
(1,96)	1:B:794:LYS:O	1:B:798:ASN:N	1	0.11
(1,96)	1:B:794:LYS:O	1:B:798:ASN:N	7	0.11
(1,95)	1:B:794:LYS:O	1:B:798:ASN:H	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:B:792:ALA:O	1:B:796:TRP:H	7	0.11
(1,90)	1:B:791:GLU:O	1:B:795:TYR:N	7	0.11
(1,9)	1:B:794:LYS:O	1:B:798:ASN:H	14	0.11
(1,76)	1:B:837:SER:O	1:B:841:ARG:N	5	0.11
(1,75)	1:B:837:SER:O	1:B:841:ARG:H	6	0.11
(1,75)	1:B:837:SER:O	1:B:841:ARG:H	8	0.11
(1,73)	1:B:836:ALA:O	1:B:840:ILE:H	3	0.11
(1,70)	1:B:834:GLN:O	1:B:838:ARG:N	8	0.11
(1,69)	1:B:834:GLN:O	1:B:838:ARG:H	4	0.11
(1,67)	1:B:833:VAL:O	1:B:837:SER:H	13	0.11
(1,62)	1:B:830:ILE:O	1:B:834:GLN:N	9	0.11
(1,61)	1:B:830:ILE:O	1:B:834:GLN:H	7	0.11
(1,59)	1:B:829:VAL:O	1:B:833:VAL:H	8	0.11
(1,55)	1:B:827:ASP:O	1:B:831:GLU:H	15	0.11
(1,5)	1:B:792:ALA:O	1:B:796:TRP:H	7	0.11
(1,47)	1:B:813:SER:O	1:B:817:ALA:H	4	0.11
(1,47)	1:B:813:SER:O	1:B:817:ALA:H	15	0.11
(1,4)	1:B:791:GLU:O	1:B:795:TYR:N	7	0.11
(1,31)	1:B:805:GLN:O	1:B:809:ASN:H	7	0.11
(1,27)	1:B:803:TRP:O	1:B:807:LEU:H	13	0.11
(1,26)	1:B:802:TYR:O	1:B:806:GLU:N	9	0.11
(1,25)	1:B:802:TYR:O	1:B:806:GLU:H	6	0.11
(1,248)	1:B:837:SER:O	1:B:841:ARG:N	5	0.11
(1,247)	1:B:837:SER:O	1:B:841:ARG:H	6	0.11
(1,247)	1:B:837:SER:O	1:B:841:ARG:H	8	0.11
(1,245)	1:B:836:ALA:O	1:B:840:ILE:H	3	0.11
(1,242)	1:B:834:GLN:O	1:B:838:ARG:N	8	0.11
(1,241)	1:B:834:GLN:O	1:B:838:ARG:H	4	0.11
(1,239)	1:B:833:VAL:O	1:B:837:SER:H	13	0.11
(1,234)	1:B:830:ILE:O	1:B:834:GLN:N	9	0.11
(1,233)	1:B:830:ILE:O	1:B:834:GLN:H	7	0.11
(1,231)	1:B:829:VAL:O	1:B:833:VAL:H	8	0.11
(1,227)	1:B:827:ASP:O	1:B:831:GLU:H	15	0.11
(1,219)	1:B:813:SER:O	1:B:817:ALA:H	4	0.11
(1,219)	1:B:813:SER:O	1:B:817:ALA:H	15	0.11
(1,203)	1:B:805:GLN:O	1:B:809:ASN:H	7	0.11
(1,20)	1:B:799:LEU:O	1:B:803:TRP:N	12	0.11
(1,199)	1:B:803:TRP:O	1:B:807:LEU:H	13	0.11
(1,198)	1:B:802:TYR:O	1:B:806:GLU:N	9	0.11
(1,197)	1:B:802:TYR:O	1:B:806:GLU:H	6	0.11
(1,192)	1:B:799:LEU:O	1:B:803:TRP:N	12	0.11
(1,184)	1:B:795:TYR:O	1:B:799:LEU:N	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:B:794:LYS:O	1:B:798:ASN:N	1	0.11
(1,182)	1:B:794:LYS:O	1:B:798:ASN:N	7	0.11
(1,181)	1:B:794:LYS:O	1:B:798:ASN:H	14	0.11
(1,177)	1:B:792:ALA:O	1:B:796:TRP:H	7	0.11
(1,176)	1:B:791:GLU:O	1:B:795:TYR:N	7	0.11
(1,162)	1:B:837:SER:O	1:B:841:ARG:N	5	0.11
(1,161)	1:B:837:SER:O	1:B:841:ARG:H	6	0.11
(1,161)	1:B:837:SER:O	1:B:841:ARG:H	8	0.11
(1,159)	1:B:836:ALA:O	1:B:840:ILE:H	3	0.11
(1,156)	1:B:834:GLN:O	1:B:838:ARG:N	8	0.11
(1,155)	1:B:834:GLN:O	1:B:838:ARG:H	4	0.11
(1,153)	1:B:833:VAL:O	1:B:837:SER:H	13	0.11
(1,148)	1:B:830:ILE:O	1:B:834:GLN:N	9	0.11
(1,147)	1:B:830:ILE:O	1:B:834:GLN:H	7	0.11
(1,145)	1:B:829:VAL:O	1:B:833:VAL:H	8	0.11
(1,141)	1:B:827:ASP:O	1:B:831:GLU:H	15	0.11
(1,133)	1:B:813:SER:O	1:B:817:ALA:H	4	0.11
(1,133)	1:B:813:SER:O	1:B:817:ALA:H	15	0.11
(1,12)	1:B:795:TYR:O	1:B:799:LEU:N	12	0.11
(1,117)	1:B:805:GLN:O	1:B:809:ASN:H	7	0.11
(1,113)	1:B:803:TRP:O	1:B:807:LEU:H	13	0.11
(1,112)	1:B:802:TYR:O	1:B:806:GLU:N	9	0.11
(1,111)	1:B:802:TYR:O	1:B:806:GLU:H	6	0.11
(1,106)	1:B:799:LEU:O	1:B:803:TRP:N	12	0.11
(1,10)	1:B:794:LYS:O	1:B:798:ASN:N	1	0.11
(1,10)	1:B:794:LYS:O	1:B:798:ASN:N	7	0.11

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

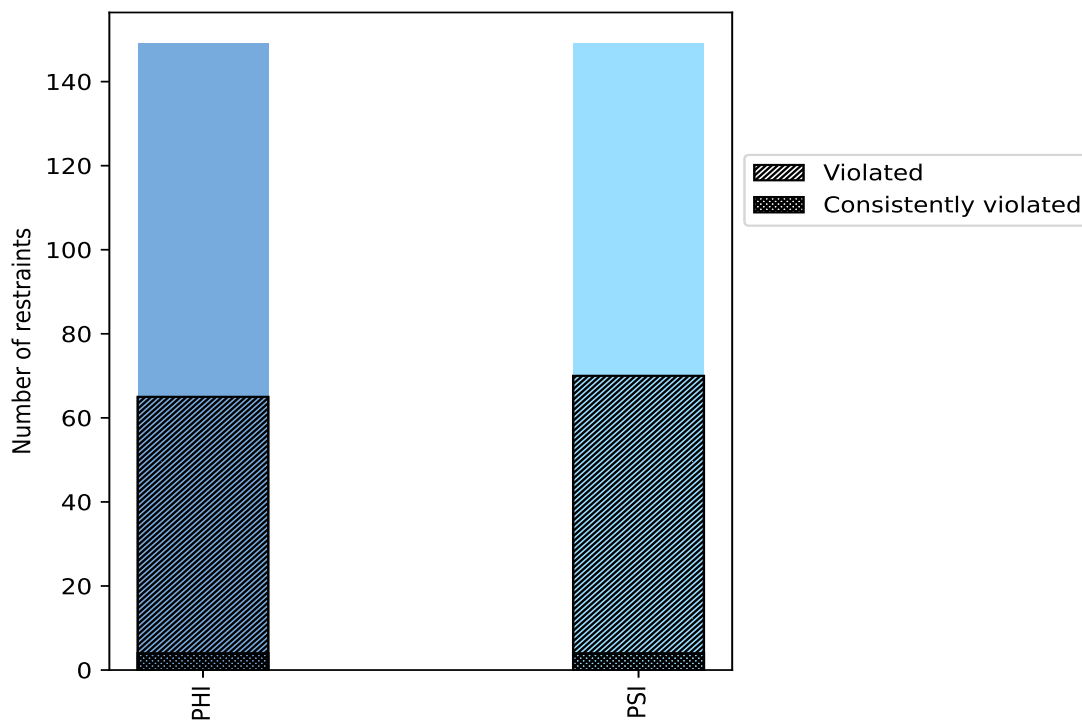
### 10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PHI	149	50.0	65	43.6	21.8	4	2.7	1.3
PSI	149	50.0	70	47.0	23.5	4	2.7	1.3
Total	298	100.0	135	45.3	45.3	8	2.7	2.7

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

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



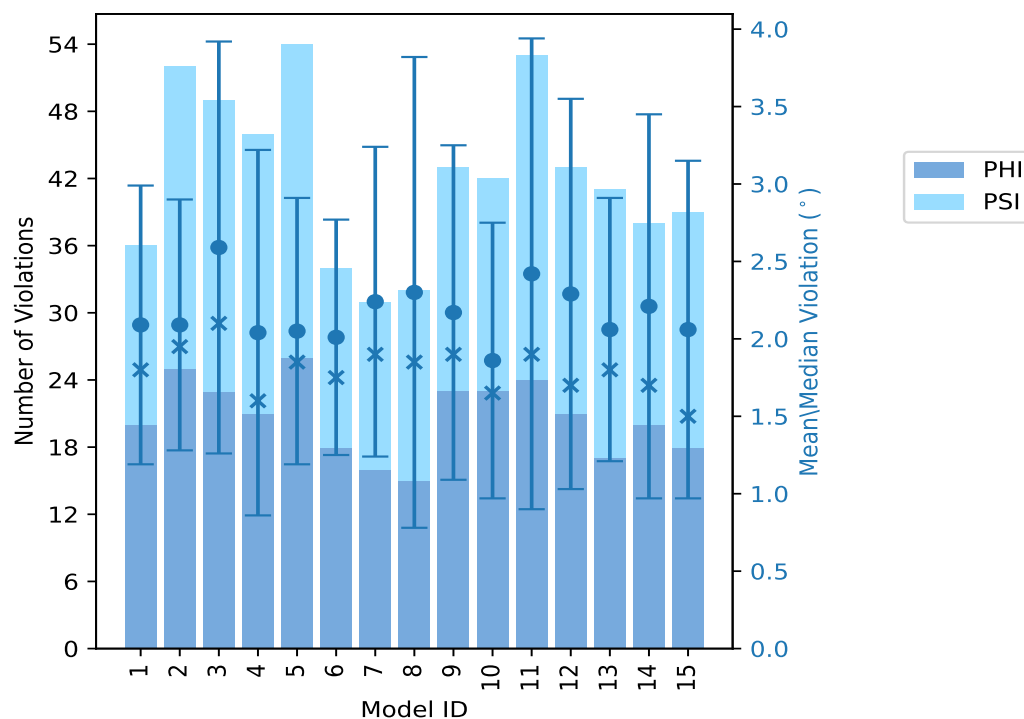
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model [\(i\)](#)

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	20	16	36	2.09	4.6	0.9	1.8
2	25	27	52	2.09	3.9	0.81	1.95
3	23	26	49	2.59	5.3	1.33	2.1
4	21	25	46	2.04	6.4	1.18	1.6
5	26	28	54	2.05	4.7	0.86	1.85
6	18	16	34	2.01	4.1	0.76	1.75
7	16	15	31	2.24	4.8	1.0	1.9
8	15	17	32	2.3	7.2	1.52	1.85
9	23	20	43	2.17	4.9	1.08	1.9
10	23	19	42	1.86	5.4	0.89	1.65
11	24	29	53	2.42	7.1	1.52	1.9
12	21	22	43	2.29	5.3	1.26	1.7
13	17	24	41	2.06	4.6	0.85	1.8
14	20	18	38	2.21	5.4	1.24	1.7
15	18	21	39	2.06	5.0	1.09	1.5

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



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

### 10.3 Dihedral-angle violation statistics for the ensemble

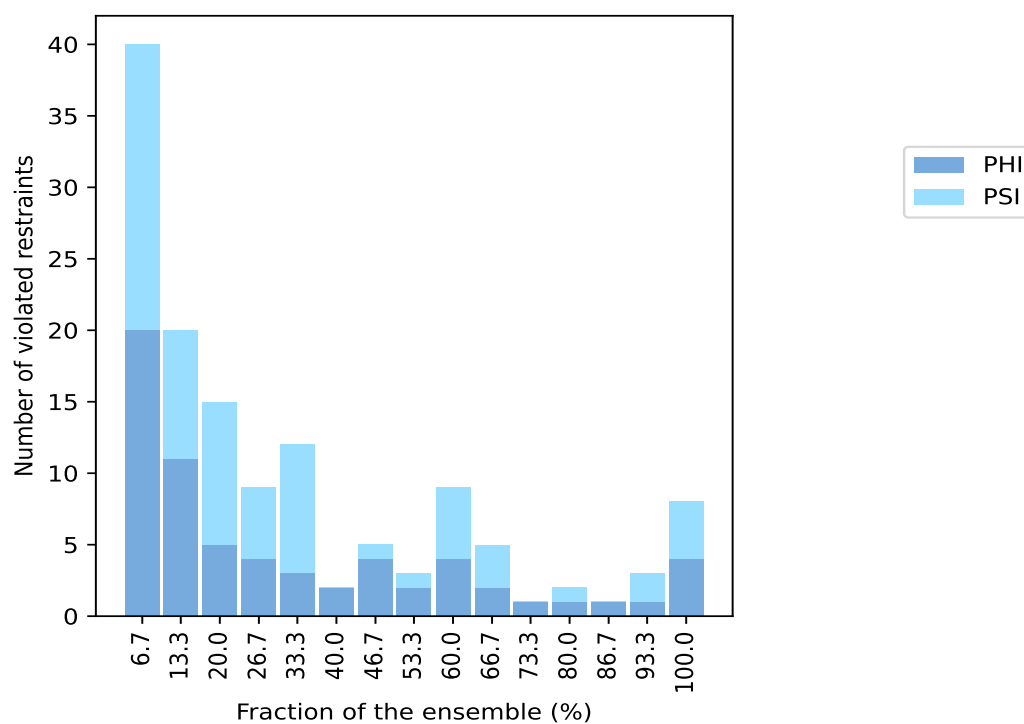
Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count <sup>1</sup>	%
20	20	40	1	6.7
11	9	20	2	13.3
5	10	15	3	20.0
4	5	9	4	26.7
3	9	12	5	33.3
2	0	2	6	40.0
4	1	5	7	46.7
2	1	3	8	53.3
4	5	9	9	60.0
2	3	5	10	66.7
1	0	1	11	73.3
1	1	2	12	80.0
1	0	1	13	86.7
1	2	3	14	93.3
4	4	8	15	100.0

<sup>1</sup> Number of models with violations



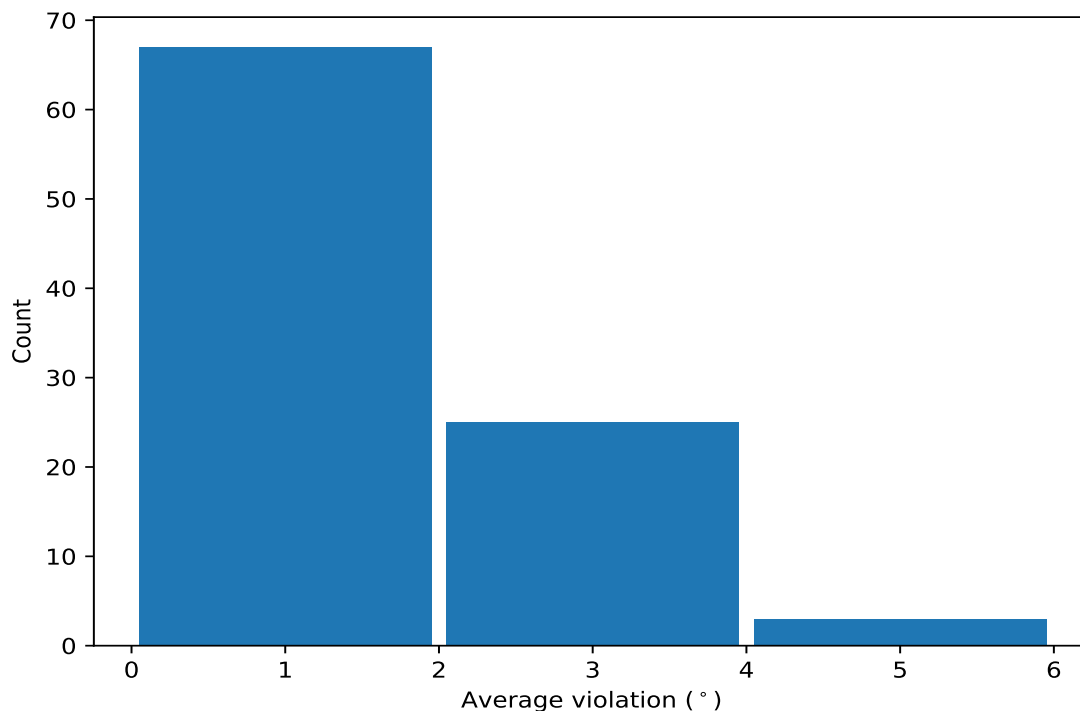
### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,148)	1:B:770:ARG:N	1:B:770:ARG:CA	1:B:770:ARG:C	1:B:771:LEU:N	15	4.51	1.33	4.6
(1,149)	1:B:770:ARG:C	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	15	4.41	1.44	4.7
(1,188)	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	1:B:791:GLU:N	15	4.09	0.66	4.1
(1,62)	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1:B:700:ALA:N	15	3.87	0.8	3.8
(1,126)	1:B:754:ALA:N	1:B:754:ALA:CA	1:B:754:ALA:C	1:B:755:LEU:N	15	3.45	1.29	3.3
(1,127)	1:B:754:ALA:C	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	15	3.27	1.31	3.1
(1,63)	1:B:699:PHE:C	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	15	3.03	0.69	3.0
(1,119)	1:B:750:ASN:C	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	15	2.57	0.61	2.8
(1,56)	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	1:B:697:ILE:N	14	2.3	0.88	2.15
(1,118)	1:B:750:ASN:N	1:B:750:ASN:CA	1:B:750:ASN:C	1:B:751:GLY:N	14	2.27	0.79	2.15
(1,195)	1:B:793:LEU:C	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	14	1.98	0.45	2.05
(1,189)	1:B:790:TRP:C	1:B:791:GLU:N	1:B:791:GLU:CA	1:B:791:GLU:C	13	1.82	0.46	1.9
(1,145)	1:B:763:LEU:C	1:B:764:SER:N	1:B:764:SER:CA	1:B:764:SER:C	12	2.17	0.59	2.1
(1,98)	1:B:740:ARG:N	1:B:740:ARG:CA	1:B:740:ARG:C	1:B:741:ASP:N	12	2.02	0.86	1.9
(1,57)	1:B:696:ARG:C	1:B:697:ILE:N	1:B:697:ILE:CA	1:B:697:ILE:C	11	1.93	0.55	1.9
(1,132)	1:B:757:TRP:N	1:B:757:TRP:CA	1:B:757:TRP:C	1:B:758:ASP:N	10	2.68	1.62	2.15
(1,18)	1:B:675:ILE:N	1:B:675:ILE:CA	1:B:675:ILE:C	1:B:676:THR:N	10	2.2	0.66	2.25
(1,99)	1:B:740:ARG:C	1:B:741:ASP:N	1:B:741:ASP:CA	1:B:741:ASP:C	10	1.89	0.83	1.7
(1,69)	1:B:702:LEU:C	1:B:703:SER:N	1:B:703:SER:CA	1:B:703:SER:C	10	1.53	0.32	1.45
(1,86)	1:B:713:SER:N	1:B:713:SER:CA	1:B:713:SER:C	1:B:714:PRO:N	10	1.4	0.2	1.35
(1,19)	1:B:675:ILE:C	1:B:676:THR:N	1:B:676:THR:CA	1:B:676:THR:C	9	2.54	0.61	2.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,142)	1:B:762:SER:N	1:B:762:SER:CA	1:B:762:SER:C	1:B:763:LEU:N	9	2.39	0.67	2.5
(1,143)	1:B:762:SER:C	1:B:763:LEU:N	1:B:763:LEU:CA	1:B:763:LEU:C	9	2.19	0.58	2.3
(1,251)	1:B:826:THR:C	1:B:827:ASP:N	1:B:827:ASP:CA	1:B:827:ASP:C	9	1.92	0.71	1.8
(1,154)	1:B:773:ASP:N	1:B:773:ASP:CA	1:B:773:ASP:C	1:B:774:LEU:N	9	1.84	0.67	1.6
(1,162)	1:B:777:ILE:N	1:B:777:ILE:CA	1:B:777:ILE:C	1:B:778:VAL:N	9	1.81	0.64	1.6
(1,46)	1:B:691:SER:N	1:B:691:SER:CA	1:B:691:SER:C	1:B:692:LEU:N	9	1.57	0.41	1.5
(1,87)	1:B:714:PRO:C	1:B:715:LEU:N	1:B:715:LEU:CA	1:B:715:LEU:C	9	1.56	0.32	1.5
(1,68)	1:B:702:LEU:N	1:B:702:LEU:CA	1:B:702:LEU:C	1:B:703:SER:N	9	1.5	0.34	1.4
(1,120)	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	1:B:752:SER:N	8	1.92	0.52	1.75
(1,197)	1:B:794:LYS:C	1:B:795:TYR:N	1:B:795:TYR:CA	1:B:795:TYR:C	8	1.59	0.53	1.45
(1,83)	1:B:709:ARG:C	1:B:710:GLN:N	1:B:710:GLN:CA	1:B:710:GLN:C	8	1.54	0.51	1.35
(1,133)	1:B:757:TRP:C	1:B:758:ASP:N	1:B:758:ASP:CA	1:B:758:ASP:C	7	3.31	1.99	2.3
(1,196)	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	1:B:795:TYR:N	7	2.01	0.67	2.1
(1,81)	1:B:708:VAL:C	1:B:709:ARG:N	1:B:709:ARG:CA	1:B:709:ARG:C	7	2.01	0.68	1.8
(1,61)	1:B:698:VAL:C	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	7	1.84	0.62	1.7
(1,47)	1:B:691:SER:C	1:B:692:LEU:N	1:B:692:LEU:CA	1:B:692:LEU:C	7	1.33	0.24	1.3
(1,135)	1:B:758:ASP:C	1:B:759:ASP:N	1:B:759:ASP:CA	1:B:759:ASP:C	6	2.42	1.12	2.3
(1,155)	1:B:773:ASP:C	1:B:774:LEU:N	1:B:774:LEU:CA	1:B:774:LEU:C	6	1.75	0.7	1.5
(1,134)	1:B:758:ASP:N	1:B:758:ASP:CA	1:B:758:ASP:C	1:B:759:ASP:N	5	2.74	1.2	2.9
(1,136)	1:B:759:ASP:N	1:B:759:ASP:CA	1:B:759:ASP:C	1:B:760:LEU:N	5	2.64	1.1	2.0
(1,80)	1:B:708:VAL:N	1:B:708:VAL:CA	1:B:708:VAL:C	1:B:709:ARG:N	5	2.02	0.65	1.8
(1,137)	1:B:759:ASP:C	1:B:760:LEU:N	1:B:760:LEU:CA	1:B:760:LEU:C	5	1.92	0.72	1.7
(1,121)	1:B:751:GLY:C	1:B:752:SER:N	1:B:752:SER:CA	1:B:752:SER:C	5	1.78	0.34	1.8
(1,144)	1:B:763:LEU:N	1:B:763:LEU:CA	1:B:763:LEU:C	1:B:764:SER:N	5	1.78	0.6	1.6
(1,156)	1:B:774:LEU:N	1:B:774:LEU:CA	1:B:774:LEU:C	1:B:775:LEU:N	5	1.68	0.69	1.4
(1,158)	1:B:775:LEU:N	1:B:775:LEU:CA	1:B:775:LEU:C	1:B:776:LEU:N	5	1.54	0.51	1.2
(1,185)	1:B:788:ARG:C	1:B:789:GLY:N	1:B:789:GLY:CA	1:B:789:GLY:C	5	1.5	0.42	1.4
(1,250)	1:B:826:THR:N	1:B:826:THR:CA	1:B:826:THR:C	1:B:827:ASP:N	5	1.46	0.27	1.6
(1,274)	1:B:838:ARG:N	1:B:838:ARG:CA	1:B:838:ARG:C	1:B:839:ALA:N	5	1.4	0.26	1.3
(1,186)	1:B:789:GLY:N	1:B:789:GLY:CA	1:B:789:GLY:C	1:B:790:TRP:N	5	1.18	0.07	1.2
(1,20)	1:B:676:THR:N	1:B:676:THR:CA	1:B:676:THR:C	1:B:677:ASN:N	4	1.95	0.78	1.85
(1,270)	1:B:836:ALA:N	1:B:836:ALA:CA	1:B:836:ALA:C	1:B:837:SER:N	4	1.92	0.48	2.05
(1,272)	1:B:837:SER:N	1:B:837:SER:CA	1:B:837:SER:C	1:B:838:ARG:N	4	1.88	0.5	1.7
(1,271)	1:B:836:ALA:C	1:B:837:SER:N	1:B:837:SER:CA	1:B:837:SER:C	4	1.78	0.38	1.8
(1,163)	1:B:777:ILE:C	1:B:778:VAL:N	1:B:778:VAL:CA	1:B:778:VAL:C	4	1.65	0.38	1.6
(1,194)	1:B:793:LEU:N	1:B:793:LEU:CA	1:B:793:LEU:C	1:B:794:LYS:N	4	1.52	0.52	1.3
(1,64)	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	1:B:701:VAL:N	4	1.33	0.08	1.35
(1,179)	1:B:785:LEU:C	1:B:786:GLY:N	1:B:786:GLY:CA	1:B:786:GLY:C	4	1.25	0.17	1.2
(1,273)	1:B:837:SER:C	1:B:838:ARG:N	1:B:838:ARG:CA	1:B:838:ARG:C	4	1.25	0.15	1.25
(1,88)	1:B:715:LEU:N	1:B:715:LEU:CA	1:B:715:LEU:C	1:B:716:SER:N	3	2.03	0.58	1.9
(1,210)	1:B:801:GLN:N	1:B:801:GLN:CA	1:B:801:GLN:C	1:B:802:TYR:N	3	2.03	0.76	1.6
(1,85)	1:B:712:TYR:C	1:B:713:SER:N	1:B:713:SER:CA	1:B:713:SER:C	3	1.97	0.66	2.1
(1,151)	1:B:771:LEU:C	1:B:772:ARG:N	1:B:772:ARG:CA	1:B:772:ARG:C	3	1.67	0.17	1.6
(1,131)	1:B:756:ILE:C	1:B:757:TRP:N	1:B:757:TRP:CA	1:B:757:TRP:C	3	1.6	0.33	1.6
(1,184)	1:B:788:ARG:N	1:B:788:ARG:CA	1:B:788:ARG:C	1:B:789:GLY:N	3	1.57	0.25	1.5
(1,84)	1:B:710:GLN:N	1:B:710:GLN:CA	1:B:710:GLN:C	1:B:711:GLY:N	3	1.53	0.26	1.4
(1,172)	1:B:782:VAL:N	1:B:782:VAL:CA	1:B:782:VAL:C	1:B:783:GLU:N	3	1.5	0.24	1.5
(1,202)	1:B:797:TRP:N	1:B:797:TRP:CA	1:B:797:TRP:C	1:B:798:ASN:N	3	1.43	0.12	1.4
(1,123)	1:B:752:SER:C	1:B:753:LEU:N	1:B:753:LEU:CA	1:B:753:LEU:C	3	1.37	0.19	1.5
(1,166)	1:B:779:THR:N	1:B:779:THR:CA	1:B:779:THR:C	1:B:780:ARG:N	3	1.37	0.05	1.4
(1,54)	1:B:695:LEU:N	1:B:695:LEU:CA	1:B:695:LEU:C	1:B:696:ARG:N	3	1.33	0.26	1.2

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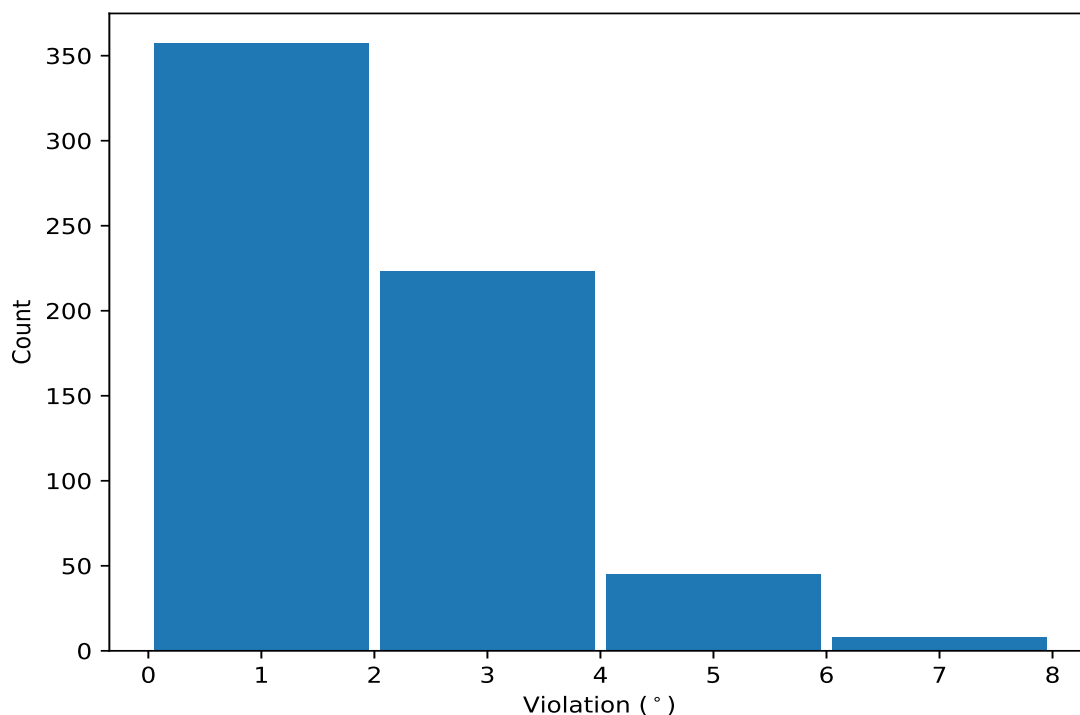
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,206)	1:B:799:LEU:N	1:B:799:LEU:CA	1:B:799:LEU:C	1:B:800:LEU:N	3	1.33	0.12	1.3
(1,192)	1:B:792:ALA:N	1:B:792:ALA:CA	1:B:792:ALA:C	1:B:793:LEU:N	3	1.23	0.12	1.2
(1,187)	1:B:789:GLY:C	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	3	1.17	0.09	1.1
(1,21)	1:B:676:THR:C	1:B:677:ASN:N	1:B:677:ASN:CA	1:B:677:ASN:C	2	2.3	0.4	2.3
(1,60)	1:B:698:VAL:N	1:B:698:VAL:CA	1:B:698:VAL:C	1:B:699:PHE:N	2	2.3	0.3	2.3
(1,247)	1:B:819:ALA:C	1:B:820:ILE:N	1:B:820:ILE:CA	1:B:820:ILE:C	2	1.95	0.45	1.95
(1,3)	1:B:664:ASP:C	1:B:665:LYS:N	1:B:665:LYS:CA	1:B:665:LYS:C	2	1.85	0.55	1.85
(1,129)	1:B:755:LEU:C	1:B:756:ILE:N	1:B:756:ILE:CA	1:B:756:ILE:C	2	1.85	0.05	1.85
(1,34)	1:B:685:PHE:N	1:B:685:PHE:CA	1:B:685:PHE:C	1:B:686:ILE:N	2	1.75	0.15	1.75
(1,113)	1:B:747:ARG:C	1:B:748:LEU:N	1:B:748:LEU:CA	1:B:748:LEU:C	2	1.55	0.05	1.55
(1,128)	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	1:B:756:ILE:N	2	1.55	0.25	1.55
(1,2)	1:B:664:ASP:N	1:B:664:ASP:CA	1:B:664:ASP:C	1:B:665:LYS:N	2	1.45	0.25	1.45
(1,170)	1:B:781:ILE:N	1:B:781:ILE:CA	1:B:781:ILE:C	1:B:782:VAL:N	2	1.45	0.25	1.45
(1,242)	1:B:817:ALA:N	1:B:817:ALA:CA	1:B:817:ALA:C	1:B:818:THR:N	2	1.4	0.1	1.4
(1,248)	1:B:820:ILE:N	1:B:820:ILE:CA	1:B:820:ILE:C	1:B:821:ALA:N	2	1.4	0.3	1.4
(1,35)	1:B:685:PHE:C	1:B:686:ILE:N	1:B:686:ILE:CA	1:B:686:ILE:C	2	1.3	0.1	1.3
(1,168)	1:B:780:ARG:N	1:B:780:ARG:CA	1:B:780:ARG:C	1:B:781:ILE:N	2	1.3	0.1	1.3
(1,111)	1:B:746:ILE:C	1:B:747:ARG:N	1:B:747:ARG:CA	1:B:747:ARG:C	2	1.25	0.15	1.25
(1,225)	1:B:808:LYS:C	1:B:809:ASN:N	1:B:809:ASN:CA	1:B:809:ASN:C	2	1.25	0.05	1.25
(1,55)	1:B:695:LEU:C	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	2	1.2	0.1	1.2
(1,211)	1:B:801:GLN:C	1:B:802:TYR:N	1:B:802:TYR:CA	1:B:802:TYR:C	2	1.2	0.1	1.2
(1,141)	1:B:761:ARG:C	1:B:762:SER:N	1:B:762:SER:CA	1:B:762:SER:C	2	1.15	0.05	1.15
(1,22)	1:B:677:ASN:N	1:B:677:ASN:CA	1:B:677:ASN:C	1:B:678:TRP:N	2	1.1	0.0	1.1

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

## 10.5 All violated dihedral-angle restraints

### 10.5.1 Histogram : Distribution of violations

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,149)	1:B:770:ARG:C	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	8	7.2
(1,148)	1:B:770:ARG:N	1:B:770:ARG:CA	1:B:770:ARG:C	1:B:771:LEU:N	8	7.2
(1,133)	1:B:757:TRP:C	1:B:758:ASP:N	1:B:758:ASP:CA	1:B:758:ASP:C	11	7.1
(1,148)	1:B:770:ARG:N	1:B:770:ARG:CA	1:B:770:ARG:C	1:B:771:LEU:N	11	7.0
(1,149)	1:B:770:ARG:C	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	11	6.8
(1,132)	1:B:757:TRP:N	1:B:757:TRP:CA	1:B:757:TRP:C	1:B:758:ASP:N	11	6.7
(1,126)	1:B:754:ALA:N	1:B:754:ALA:CA	1:B:754:ALA:C	1:B:755:LEU:N	4	6.4
(1,127)	1:B:754:ALA:C	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	4	6.1
(1,188)	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	1:B:791:GLU:N	10	5.4
(1,149)	1:B:770:ARG:C	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	14	5.4
(1,148)	1:B:770:ARG:N	1:B:770:ARG:CA	1:B:770:ARG:C	1:B:771:LEU:N	14	5.4
(1,148)	1:B:770:ARG:N	1:B:770:ARG:CA	1:B:770:ARG:C	1:B:771:LEU:N	12	5.3
(1,126)	1:B:754:ALA:N	1:B:754:ALA:CA	1:B:754:ALA:C	1:B:755:LEU:N	3	5.3
(1,133)	1:B:757:TRP:C	1:B:758:ASP:N	1:B:758:ASP:CA	1:B:758:ASP:C	3	5.1
(1,62)	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1:B:700:ALA:N	14	5.0
(1,149)	1:B:770:ARG:C	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	12	5.0
(1,148)	1:B:770:ARG:N	1:B:770:ARG:CA	1:B:770:ARG:C	1:B:771:LEU:N	15	5.0
(1,62)	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1:B:700:ALA:N	12	4.9
(1,149)	1:B:770:ARG:C	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	15	4.9
(1,148)	1:B:770:ARG:N	1:B:770:ARG:CA	1:B:770:ARG:C	1:B:771:LEU:N	9	4.9
(1,126)	1:B:754:ALA:N	1:B:754:ALA:CA	1:B:754:ALA:C	1:B:755:LEU:N	12	4.9

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,149)	1:B:770:ARG:C	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	9	4.8
(1,127)	1:B:754:ALA:C	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	7	4.8
(1,62)	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1:B:700:ALA:N	15	4.7
(1,188)	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	1:B:791:GLU:N	7	4.7
(1,188)	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	1:B:791:GLU:N	12	4.7
(1,149)	1:B:770:ARG:C	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	3	4.7
(1,149)	1:B:770:ARG:C	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	5	4.7
(1,148)	1:B:770:ARG:N	1:B:770:ARG:CA	1:B:770:ARG:C	1:B:771:LEU:N	3	4.7
(1,127)	1:B:754:ALA:C	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	3	4.7
(1,127)	1:B:754:ALA:C	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	12	4.7
(1,98)	1:B:740:ARG:N	1:B:740:ARG:CA	1:B:740:ARG:C	1:B:741:ASP:N	3	4.6
(1,62)	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1:B:700:ALA:N	1	4.6
(1,62)	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1:B:700:ALA:N	10	4.6
(1,188)	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	1:B:791:GLU:N	8	4.6
(1,149)	1:B:770:ARG:C	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	4	4.6
(1,148)	1:B:770:ARG:N	1:B:770:ARG:CA	1:B:770:ARG:C	1:B:771:LEU:N	13	4.6
(1,188)	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	1:B:791:GLU:N	3	4.5
(1,188)	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	1:B:791:GLU:N	14	4.5
(1,62)	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1:B:700:ALA:N	3	4.4
(1,149)	1:B:770:ARG:C	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	13	4.4
(1,134)	1:B:758:ASP:N	1:B:758:ASP:CA	1:B:758:ASP:C	1:B:759:ASP:N	3	4.4
(1,132)	1:B:757:TRP:N	1:B:757:TRP:CA	1:B:757:TRP:C	1:B:758:ASP:N	3	4.4
(1,56)	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	1:B:697:ILE:N	14	4.3
(1,188)	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	1:B:791:GLU:N	11	4.3
(1,136)	1:B:759:ASP:N	1:B:759:ASP:CA	1:B:759:ASP:C	1:B:760:LEU:N	5	4.3
(1,99)	1:B:740:ARG:C	1:B:741:ASP:N	1:B:741:ASP:CA	1:B:741:ASP:C	3	4.2
(1,63)	1:B:699:PHE:C	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	1	4.2
(1,135)	1:B:758:ASP:C	1:B:759:ASP:N	1:B:759:ASP:CA	1:B:759:ASP:C	3	4.2
(1,63)	1:B:699:PHE:C	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	12	4.1
(1,188)	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	1:B:791:GLU:N	6	4.1
(1,148)	1:B:770:ARG:N	1:B:770:ARG:CA	1:B:770:ARG:C	1:B:771:LEU:N	4	4.1
(1,126)	1:B:754:ALA:N	1:B:754:ALA:CA	1:B:754:ALA:C	1:B:755:LEU:N	7	4.1
(1,62)	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1:B:700:ALA:N	11	3.9
(1,19)	1:B:675:ILE:C	1:B:676:THR:N	1:B:676:THR:CA	1:B:676:THR:C	2	3.9
(1,188)	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	1:B:791:GLU:N	1	3.9
(1,188)	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	1:B:791:GLU:N	4	3.9
(1,127)	1:B:754:ALA:C	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	9	3.9
(1,126)	1:B:754:ALA:N	1:B:754:ALA:CA	1:B:754:ALA:C	1:B:755:LEU:N	9	3.9
(1,62)	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1:B:700:ALA:N	2	3.8
(1,188)	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	1:B:791:GLU:N	13	3.8
(1,148)	1:B:770:ARG:N	1:B:770:ARG:CA	1:B:770:ARG:C	1:B:771:LEU:N	1	3.8
(1,148)	1:B:770:ARG:N	1:B:770:ARG:CA	1:B:770:ARG:C	1:B:771:LEU:N	5	3.8
(1,133)	1:B:757:TRP:C	1:B:758:ASP:N	1:B:758:ASP:CA	1:B:758:ASP:C	5	3.8
(1,63)	1:B:699:PHE:C	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	14	3.7
(1,62)	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1:B:700:ALA:N	9	3.7
(1,188)	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	1:B:791:GLU:N	9	3.7
(1,126)	1:B:754:ALA:N	1:B:754:ALA:CA	1:B:754:ALA:C	1:B:755:LEU:N	11	3.7
(1,63)	1:B:699:PHE:C	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	10	3.6
(1,56)	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	1:B:697:ILE:N	9	3.6
(1,154)	1:B:773:ASP:N	1:B:773:ASP:CA	1:B:773:ASP:C	1:B:774:LEU:N	3	3.6
(1,149)	1:B:770:ARG:C	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	1	3.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,145)	1:B:763:LEU:C	1:B:764:SER:N	1:B:764:SER:CA	1:B:764:SER:C	2	3.6
(1,136)	1:B:759:ASP:N	1:B:759:ASP:CA	1:B:759:ASP:C	1:B:760:LEU:N	3	3.6
(1,134)	1:B:758:ASP:N	1:B:758:ASP:CA	1:B:758:ASP:C	1:B:759:ASP:N	11	3.6
(1,118)	1:B:750:ASN:N	1:B:750:ASN:CA	1:B:750:ASN:C	1:B:751:GLY:N	11	3.6
(1,62)	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1:B:700:ALA:N	7	3.5
(1,62)	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1:B:700:ALA:N	13	3.5
(1,251)	1:B:826:THR:C	1:B:827:ASP:N	1:B:827:ASP:CA	1:B:827:ASP:C	15	3.5
(1,63)	1:B:699:PHE:C	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	3	3.4
(1,63)	1:B:699:PHE:C	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	15	3.4
(1,62)	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1:B:700:ALA:N	8	3.4
(1,212)	1:B:802:TYR:N	1:B:802:TYR:CA	1:B:802:TYR:C	1:B:803:TRP:N	9	3.4
(1,196)	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	1:B:795:TYR:N	12	3.4
(1,188)	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	1:B:791:GLU:N	5	3.4
(1,148)	1:B:770:ARG:N	1:B:770:ARG:CA	1:B:770:ARG:C	1:B:771:LEU:N	6	3.4
(1,126)	1:B:754:ALA:N	1:B:754:ALA:CA	1:B:754:ALA:C	1:B:755:LEU:N	14	3.4
(1,119)	1:B:750:ASN:C	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	6	3.4
(1,63)	1:B:699:PHE:C	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	11	3.3
(1,149)	1:B:770:ARG:C	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	6	3.3
(1,127)	1:B:754:ALA:C	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	8	3.3
(1,126)	1:B:754:ALA:N	1:B:754:ALA:CA	1:B:754:ALA:C	1:B:755:LEU:N	2	3.3
(1,126)	1:B:754:ALA:N	1:B:754:ALA:CA	1:B:754:ALA:C	1:B:755:LEU:N	8	3.3
(1,119)	1:B:750:ASN:C	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	3	3.3
(1,118)	1:B:750:ASN:N	1:B:750:ASN:CA	1:B:750:ASN:C	1:B:751:GLY:N	2	3.3
(1,62)	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1:B:700:ALA:N	6	3.2
(1,18)	1:B:675:ILE:N	1:B:675:ILE:CA	1:B:675:ILE:C	1:B:676:THR:N	13	3.2
(1,155)	1:B:773:ASP:C	1:B:774:LEU:N	1:B:774:LEU:CA	1:B:774:LEU:C	3	3.2
(1,148)	1:B:770:ARG:N	1:B:770:ARG:CA	1:B:770:ARG:C	1:B:771:LEU:N	7	3.2
(1,142)	1:B:762:SER:N	1:B:762:SER:CA	1:B:762:SER:C	1:B:763:LEU:N	8	3.2
(1,142)	1:B:762:SER:N	1:B:762:SER:CA	1:B:762:SER:C	1:B:763:LEU:N	12	3.2
(1,119)	1:B:750:ASN:C	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	15	3.2
(1,81)	1:B:708:VAL:C	1:B:709:ARG:N	1:B:709:ARG:CA	1:B:709:ARG:C	2	3.1
(1,57)	1:B:696:ARG:C	1:B:697:ILE:N	1:B:697:ILE:CA	1:B:697:ILE:C	14	3.1
(1,210)	1:B:801:GLN:N	1:B:801:GLN:CA	1:B:801:GLN:C	1:B:802:TYR:N	9	3.1
(1,143)	1:B:762:SER:C	1:B:763:LEU:N	1:B:763:LEU:CA	1:B:763:LEU:C	12	3.1
(1,142)	1:B:762:SER:N	1:B:762:SER:CA	1:B:762:SER:C	1:B:763:LEU:N	15	3.1
(1,135)	1:B:758:ASP:C	1:B:759:ASP:N	1:B:759:ASP:CA	1:B:759:ASP:C	5	3.1
(1,135)	1:B:758:ASP:C	1:B:759:ASP:N	1:B:759:ASP:CA	1:B:759:ASP:C	11	3.1
(1,132)	1:B:757:TRP:N	1:B:757:TRP:CA	1:B:757:TRP:C	1:B:758:ASP:N	5	3.1
(1,127)	1:B:754:ALA:C	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	11	3.1
(1,127)	1:B:754:ALA:C	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	14	3.1
(1,127)	1:B:754:ALA:C	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	15	3.1
(1,119)	1:B:750:ASN:C	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	11	3.1
(1,118)	1:B:750:ASN:N	1:B:750:ASN:CA	1:B:750:ASN:C	1:B:751:GLY:N	3	3.1
(1,63)	1:B:699:PHE:C	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	7	3.0
(1,61)	1:B:698:VAL:C	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	11	3.0
(1,56)	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	1:B:697:ILE:N	4	3.0
(1,20)	1:B:676:THR:N	1:B:676:THR:CA	1:B:676:THR:C	1:B:677:ASN:N	2	3.0
(1,19)	1:B:675:ILE:C	1:B:676:THR:N	1:B:676:THR:CA	1:B:676:THR:C	13	3.0
(1,188)	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	1:B:791:GLU:N	2	3.0
(1,18)	1:B:675:ILE:N	1:B:675:ILE:CA	1:B:675:ILE:C	1:B:676:THR:N	2	3.0
(1,156)	1:B:774:LEU:N	1:B:774:LEU:CA	1:B:774:LEU:C	1:B:775:LEU:N	2	3.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,137)	1:B:759:ASP:C	1:B:760:LEU:N	1:B:760:LEU:CA	1:B:760:LEU:C	5	3.0
(1,127)	1:B:754:ALA:C	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	2	3.0
(1,80)	1:B:708:VAL:N	1:B:708:VAL:CA	1:B:708:VAL:C	1:B:709:ARG:N	12	2.9
(1,188)	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	1:B:791:GLU:N	15	2.9
(1,162)	1:B:777:ILE:N	1:B:777:ILE:CA	1:B:777:ILE:C	1:B:778:VAL:N	14	2.9
(1,148)	1:B:770:ARG:N	1:B:770:ARG:CA	1:B:770:ARG:C	1:B:771:LEU:N	10	2.9
(1,144)	1:B:763:LEU:N	1:B:763:LEU:CA	1:B:763:LEU:C	1:B:764:SER:N	2	2.9
(1,134)	1:B:758:ASP:N	1:B:758:ASP:CA	1:B:758:ASP:C	1:B:759:ASP:N	5	2.9
(1,119)	1:B:750:ASN:C	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	2	2.9
(1,119)	1:B:750:ASN:C	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	5	2.9
(1,119)	1:B:750:ASN:C	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	7	2.9
(1,118)	1:B:750:ASN:N	1:B:750:ASN:CA	1:B:750:ASN:C	1:B:751:GLY:N	7	2.9
(1,88)	1:B:715:LEU:N	1:B:715:LEU:CA	1:B:715:LEU:C	1:B:716:SER:N	9	2.8
(1,63)	1:B:699:PHE:C	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	2	2.8
(1,63)	1:B:699:PHE:C	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	9	2.8
(1,56)	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	1:B:697:ILE:N	13	2.8
(1,162)	1:B:777:ILE:N	1:B:777:ILE:CA	1:B:777:ILE:C	1:B:778:VAL:N	2	2.8
(1,126)	1:B:754:ALA:N	1:B:754:ALA:CA	1:B:754:ALA:C	1:B:755:LEU:N	1	2.8
(1,120)	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	1:B:752:SER:N	5	2.8
(1,119)	1:B:750:ASN:C	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	1	2.8
(1,118)	1:B:750:ASN:N	1:B:750:ASN:CA	1:B:750:ASN:C	1:B:751:GLY:N	6	2.8
(1,118)	1:B:750:ASN:N	1:B:750:ASN:CA	1:B:750:ASN:C	1:B:751:GLY:N	15	2.8
(1,85)	1:B:712:TYR:C	1:B:713:SER:N	1:B:713:SER:CA	1:B:713:SER:C	5	2.7
(1,83)	1:B:709:ARG:C	1:B:710:GLN:N	1:B:710:GLN:CA	1:B:710:GLN:C	3	2.7
(1,81)	1:B:708:VAL:C	1:B:709:ARG:N	1:B:709:ARG:CA	1:B:709:ARG:C	12	2.7
(1,62)	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1:B:700:ALA:N	4	2.7
(1,58)	1:B:697:ILE:N	1:B:697:ILE:CA	1:B:697:ILE:C	1:B:698:VAL:N	3	2.7
(1,56)	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	1:B:697:ILE:N	1	2.7
(1,272)	1:B:837:SER:N	1:B:837:SER:CA	1:B:837:SER:C	1:B:838:ARG:N	5	2.7
(1,251)	1:B:826:THR:C	1:B:827:ASP:N	1:B:827:ASP:CA	1:B:827:ASP:C	6	2.7
(1,21)	1:B:676:THR:C	1:B:677:ASN:N	1:B:677:ASN:CA	1:B:677:ASN:C	2	2.7
(1,195)	1:B:793:LEU:C	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	13	2.7
(1,19)	1:B:675:ILE:C	1:B:676:THR:N	1:B:676:THR:CA	1:B:676:THR:C	8	2.7
(1,19)	1:B:675:ILE:C	1:B:676:THR:N	1:B:676:THR:CA	1:B:676:THR:C	9	2.7
(1,18)	1:B:675:ILE:N	1:B:675:ILE:CA	1:B:675:ILE:C	1:B:676:THR:N	9	2.7
(1,143)	1:B:762:SER:C	1:B:763:LEU:N	1:B:763:LEU:CA	1:B:763:LEU:C	7	2.7
(1,143)	1:B:762:SER:C	1:B:763:LEU:N	1:B:763:LEU:CA	1:B:763:LEU:C	15	2.7
(1,142)	1:B:762:SER:N	1:B:762:SER:CA	1:B:762:SER:C	1:B:763:LEU:N	11	2.7
(1,80)	1:B:708:VAL:N	1:B:708:VAL:CA	1:B:708:VAL:C	1:B:709:ARG:N	2	2.6
(1,60)	1:B:698:VAL:N	1:B:698:VAL:CA	1:B:698:VAL:C	1:B:699:PHE:N	11	2.6
(1,197)	1:B:794:LYS:C	1:B:795:TYR:N	1:B:795:TYR:CA	1:B:795:TYR:C	12	2.6
(1,195)	1:B:793:LEU:C	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	5	2.6
(1,189)	1:B:790:TRP:C	1:B:791:GLU:N	1:B:791:GLU:CA	1:B:791:GLU:C	11	2.6
(1,18)	1:B:675:ILE:N	1:B:675:ILE:CA	1:B:675:ILE:C	1:B:676:THR:N	8	2.6
(1,145)	1:B:763:LEU:C	1:B:764:SER:N	1:B:764:SER:CA	1:B:764:SER:C	7	2.6
(1,145)	1:B:763:LEU:C	1:B:764:SER:N	1:B:764:SER:CA	1:B:764:SER:C	9	2.6
(1,126)	1:B:754:ALA:N	1:B:754:ALA:CA	1:B:754:ALA:C	1:B:755:LEU:N	15	2.6
(1,120)	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	1:B:752:SER:N	6	2.6
(1,63)	1:B:699:PHE:C	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	6	2.5
(1,57)	1:B:696:ARG:C	1:B:697:ILE:N	1:B:697:ILE:CA	1:B:697:ILE:C	9	2.5
(1,195)	1:B:793:LEU:C	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	9	2.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,19)	1:B:675:ILE:C	1:B:676:THR:N	1:B:676:THR:CA	1:B:676:THR:C	11	2.5
(1,142)	1:B:762:SER:N	1:B:762:SER:CA	1:B:762:SER:C	1:B:763:LEU:N	7	2.5
(1,137)	1:B:759:ASP:C	1:B:760:LEU:N	1:B:760:LEU:CA	1:B:760:LEU:C	3	2.5
(1,119)	1:B:750:ASN:C	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	12	2.5
(1,98)	1:B:740:ARG:N	1:B:740:ARG:CA	1:B:740:ARG:C	1:B:741:ASP:N	7	2.4
(1,81)	1:B:708:VAL:C	1:B:709:ARG:N	1:B:709:ARG:CA	1:B:709:ARG:C	13	2.4
(1,63)	1:B:699:PHE:C	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	8	2.4
(1,61)	1:B:698:VAL:C	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	3	2.4
(1,56)	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	1:B:697:ILE:N	10	2.4
(1,46)	1:B:691:SER:N	1:B:691:SER:CA	1:B:691:SER:C	1:B:692:LEU:N	1	2.4
(1,3)	1:B:664:ASP:C	1:B:665:LYS:N	1:B:665:LYS:CA	1:B:665:LYS:C	9	2.4
(1,270)	1:B:836:ALA:N	1:B:836:ALA:CA	1:B:836:ALA:C	1:B:837:SER:N	4	2.4
(1,247)	1:B:819:ALA:C	1:B:820:ILE:N	1:B:820:ILE:CA	1:B:820:ILE:C	13	2.4
(1,20)	1:B:676:THR:N	1:B:676:THR:CA	1:B:676:THR:C	1:B:677:ASN:N	8	2.4
(1,194)	1:B:793:LEU:N	1:B:793:LEU:CA	1:B:793:LEU:C	1:B:794:LYS:N	5	2.4
(1,18)	1:B:675:ILE:N	1:B:675:ILE:CA	1:B:675:ILE:C	1:B:676:THR:N	10	2.4
(1,149)	1:B:770:ARG:C	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	10	2.4
(1,148)	1:B:770:ARG:N	1:B:770:ARG:CA	1:B:770:ARG:C	1:B:771:LEU:N	2	2.4
(1,143)	1:B:762:SER:C	1:B:763:LEU:N	1:B:763:LEU:CA	1:B:763:LEU:C	11	2.4
(1,132)	1:B:757:TRP:N	1:B:757:TRP:CA	1:B:757:TRP:C	1:B:758:ASP:N	2	2.4
(1,132)	1:B:757:TRP:N	1:B:757:TRP:CA	1:B:757:TRP:C	1:B:758:ASP:N	4	2.4
(1,127)	1:B:754:ALA:C	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	1	2.4
(1,126)	1:B:754:ALA:N	1:B:754:ALA:CA	1:B:754:ALA:C	1:B:755:LEU:N	5	2.4
(1,119)	1:B:750:ASN:C	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	9	2.4
(1,119)	1:B:750:ASN:C	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	13	2.4
(1,63)	1:B:699:PHE:C	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	13	2.3
(1,57)	1:B:696:ARG:C	1:B:697:ILE:N	1:B:697:ILE:CA	1:B:697:ILE:C	4	2.3
(1,56)	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	1:B:697:ILE:N	2	2.3
(1,270)	1:B:836:ALA:N	1:B:836:ALA:CA	1:B:836:ALA:C	1:B:837:SER:N	5	2.3
(1,197)	1:B:794:LYS:C	1:B:795:TYR:N	1:B:795:TYR:CA	1:B:795:TYR:C	14	2.3
(1,196)	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	1:B:795:TYR:N	13	2.3
(1,195)	1:B:793:LEU:C	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	7	2.3
(1,195)	1:B:793:LEU:C	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	12	2.3
(1,19)	1:B:675:ILE:C	1:B:676:THR:N	1:B:676:THR:CA	1:B:676:THR:C	10	2.3
(1,185)	1:B:788:ARG:C	1:B:789:GLY:N	1:B:789:GLY:CA	1:B:789:GLY:C	11	2.3
(1,158)	1:B:775:LEU:N	1:B:775:LEU:CA	1:B:775:LEU:C	1:B:776:LEU:N	15	2.3
(1,145)	1:B:763:LEU:C	1:B:764:SER:N	1:B:764:SER:CA	1:B:764:SER:C	11	2.3
(1,143)	1:B:762:SER:C	1:B:763:LEU:N	1:B:763:LEU:CA	1:B:763:LEU:C	8	2.3
(1,133)	1:B:757:TRP:C	1:B:758:ASP:N	1:B:758:ASP:CA	1:B:758:ASP:C	4	2.3
(1,98)	1:B:740:ARG:N	1:B:740:ARG:CA	1:B:740:ARG:C	1:B:741:ASP:N	6	2.2
(1,87)	1:B:714:PRO:C	1:B:715:LEU:N	1:B:715:LEU:CA	1:B:715:LEU:C	9	2.2
(1,69)	1:B:702:LEU:C	1:B:703:SER:N	1:B:703:SER:CA	1:B:703:SER:C	3	2.2
(1,68)	1:B:702:LEU:N	1:B:702:LEU:CA	1:B:702:LEU:C	1:B:703:SER:N	3	2.2
(1,62)	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1:B:700:ALA:N	5	2.2
(1,57)	1:B:696:ARG:C	1:B:697:ILE:N	1:B:697:ILE:CA	1:B:697:ILE:C	13	2.2
(1,28)	1:B:682:ILE:N	1:B:682:ILE:CA	1:B:682:ILE:C	1:B:683:ARG:N	10	2.2
(1,271)	1:B:836:ALA:C	1:B:837:SER:N	1:B:837:SER:CA	1:B:837:SER:C	4	2.2
(1,195)	1:B:793:LEU:C	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	8	2.2
(1,189)	1:B:790:TRP:C	1:B:791:GLU:N	1:B:791:GLU:CA	1:B:791:GLU:C	10	2.2
(1,189)	1:B:790:TRP:C	1:B:791:GLU:N	1:B:791:GLU:CA	1:B:791:GLU:C	12	2.2
(1,189)	1:B:790:TRP:C	1:B:791:GLU:N	1:B:791:GLU:CA	1:B:791:GLU:C	13	2.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,163)	1:B:777:ILE:C	1:B:778:VAL:N	1:B:778:VAL:CA	1:B:778:VAL:C	2	2.2
(1,149)	1:B:770:ARG:C	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	2	2.2
(1,149)	1:B:770:ARG:C	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	7	2.2
(1,145)	1:B:763:LEU:C	1:B:764:SER:N	1:B:764:SER:CA	1:B:764:SER:C	14	2.2
(1,133)	1:B:757:TRP:C	1:B:758:ASP:N	1:B:758:ASP:CA	1:B:758:ASP:C	2	2.2
(1,126)	1:B:754:ALA:N	1:B:754:ALA:CA	1:B:754:ALA:C	1:B:755:LEU:N	6	2.2
(1,121)	1:B:751:GLY:C	1:B:752:SER:N	1:B:752:SER:CA	1:B:752:SER:C	5	2.2
(1,120)	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	1:B:752:SER:N	9	2.2
(1,118)	1:B:750:ASN:N	1:B:750:ASN:CA	1:B:750:ASN:C	1:B:751:GLY:N	12	2.2
(1,99)	1:B:740:ARG:C	1:B:741:ASP:N	1:B:741:ASP:CA	1:B:741:ASP:C	7	2.1
(1,85)	1:B:712:TYR:C	1:B:713:SER:N	1:B:713:SER:CA	1:B:713:SER:C	4	2.1
(1,63)	1:B:699:PHE:C	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	4	2.1
(1,59)	1:B:697:ILE:C	1:B:698:VAL:N	1:B:698:VAL:CA	1:B:698:VAL:C	3	2.1
(1,46)	1:B:691:SER:N	1:B:691:SER:CA	1:B:691:SER:C	1:B:692:LEU:N	13	2.1
(1,271)	1:B:836:ALA:C	1:B:837:SER:N	1:B:837:SER:CA	1:B:837:SER:C	5	2.1
(1,196)	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	1:B:795:TYR:N	5	2.1
(1,196)	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	1:B:795:TYR:N	15	2.1
(1,195)	1:B:793:LEU:C	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	2	2.1
(1,189)	1:B:790:TRP:C	1:B:791:GLU:N	1:B:791:GLU:CA	1:B:791:GLU:C	1	2.1
(1,18)	1:B:675:ILE:N	1:B:675:ILE:CA	1:B:675:ILE:C	1:B:676:THR:N	11	2.1
(1,162)	1:B:777:ILE:N	1:B:777:ILE:CA	1:B:777:ILE:C	1:B:778:VAL:N	5	2.1
(1,157)	1:B:774:LEU:C	1:B:775:LEU:N	1:B:775:LEU:CA	1:B:775:LEU:C	2	2.1
(1,145)	1:B:763:LEU:C	1:B:764:SER:N	1:B:764:SER:CA	1:B:764:SER:C	1	2.1
(1,145)	1:B:763:LEU:C	1:B:764:SER:N	1:B:764:SER:CA	1:B:764:SER:C	5	2.1
(1,145)	1:B:763:LEU:C	1:B:764:SER:N	1:B:764:SER:CA	1:B:764:SER:C	6	2.1
(1,145)	1:B:763:LEU:C	1:B:764:SER:N	1:B:764:SER:CA	1:B:764:SER:C	13	2.1
(1,121)	1:B:751:GLY:C	1:B:752:SER:N	1:B:752:SER:CA	1:B:752:SER:C	9	2.1
(1,119)	1:B:750:ASN:C	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	4	2.1
(1,118)	1:B:750:ASN:N	1:B:750:ASN:CA	1:B:750:ASN:C	1:B:751:GLY:N	1	2.1
(1,99)	1:B:740:ARG:C	1:B:741:ASP:N	1:B:741:ASP:CA	1:B:741:ASP:C	5	2.0
(1,99)	1:B:740:ARG:C	1:B:741:ASP:N	1:B:741:ASP:CA	1:B:741:ASP:C	6	2.0
(1,98)	1:B:740:ARG:N	1:B:740:ARG:CA	1:B:740:ARG:C	1:B:741:ASP:N	5	2.0
(1,98)	1:B:740:ARG:N	1:B:740:ARG:CA	1:B:740:ARG:C	1:B:741:ASP:N	8	2.0
(1,98)	1:B:740:ARG:N	1:B:740:ARG:CA	1:B:740:ARG:C	1:B:741:ASP:N	12	2.0
(1,60)	1:B:698:VAL:N	1:B:698:VAL:CA	1:B:698:VAL:C	1:B:699:PHE:N	3	2.0
(1,57)	1:B:696:ARG:C	1:B:697:ILE:N	1:B:697:ILE:CA	1:B:697:ILE:C	1	2.0
(1,56)	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	1:B:697:ILE:N	11	2.0
(1,195)	1:B:793:LEU:C	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	4	2.0
(1,191)	1:B:791:GLU:C	1:B:792:ALA:N	1:B:792:ALA:CA	1:B:792:ALA:C	11	2.0
(1,19)	1:B:675:ILE:C	1:B:676:THR:N	1:B:676:THR:CA	1:B:676:THR:C	4	2.0
(1,19)	1:B:675:ILE:C	1:B:676:THR:N	1:B:676:THR:CA	1:B:676:THR:C	6	2.0
(1,189)	1:B:790:TRP:C	1:B:791:GLU:N	1:B:791:GLU:CA	1:B:791:GLU:C	3	2.0
(1,169)	1:B:780:ARG:C	1:B:781:ILE:N	1:B:781:ILE:CA	1:B:781:ILE:C	15	2.0
(1,158)	1:B:775:LEU:N	1:B:775:LEU:CA	1:B:775:LEU:C	1:B:776:LEU:N	1	2.0
(1,154)	1:B:773:ASP:N	1:B:773:ASP:CA	1:B:773:ASP:C	1:B:774:LEU:N	10	2.0
(1,143)	1:B:762:SER:C	1:B:763:LEU:N	1:B:763:LEU:CA	1:B:763:LEU:C	10	2.0
(1,142)	1:B:762:SER:N	1:B:762:SER:CA	1:B:762:SER:C	1:B:763:LEU:N	10	2.0
(1,136)	1:B:759:ASP:N	1:B:759:ASP:CA	1:B:759:ASP:C	1:B:760:LEU:N	11	2.0
(1,131)	1:B:756:ILE:C	1:B:757:TRP:N	1:B:757:TRP:CA	1:B:757:TRP:C	2	2.0
(1,127)	1:B:754:ALA:C	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	5	2.0
(1,127)	1:B:754:ALA:C	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	13	2.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,88)	1:B:715:LEU:N	1:B:715:LEU:CA	1:B:715:LEU:C	1:B:716:SER:N	10	1.9
(1,84)	1:B:710:GLN:N	1:B:710:GLN:CA	1:B:710:GLN:C	1:B:711:GLY:N	4	1.9
(1,83)	1:B:709:ARG:C	1:B:710:GLN:N	1:B:710:GLN:CA	1:B:710:GLN:C	7	1.9
(1,63)	1:B:699:PHE:C	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	5	1.9
(1,61)	1:B:698:VAL:C	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	14	1.9
(1,57)	1:B:696:ARG:C	1:B:697:ILE:N	1:B:697:ILE:CA	1:B:697:ILE:C	6	1.9
(1,56)	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	1:B:697:ILE:N	6	1.9
(1,34)	1:B:685:PHE:N	1:B:685:PHE:CA	1:B:685:PHE:C	1:B:686:ILE:N	10	1.9
(1,29)	1:B:682:ILE:C	1:B:683:ARG:N	1:B:683:ARG:CA	1:B:683:ARG:C	10	1.9
(1,274)	1:B:838:ARG:N	1:B:838:ARG:CA	1:B:838:ARG:C	1:B:839:ALA:N	2	1.9
(1,251)	1:B:826:THR:C	1:B:827:ASP:N	1:B:827:ASP:CA	1:B:827:ASP:C	4	1.9
(1,251)	1:B:826:THR:C	1:B:827:ASP:N	1:B:827:ASP:CA	1:B:827:ASP:C	13	1.9
(1,21)	1:B:676:THR:C	1:B:677:ASN:N	1:B:677:ASN:CA	1:B:677:ASN:C	8	1.9
(1,189)	1:B:790:TRP:C	1:B:791:GLU:N	1:B:791:GLU:CA	1:B:791:GLU:C	7	1.9
(1,189)	1:B:790:TRP:C	1:B:791:GLU:N	1:B:791:GLU:CA	1:B:791:GLU:C	9	1.9
(1,184)	1:B:788:ARG:N	1:B:788:ARG:CA	1:B:788:ARG:C	1:B:789:GLY:N	11	1.9
(1,162)	1:B:777:ILE:N	1:B:777:ILE:CA	1:B:777:ILE:C	1:B:778:VAL:N	11	1.9
(1,155)	1:B:773:ASP:C	1:B:774:LEU:N	1:B:774:LEU:CA	1:B:774:LEU:C	10	1.9
(1,154)	1:B:773:ASP:N	1:B:773:ASP:CA	1:B:773:ASP:C	1:B:774:LEU:N	2	1.9
(1,151)	1:B:771:LEU:C	1:B:772:ARG:N	1:B:772:ARG:CA	1:B:772:ARG:C	14	1.9
(1,142)	1:B:762:SER:N	1:B:762:SER:CA	1:B:762:SER:C	1:B:763:LEU:N	14	1.9
(1,132)	1:B:757:TRP:N	1:B:757:TRP:CA	1:B:757:TRP:C	1:B:758:ASP:N	8	1.9
(1,129)	1:B:755:LEU:C	1:B:756:ILE:N	1:B:756:ILE:CA	1:B:756:ILE:C	7	1.9
(1,118)	1:B:750:ASN:N	1:B:750:ASN:CA	1:B:750:ASN:C	1:B:751:GLY:N	13	1.9
(1,99)	1:B:740:ARG:C	1:B:741:ASP:N	1:B:741:ASP:CA	1:B:741:ASP:C	8	1.8
(1,98)	1:B:740:ARG:N	1:B:740:ARG:CA	1:B:740:ARG:C	1:B:741:ASP:N	1	1.8
(1,98)	1:B:740:ARG:N	1:B:740:ARG:CA	1:B:740:ARG:C	1:B:741:ASP:N	11	1.8
(1,87)	1:B:714:PRO:C	1:B:715:LEU:N	1:B:715:LEU:CA	1:B:715:LEU:C	1	1.8
(1,87)	1:B:714:PRO:C	1:B:715:LEU:N	1:B:715:LEU:CA	1:B:715:LEU:C	14	1.8
(1,81)	1:B:708:VAL:C	1:B:709:ARG:N	1:B:709:ARG:CA	1:B:709:ARG:C	14	1.8
(1,80)	1:B:708:VAL:N	1:B:708:VAL:CA	1:B:708:VAL:C	1:B:709:ARG:N	3	1.8
(1,69)	1:B:702:LEU:C	1:B:703:SER:N	1:B:703:SER:CA	1:B:703:SER:C	4	1.8
(1,69)	1:B:702:LEU:C	1:B:703:SER:N	1:B:703:SER:CA	1:B:703:SER:C	11	1.8
(1,68)	1:B:702:LEU:N	1:B:702:LEU:CA	1:B:702:LEU:C	1:B:703:SER:N	5	1.8
(1,56)	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	1:B:697:ILE:N	5	1.8
(1,47)	1:B:691:SER:C	1:B:692:LEU:N	1:B:692:LEU:CA	1:B:692:LEU:C	1	1.8
(1,272)	1:B:837:SER:N	1:B:837:SER:CA	1:B:837:SER:C	1:B:838:ARG:N	2	1.8
(1,270)	1:B:836:ALA:N	1:B:836:ALA:CA	1:B:836:ALA:C	1:B:837:SER:N	2	1.8
(1,251)	1:B:826:THR:C	1:B:827:ASP:N	1:B:827:ASP:CA	1:B:827:ASP:C	1	1.8
(1,250)	1:B:826:THR:N	1:B:826:THR:CA	1:B:826:THR:C	1:B:827:ASP:N	6	1.8
(1,19)	1:B:675:ILE:C	1:B:676:THR:N	1:B:676:THR:CA	1:B:676:THR:C	12	1.8
(1,18)	1:B:675:ILE:N	1:B:675:ILE:CA	1:B:675:ILE:C	1:B:676:THR:N	4	1.8
(1,172)	1:B:782:VAL:N	1:B:782:VAL:CA	1:B:782:VAL:C	1:B:783:GLU:N	13	1.8
(1,163)	1:B:777:ILE:C	1:B:778:VAL:N	1:B:778:VAL:CA	1:B:778:VAL:C	1	1.8
(1,144)	1:B:763:LEU:N	1:B:763:LEU:CA	1:B:763:LEU:C	1:B:764:SER:N	13	1.8
(1,143)	1:B:762:SER:C	1:B:763:LEU:N	1:B:763:LEU:CA	1:B:763:LEU:C	14	1.8
(1,132)	1:B:757:TRP:N	1:B:757:TRP:CA	1:B:757:TRP:C	1:B:758:ASP:N	7	1.8
(1,129)	1:B:755:LEU:C	1:B:756:ILE:N	1:B:756:ILE:CA	1:B:756:ILE:C	2	1.8
(1,128)	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	1:B:756:ILE:N	11	1.8
(1,127)	1:B:754:ALA:C	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	10	1.8
(1,121)	1:B:751:GLY:C	1:B:752:SER:N	1:B:752:SER:CA	1:B:752:SER:C	1	1.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,120)	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	1:B:752:SER:N	11	1.8
(1,118)	1:B:750:ASN:N	1:B:750:ASN:CA	1:B:750:ASN:C	1:B:751:GLY:N	5	1.8
(1,86)	1:B:713:SER:N	1:B:713:SER:CA	1:B:713:SER:C	1:B:714:PRO:N	12	1.7
(1,80)	1:B:708:VAL:N	1:B:708:VAL:CA	1:B:708:VAL:C	1:B:709:ARG:N	13	1.7
(1,69)	1:B:702:LEU:C	1:B:703:SER:N	1:B:703:SER:CA	1:B:703:SER:C	14	1.7
(1,68)	1:B:702:LEU:N	1:B:702:LEU:CA	1:B:702:LEU:C	1:B:703:SER:N	13	1.7
(1,61)	1:B:698:VAL:C	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	15	1.7
(1,57)	1:B:696:ARG:C	1:B:697:ILE:N	1:B:697:ILE:CA	1:B:697:ILE:C	2	1.7
(1,57)	1:B:696:ARG:C	1:B:697:ILE:N	1:B:697:ILE:CA	1:B:697:ILE:C	11	1.7
(1,56)	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	1:B:697:ILE:N	12	1.7
(1,54)	1:B:695:LEU:N	1:B:695:LEU:CA	1:B:695:LEU:C	1:B:696:ARG:N	12	1.7
(1,251)	1:B:826:THR:C	1:B:827:ASP:N	1:B:827:ASP:CA	1:B:827:ASP:C	10	1.7
(1,248)	1:B:820:ILE:N	1:B:820:ILE:CA	1:B:820:ILE:C	1:B:821:ALA:N	12	1.7
(1,213)	1:B:802:TYR:C	1:B:803:TRP:N	1:B:803:TRP:CA	1:B:803:TRP:C	9	1.7
(1,2)	1:B:664:ASP:N	1:B:664:ASP:CA	1:B:664:ASP:C	1:B:665:LYS:N	9	1.7
(1,170)	1:B:781:ILE:N	1:B:781:ILE:CA	1:B:781:ILE:C	1:B:782:VAL:N	15	1.7
(1,156)	1:B:774:LEU:N	1:B:774:LEU:CA	1:B:774:LEU:C	1:B:775:LEU:N	14	1.7
(1,155)	1:B:773:ASP:C	1:B:774:LEU:N	1:B:774:LEU:CA	1:B:774:LEU:C	6	1.7
(1,154)	1:B:773:ASP:N	1:B:773:ASP:CA	1:B:773:ASP:C	1:B:774:LEU:N	13	1.7
(1,137)	1:B:759:ASP:C	1:B:760:LEU:N	1:B:760:LEU:CA	1:B:760:LEU:C	1	1.7
(1,136)	1:B:759:ASP:N	1:B:759:ASP:CA	1:B:759:ASP:C	1:B:760:LEU:N	2	1.7
(1,126)	1:B:754:ALA:N	1:B:754:ALA:CA	1:B:754:ALA:C	1:B:755:LEU:N	10	1.7
(1,126)	1:B:754:ALA:N	1:B:754:ALA:CA	1:B:754:ALA:C	1:B:755:LEU:N	13	1.7
(1,120)	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	1:B:752:SER:N	1	1.7
(1,119)	1:B:750:ASN:C	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	10	1.7
(1,118)	1:B:750:ASN:N	1:B:750:ASN:CA	1:B:750:ASN:C	1:B:751:GLY:N	4	1.7
(1,99)	1:B:740:ARG:C	1:B:741:ASP:N	1:B:741:ASP:CA	1:B:741:ASP:C	11	1.6
(1,87)	1:B:714:PRO:C	1:B:715:LEU:N	1:B:715:LEU:CA	1:B:715:LEU:C	2	1.6
(1,86)	1:B:713:SER:N	1:B:713:SER:CA	1:B:713:SER:C	1:B:714:PRO:N	5	1.6
(1,86)	1:B:713:SER:N	1:B:713:SER:CA	1:B:713:SER:C	1:B:714:PRO:N	11	1.6
(1,86)	1:B:713:SER:N	1:B:713:SER:CA	1:B:713:SER:C	1:B:714:PRO:N	14	1.6
(1,83)	1:B:709:ARG:C	1:B:710:GLN:N	1:B:710:GLN:CA	1:B:710:GLN:C	9	1.6
(1,81)	1:B:708:VAL:C	1:B:709:ARG:N	1:B:709:ARG:CA	1:B:709:ARG:C	6	1.6
(1,68)	1:B:702:LEU:N	1:B:702:LEU:CA	1:B:702:LEU:C	1:B:703:SER:N	6	1.6
(1,61)	1:B:698:VAL:C	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	10	1.6
(1,46)	1:B:691:SER:N	1:B:691:SER:CA	1:B:691:SER:C	1:B:692:LEU:N	7	1.6
(1,46)	1:B:691:SER:N	1:B:691:SER:CA	1:B:691:SER:C	1:B:692:LEU:N	14	1.6
(1,34)	1:B:685:PHE:N	1:B:685:PHE:CA	1:B:685:PHE:C	1:B:686:ILE:N	15	1.6
(1,272)	1:B:837:SER:N	1:B:837:SER:CA	1:B:837:SER:C	1:B:838:ARG:N	4	1.6
(1,250)	1:B:826:THR:N	1:B:826:THR:CA	1:B:826:THR:C	1:B:827:ASP:N	1	1.6
(1,250)	1:B:826:THR:N	1:B:826:THR:CA	1:B:826:THR:C	1:B:827:ASP:N	4	1.6
(1,222)	1:B:807:LEU:N	1:B:807:LEU:CA	1:B:807:LEU:C	1:B:808:LYS:N	4	1.6
(1,210)	1:B:801:GLN:N	1:B:801:GLN:CA	1:B:801:GLN:C	1:B:802:TYR:N	13	1.6
(1,202)	1:B:797:TRP:N	1:B:797:TRP:CA	1:B:797:TRP:C	1:B:798:ASN:N	9	1.6
(1,195)	1:B:793:LEU:C	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	6	1.6
(1,189)	1:B:790:TRP:C	1:B:791:GLU:N	1:B:791:GLU:CA	1:B:791:GLU:C	5	1.6
(1,18)	1:B:675:ILE:N	1:B:675:ILE:CA	1:B:675:ILE:C	1:B:676:THR:N	6	1.6
(1,162)	1:B:777:ILE:N	1:B:777:ILE:CA	1:B:777:ILE:C	1:B:778:VAL:N	12	1.6
(1,154)	1:B:773:ASP:N	1:B:773:ASP:CA	1:B:773:ASP:C	1:B:774:LEU:N	5	1.6
(1,154)	1:B:773:ASP:N	1:B:773:ASP:CA	1:B:773:ASP:C	1:B:774:LEU:N	11	1.6
(1,154)	1:B:773:ASP:N	1:B:773:ASP:CA	1:B:773:ASP:C	1:B:774:LEU:N	15	1.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,151)	1:B:771:LEU:C	1:B:772:ARG:N	1:B:772:ARG:CA	1:B:772:ARG:C	3	1.6
(1,145)	1:B:763:LEU:C	1:B:764:SER:N	1:B:764:SER:CA	1:B:764:SER:C	12	1.6
(1,144)	1:B:763:LEU:N	1:B:763:LEU:CA	1:B:763:LEU:C	1:B:764:SER:N	6	1.6
(1,136)	1:B:759:ASP:N	1:B:759:ASP:CA	1:B:759:ASP:C	1:B:760:LEU:N	1	1.6
(1,134)	1:B:758:ASP:N	1:B:758:ASP:CA	1:B:758:ASP:C	1:B:759:ASP:N	4	1.6
(1,132)	1:B:757:TRP:N	1:B:757:TRP:CA	1:B:757:TRP:C	1:B:758:ASP:N	12	1.6
(1,131)	1:B:756:ILE:C	1:B:757:TRP:N	1:B:757:TRP:CA	1:B:757:TRP:C	3	1.6
(1,122)	1:B:752:SER:N	1:B:752:SER:CA	1:B:752:SER:C	1:B:753:LEU:N	3	1.6
(1,120)	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	1:B:752:SER:N	12	1.6
(1,113)	1:B:747:ARG:C	1:B:748:LEU:N	1:B:748:LEU:CA	1:B:748:LEU:C	13	1.6
(1,100)	1:B:741:ASP:N	1:B:741:ASP:CA	1:B:741:ASP:C	1:B:742:ARG:N	3	1.6
(1,98)	1:B:740:ARG:N	1:B:740:ARG:CA	1:B:740:ARG:C	1:B:741:ASP:N	15	1.5
(1,87)	1:B:714:PRO:C	1:B:715:LEU:N	1:B:715:LEU:CA	1:B:715:LEU:C	10	1.5
(1,69)	1:B:702:LEU:C	1:B:703:SER:N	1:B:703:SER:CA	1:B:703:SER:C	13	1.5
(1,47)	1:B:691:SER:C	1:B:692:LEU:N	1:B:692:LEU:CA	1:B:692:LEU:C	14	1.5
(1,46)	1:B:691:SER:N	1:B:691:SER:CA	1:B:691:SER:C	1:B:692:LEU:N	2	1.5
(1,271)	1:B:836:ALA:C	1:B:837:SER:N	1:B:837:SER:CA	1:B:837:SER:C	2	1.5
(1,247)	1:B:819:ALA:C	1:B:820:ILE:N	1:B:820:ILE:CA	1:B:820:ILE:C	6	1.5
(1,246)	1:B:819:ALA:N	1:B:819:ALA:CA	1:B:819:ALA:C	1:B:820:ILE:N	13	1.5
(1,242)	1:B:817:ALA:N	1:B:817:ALA:CA	1:B:817:ALA:C	1:B:818:THR:N	12	1.5
(1,206)	1:B:799:LEU:N	1:B:799:LEU:CA	1:B:799:LEU:C	1:B:800:LEU:N	13	1.5
(1,198)	1:B:795:TYR:N	1:B:795:TYR:CA	1:B:795:TYR:C	1:B:796:TRP:N	8	1.5
(1,197)	1:B:794:LYS:C	1:B:795:TYR:N	1:B:795:TYR:CA	1:B:795:TYR:C	11	1.5
(1,197)	1:B:794:LYS:C	1:B:795:TYR:N	1:B:795:TYR:CA	1:B:795:TYR:C	15	1.5
(1,196)	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	1:B:795:TYR:N	11	1.5
(1,195)	1:B:793:LEU:C	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	1	1.5
(1,195)	1:B:793:LEU:C	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	10	1.5
(1,195)	1:B:793:LEU:C	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	11	1.5
(1,195)	1:B:793:LEU:C	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	14	1.5
(1,185)	1:B:788:ARG:C	1:B:789:GLY:N	1:B:789:GLY:CA	1:B:789:GLY:C	3	1.5
(1,184)	1:B:788:ARG:N	1:B:788:ARG:CA	1:B:788:ARG:C	1:B:789:GLY:N	3	1.5
(1,18)	1:B:675:ILE:N	1:B:675:ILE:CA	1:B:675:ILE:C	1:B:676:THR:N	12	1.5
(1,179)	1:B:785:LEU:C	1:B:786:GLY:N	1:B:786:GLY:CA	1:B:786:GLY:C	4	1.5
(1,172)	1:B:782:VAL:N	1:B:782:VAL:CA	1:B:782:VAL:C	1:B:783:GLU:N	10	1.5
(1,162)	1:B:777:ILE:N	1:B:777:ILE:CA	1:B:777:ILE:C	1:B:778:VAL:N	1	1.5
(1,154)	1:B:773:ASP:N	1:B:773:ASP:CA	1:B:773:ASP:C	1:B:774:LEU:N	6	1.5
(1,151)	1:B:771:LEU:C	1:B:772:ARG:N	1:B:772:ARG:CA	1:B:772:ARG:C	1	1.5
(1,150)	1:B:771:LEU:N	1:B:771:LEU:CA	1:B:771:LEU:C	1:B:772:ARG:N	11	1.5
(1,145)	1:B:763:LEU:C	1:B:764:SER:N	1:B:764:SER:CA	1:B:764:SER:C	15	1.5
(1,144)	1:B:763:LEU:N	1:B:763:LEU:CA	1:B:763:LEU:C	1:B:764:SER:N	3	1.5
(1,143)	1:B:762:SER:C	1:B:763:LEU:N	1:B:763:LEU:CA	1:B:763:LEU:C	4	1.5
(1,142)	1:B:762:SER:N	1:B:762:SER:CA	1:B:762:SER:C	1:B:763:LEU:N	5	1.5
(1,135)	1:B:758:ASP:C	1:B:759:ASP:N	1:B:759:ASP:CA	1:B:759:ASP:C	4	1.5
(1,123)	1:B:752:SER:C	1:B:753:LEU:N	1:B:753:LEU:CA	1:B:753:LEU:C	3	1.5
(1,123)	1:B:752:SER:C	1:B:753:LEU:N	1:B:753:LEU:CA	1:B:753:LEU:C	6	1.5
(1,121)	1:B:751:GLY:C	1:B:752:SER:N	1:B:752:SER:CA	1:B:752:SER:C	6	1.5
(1,119)	1:B:750:ASN:C	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	8	1.5
(1,119)	1:B:750:ASN:C	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	14	1.5
(1,113)	1:B:747:ARG:C	1:B:748:LEU:N	1:B:748:LEU:CA	1:B:748:LEU:C	3	1.5
(1,99)	1:B:740:ARG:C	1:B:741:ASP:N	1:B:741:ASP:CA	1:B:741:ASP:C	1	1.4
(1,99)	1:B:740:ARG:C	1:B:741:ASP:N	1:B:741:ASP:CA	1:B:741:ASP:C	12	1.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,98)	1:B:740:ARG:N	1:B:740:ARG:CA	1:B:740:ARG:C	1:B:741:ASP:N	2	1.4
(1,98)	1:B:740:ARG:N	1:B:740:ARG:CA	1:B:740:ARG:C	1:B:741:ASP:N	4	1.4
(1,97)	1:B:739:GLU:C	1:B:740:ARG:N	1:B:740:ARG:CA	1:B:740:ARG:C	14	1.4
(1,88)	1:B:715:LEU:N	1:B:715:LEU:CA	1:B:715:LEU:C	1:B:716:SER:N	3	1.4
(1,87)	1:B:714:PRO:C	1:B:715:LEU:N	1:B:715:LEU:CA	1:B:715:LEU:C	5	1.4
(1,87)	1:B:714:PRO:C	1:B:715:LEU:N	1:B:715:LEU:CA	1:B:715:LEU:C	12	1.4
(1,86)	1:B:713:SER:N	1:B:713:SER:CA	1:B:713:SER:C	1:B:714:PRO:N	4	1.4
(1,84)	1:B:710:GLN:N	1:B:710:GLN:CA	1:B:710:GLN:C	1:B:711:GLY:N	3	1.4
(1,83)	1:B:709:ARG:C	1:B:710:GLN:N	1:B:710:GLN:CA	1:B:710:GLN:C	14	1.4
(1,81)	1:B:708:VAL:C	1:B:709:ARG:N	1:B:709:ARG:CA	1:B:709:ARG:C	3	1.4
(1,69)	1:B:702:LEU:C	1:B:703:SER:N	1:B:703:SER:CA	1:B:703:SER:C	15	1.4
(1,68)	1:B:702:LEU:N	1:B:702:LEU:CA	1:B:702:LEU:C	1:B:703:SER:N	11	1.4
(1,64)	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	1:B:701:VAL:N	10	1.4
(1,64)	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	1:B:701:VAL:N	14	1.4
(1,57)	1:B:696:ARG:C	1:B:697:ILE:N	1:B:697:ILE:CA	1:B:697:ILE:C	5	1.4
(1,56)	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	1:B:697:ILE:N	15	1.4
(1,47)	1:B:691:SER:C	1:B:692:LEU:N	1:B:692:LEU:CA	1:B:692:LEU:C	7	1.4
(1,35)	1:B:685:PHE:C	1:B:686:ILE:N	1:B:686:ILE:CA	1:B:686:ILE:C	10	1.4
(1,274)	1:B:838:ARG:N	1:B:838:ARG:CA	1:B:838:ARG:C	1:B:839:ALA:N	12	1.4
(1,273)	1:B:837:SER:C	1:B:838:ARG:N	1:B:838:ARG:CA	1:B:838:ARG:C	2	1.4
(1,273)	1:B:837:SER:C	1:B:838:ARG:N	1:B:838:ARG:CA	1:B:838:ARG:C	5	1.4
(1,272)	1:B:837:SER:N	1:B:837:SER:CA	1:B:837:SER:C	1:B:838:ARG:N	8	1.4
(1,27)	1:B:681:TYR:C	1:B:682:ILE:N	1:B:682:ILE:CA	1:B:682:ILE:C	10	1.4
(1,251)	1:B:826:THR:C	1:B:827:ASP:N	1:B:827:ASP:CA	1:B:827:ASP:C	2	1.4
(1,243)	1:B:817:ALA:C	1:B:818:THR:N	1:B:818:THR:CA	1:B:818:THR:C	12	1.4
(1,210)	1:B:801:GLN:N	1:B:801:GLN:CA	1:B:801:GLN:C	1:B:802:TYR:N	7	1.4
(1,202)	1:B:797:TRP:N	1:B:797:TRP:CA	1:B:797:TRP:C	1:B:798:ASN:N	3	1.4
(1,197)	1:B:794:LYS:C	1:B:795:TYR:N	1:B:795:TYR:CA	1:B:795:TYR:C	5	1.4
(1,196)	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	1:B:795:TYR:N	14	1.4
(1,195)	1:B:793:LEU:C	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	15	1.4
(1,194)	1:B:793:LEU:N	1:B:793:LEU:CA	1:B:793:LEU:C	1:B:794:LYS:N	13	1.4
(1,192)	1:B:792:ALA:N	1:B:792:ALA:CA	1:B:792:ALA:C	1:B:793:LEU:N	5	1.4
(1,189)	1:B:790:TRP:C	1:B:791:GLU:N	1:B:791:GLU:CA	1:B:791:GLU:C	4	1.4
(1,185)	1:B:788:ARG:C	1:B:789:GLY:N	1:B:789:GLY:CA	1:B:789:GLY:C	10	1.4
(1,168)	1:B:780:ARG:N	1:B:780:ARG:CA	1:B:780:ARG:C	1:B:781:ILE:N	15	1.4
(1,166)	1:B:779:THR:N	1:B:779:THR:CA	1:B:779:THR:C	1:B:780:ARG:N	5	1.4
(1,166)	1:B:779:THR:N	1:B:779:THR:CA	1:B:779:THR:C	1:B:780:ARG:N	13	1.4
(1,163)	1:B:777:ILE:C	1:B:778:VAL:N	1:B:778:VAL:CA	1:B:778:VAL:C	14	1.4
(1,156)	1:B:774:LEU:N	1:B:774:LEU:CA	1:B:774:LEU:C	1:B:775:LEU:N	5	1.4
(1,142)	1:B:762:SER:N	1:B:762:SER:CA	1:B:762:SER:C	1:B:763:LEU:N	4	1.4
(1,135)	1:B:758:ASP:C	1:B:759:ASP:N	1:B:759:ASP:CA	1:B:759:ASP:C	2	1.4
(1,133)	1:B:757:TRP:C	1:B:758:ASP:N	1:B:758:ASP:CA	1:B:758:ASP:C	8	1.4
(1,120)	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	1:B:752:SER:N	4	1.4
(1,111)	1:B:746:ILE:C	1:B:747:ARG:N	1:B:747:ARG:CA	1:B:747:ARG:C	7	1.4
(1,86)	1:B:713:SER:N	1:B:713:SER:CA	1:B:713:SER:C	1:B:714:PRO:N	6	1.3
(1,86)	1:B:713:SER:N	1:B:713:SER:CA	1:B:713:SER:C	1:B:714:PRO:N	15	1.3
(1,84)	1:B:710:GLN:N	1:B:710:GLN:CA	1:B:710:GLN:C	1:B:711:GLY:N	11	1.3
(1,83)	1:B:709:ARG:C	1:B:710:GLN:N	1:B:710:GLN:CA	1:B:710:GLN:C	1	1.3
(1,69)	1:B:702:LEU:C	1:B:703:SER:N	1:B:703:SER:CA	1:B:703:SER:C	5	1.3
(1,69)	1:B:702:LEU:C	1:B:703:SER:N	1:B:703:SER:CA	1:B:703:SER:C	6	1.3
(1,68)	1:B:702:LEU:N	1:B:702:LEU:CA	1:B:702:LEU:C	1:B:703:SER:N	15	1.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,64)	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	1:B:701:VAL:N	1	1.3
(1,57)	1:B:696:ARG:C	1:B:697:ILE:N	1:B:697:ILE:CA	1:B:697:ILE:C	12	1.3
(1,55)	1:B:695:LEU:C	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	12	1.3
(1,47)	1:B:691:SER:C	1:B:692:LEU:N	1:B:692:LEU:CA	1:B:692:LEU:C	13	1.3
(1,46)	1:B:691:SER:N	1:B:691:SER:CA	1:B:691:SER:C	1:B:692:LEU:N	5	1.3
(1,46)	1:B:691:SER:N	1:B:691:SER:CA	1:B:691:SER:C	1:B:692:LEU:N	11	1.3
(1,3)	1:B:664:ASP:C	1:B:665:LYS:N	1:B:665:LYS:CA	1:B:665:LYS:C	14	1.3
(1,274)	1:B:838:ARG:N	1:B:838:ARG:CA	1:B:838:ARG:C	1:B:839:ALA:N	5	1.3
(1,271)	1:B:836:ALA:C	1:B:837:SER:N	1:B:837:SER:CA	1:B:837:SER:C	8	1.3
(1,25)	1:B:678:TRP:C	1:B:679:LEU:N	1:B:679:LEU:CA	1:B:679:LEU:C	10	1.3
(1,242)	1:B:817:ALA:N	1:B:817:ALA:CA	1:B:817:ALA:C	1:B:818:THR:N	4	1.3
(1,225)	1:B:808:LYS:C	1:B:809:ASN:N	1:B:809:ASN:CA	1:B:809:ASN:C	8	1.3
(1,216)	1:B:804:SER:N	1:B:804:SER:CA	1:B:804:SER:C	1:B:805:GLN:N	7	1.3
(1,214)	1:B:803:TRP:N	1:B:803:TRP:CA	1:B:803:TRP:C	1:B:804:SER:N	9	1.3
(1,211)	1:B:801:GLN:C	1:B:802:TYR:N	1:B:802:TYR:CA	1:B:802:TYR:C	7	1.3
(1,206)	1:B:799:LEU:N	1:B:799:LEU:CA	1:B:799:LEU:C	1:B:800:LEU:N	5	1.3
(1,202)	1:B:797:TRP:N	1:B:797:TRP:CA	1:B:797:TRP:C	1:B:798:ASN:N	10	1.3
(1,20)	1:B:676:THR:N	1:B:676:THR:CA	1:B:676:THR:C	1:B:677:ASN:N	7	1.3
(1,196)	1:B:794:LYS:N	1:B:794:LYS:CA	1:B:794:LYS:C	1:B:795:TYR:N	9	1.3
(1,189)	1:B:790:TRP:C	1:B:791:GLU:N	1:B:791:GLU:CA	1:B:791:GLU:C	8	1.3
(1,187)	1:B:789:GLY:C	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	7	1.3
(1,186)	1:B:789:GLY:N	1:B:789:GLY:CA	1:B:789:GLY:C	1:B:790:TRP:N	7	1.3
(1,184)	1:B:788:ARG:N	1:B:788:ARG:CA	1:B:788:ARG:C	1:B:789:GLY:N	10	1.3
(1,179)	1:B:785:LEU:C	1:B:786:GLY:N	1:B:786:GLY:CA	1:B:786:GLY:C	9	1.3
(1,178)	1:B:785:LEU:N	1:B:785:LEU:CA	1:B:785:LEU:C	1:B:786:GLY:N	4	1.3
(1,171)	1:B:781:ILE:C	1:B:782:VAL:N	1:B:782:VAL:CA	1:B:782:VAL:C	3	1.3
(1,166)	1:B:779:THR:N	1:B:779:THR:CA	1:B:779:THR:C	1:B:780:ARG:N	1	1.3
(1,162)	1:B:777:ILE:N	1:B:777:ILE:CA	1:B:777:ILE:C	1:B:778:VAL:N	4	1.3
(1,155)	1:B:773:ASP:C	1:B:774:LEU:N	1:B:774:LEU:CA	1:B:774:LEU:C	11	1.3
(1,155)	1:B:773:ASP:C	1:B:774:LEU:N	1:B:774:LEU:CA	1:B:774:LEU:C	12	1.3
(1,133)	1:B:757:TRP:C	1:B:758:ASP:N	1:B:758:ASP:CA	1:B:758:ASP:C	7	1.3
(1,132)	1:B:757:TRP:N	1:B:757:TRP:CA	1:B:757:TRP:C	1:B:758:ASP:N	13	1.3
(1,128)	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	1:B:756:ILE:N	6	1.3
(1,121)	1:B:751:GLY:C	1:B:752:SER:N	1:B:752:SER:CA	1:B:752:SER:C	12	1.3
(1,120)	1:B:751:GLY:N	1:B:751:GLY:CA	1:B:751:GLY:C	1:B:752:SER:N	14	1.3
(1,1)	1:B:663:LEU:C	1:B:664:ASP:N	1:B:664:ASP:CA	1:B:664:ASP:C	10	1.3
(1,99)	1:B:740:ARG:C	1:B:741:ASP:N	1:B:741:ASP:CA	1:B:741:ASP:C	2	1.2
(1,99)	1:B:740:ARG:C	1:B:741:ASP:N	1:B:741:ASP:CA	1:B:741:ASP:C	15	1.2
(1,87)	1:B:714:PRO:C	1:B:715:LEU:N	1:B:715:LEU:CA	1:B:715:LEU:C	6	1.2
(1,86)	1:B:713:SER:N	1:B:713:SER:CA	1:B:713:SER:C	1:B:714:PRO:N	3	1.2
(1,86)	1:B:713:SER:N	1:B:713:SER:CA	1:B:713:SER:C	1:B:714:PRO:N	8	1.2
(1,83)	1:B:709:ARG:C	1:B:710:GLN:N	1:B:710:GLN:CA	1:B:710:GLN:C	15	1.2
(1,79)	1:B:707:ARG:C	1:B:708:VAL:N	1:B:708:VAL:CA	1:B:708:VAL:C	3	1.2
(1,72)	1:B:704:LEU:N	1:B:704:LEU:CA	1:B:704:LEU:C	1:B:705:VAL:N	10	1.2
(1,69)	1:B:702:LEU:C	1:B:703:SER:N	1:B:703:SER:CA	1:B:703:SER:C	8	1.2
(1,68)	1:B:702:LEU:N	1:B:702:LEU:CA	1:B:702:LEU:C	1:B:703:SER:N	8	1.2
(1,68)	1:B:702:LEU:N	1:B:702:LEU:CA	1:B:702:LEU:C	1:B:703:SER:N	14	1.2
(1,64)	1:B:700:ALA:N	1:B:700:ALA:CA	1:B:700:ALA:C	1:B:701:VAL:N	12	1.2
(1,61)	1:B:698:VAL:C	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	9	1.2
(1,56)	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	1:B:697:ILE:N	7	1.2
(1,54)	1:B:695:LEU:N	1:B:695:LEU:CA	1:B:695:LEU:C	1:B:696:ARG:N	5	1.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,46)	1:B:691:SER:N	1:B:691:SER:CA	1:B:691:SER:C	1:B:692:LEU:N	3	1.2
(1,35)	1:B:685:PHE:C	1:B:686:ILE:N	1:B:686:ILE:CA	1:B:686:ILE:C	15	1.2
(1,274)	1:B:838:ARG:N	1:B:838:ARG:CA	1:B:838:ARG:C	1:B:839:ALA:N	4	1.2
(1,274)	1:B:838:ARG:N	1:B:838:ARG:CA	1:B:838:ARG:C	1:B:839:ALA:N	8	1.2
(1,270)	1:B:836:ALA:N	1:B:836:ALA:CA	1:B:836:ALA:C	1:B:837:SER:N	8	1.2
(1,251)	1:B:826:THR:C	1:B:827:ASP:N	1:B:827:ASP:CA	1:B:827:ASP:C	9	1.2
(1,251)	1:B:826:THR:C	1:B:827:ASP:N	1:B:827:ASP:CA	1:B:827:ASP:C	11	1.2
(1,250)	1:B:826:THR:N	1:B:826:THR:CA	1:B:826:THR:C	1:B:827:ASP:N	15	1.2
(1,23)	1:B:677:ASN:C	1:B:678:TRP:N	1:B:678:TRP:CA	1:B:678:TRP:C	4	1.2
(1,225)	1:B:808:LYS:C	1:B:809:ASN:N	1:B:809:ASN:CA	1:B:809:ASN:C	11	1.2
(1,206)	1:B:799:LEU:N	1:B:799:LEU:CA	1:B:799:LEU:C	1:B:800:LEU:N	7	1.2
(1,203)	1:B:797:TRP:C	1:B:798:ASN:N	1:B:798:ASN:CA	1:B:798:ASN:C	9	1.2
(1,2)	1:B:664:ASP:N	1:B:664:ASP:CA	1:B:664:ASP:C	1:B:665:LYS:N	14	1.2
(1,197)	1:B:794:LYS:C	1:B:795:TYR:N	1:B:795:TYR:CA	1:B:795:TYR:C	13	1.2
(1,194)	1:B:793:LEU:N	1:B:793:LEU:CA	1:B:793:LEU:C	1:B:794:LYS:N	11	1.2
(1,192)	1:B:792:ALA:N	1:B:792:ALA:CA	1:B:792:ALA:C	1:B:793:LEU:N	11	1.2
(1,186)	1:B:789:GLY:N	1:B:789:GLY:CA	1:B:789:GLY:C	1:B:790:TRP:N	3	1.2
(1,186)	1:B:789:GLY:N	1:B:789:GLY:CA	1:B:789:GLY:C	1:B:790:TRP:N	11	1.2
(1,185)	1:B:788:ARG:C	1:B:789:GLY:N	1:B:789:GLY:CA	1:B:789:GLY:C	5	1.2
(1,175)	1:B:783:GLU:C	1:B:784:LEU:N	1:B:784:LEU:CA	1:B:784:LEU:C	15	1.2
(1,172)	1:B:782:VAL:N	1:B:782:VAL:CA	1:B:782:VAL:C	1:B:783:GLU:N	15	1.2
(1,170)	1:B:781:ILE:N	1:B:781:ILE:CA	1:B:781:ILE:C	1:B:782:VAL:N	14	1.2
(1,168)	1:B:780:ARG:N	1:B:780:ARG:CA	1:B:780:ARG:C	1:B:781:ILE:N	11	1.2
(1,163)	1:B:777:ILE:C	1:B:778:VAL:N	1:B:778:VAL:CA	1:B:778:VAL:C	5	1.2
(1,159)	1:B:775:LEU:C	1:B:776:LEU:N	1:B:776:LEU:CA	1:B:776:LEU:C	10	1.2
(1,158)	1:B:775:LEU:N	1:B:775:LEU:CA	1:B:775:LEU:C	1:B:776:LEU:N	9	1.2
(1,156)	1:B:774:LEU:N	1:B:774:LEU:CA	1:B:774:LEU:C	1:B:775:LEU:N	13	1.2
(1,145)	1:B:763:LEU:C	1:B:764:SER:N	1:B:764:SER:CA	1:B:764:SER:C	4	1.2
(1,143)	1:B:762:SER:C	1:B:763:LEU:N	1:B:763:LEU:CA	1:B:763:LEU:C	5	1.2
(1,141)	1:B:761:ARG:C	1:B:762:SER:N	1:B:762:SER:CA	1:B:762:SER:C	12	1.2
(1,138)	1:B:760:LEU:N	1:B:760:LEU:CA	1:B:760:LEU:C	1:B:761:ARG:N	13	1.2
(1,137)	1:B:759:ASP:C	1:B:760:LEU:N	1:B:760:LEU:CA	1:B:760:LEU:C	2	1.2
(1,137)	1:B:759:ASP:C	1:B:760:LEU:N	1:B:760:LEU:CA	1:B:760:LEU:C	12	1.2
(1,135)	1:B:758:ASP:C	1:B:759:ASP:N	1:B:759:ASP:CA	1:B:759:ASP:C	8	1.2
(1,134)	1:B:758:ASP:N	1:B:758:ASP:CA	1:B:758:ASP:C	1:B:759:ASP:N	2	1.2
(1,132)	1:B:757:TRP:N	1:B:757:TRP:CA	1:B:757:TRP:C	1:B:758:ASP:N	15	1.2
(1,131)	1:B:756:ILE:C	1:B:757:TRP:N	1:B:757:TRP:CA	1:B:757:TRP:C	15	1.2
(1,118)	1:B:750:ASN:N	1:B:750:ASN:CA	1:B:750:ASN:C	1:B:751:GLY:N	9	1.2
(1,118)	1:B:750:ASN:N	1:B:750:ASN:CA	1:B:750:ASN:C	1:B:751:GLY:N	10	1.2
(1,118)	1:B:750:ASN:N	1:B:750:ASN:CA	1:B:750:ASN:C	1:B:751:GLY:N	14	1.2
(1,98)	1:B:740:ARG:N	1:B:740:ARG:CA	1:B:740:ARG:C	1:B:741:ASP:N	10	1.1
(1,87)	1:B:714:PRO:C	1:B:715:LEU:N	1:B:715:LEU:CA	1:B:715:LEU:C	11	1.1
(1,86)	1:B:713:SER:N	1:B:713:SER:CA	1:B:713:SER:C	1:B:714:PRO:N	2	1.1
(1,85)	1:B:712:TYR:C	1:B:713:SER:N	1:B:713:SER:CA	1:B:713:SER:C	9	1.1
(1,83)	1:B:709:ARG:C	1:B:710:GLN:N	1:B:710:GLN:CA	1:B:710:GLN:C	2	1.1
(1,83)	1:B:709:ARG:C	1:B:710:GLN:N	1:B:710:GLN:CA	1:B:710:GLN:C	10	1.1
(1,81)	1:B:708:VAL:C	1:B:709:ARG:N	1:B:709:ARG:CA	1:B:709:ARG:C	9	1.1
(1,80)	1:B:708:VAL:N	1:B:708:VAL:CA	1:B:708:VAL:C	1:B:709:ARG:N	14	1.1
(1,76)	1:B:706:ASN:N	1:B:706:ASN:CA	1:B:706:ASN:C	1:B:707:ARG:N	5	1.1
(1,69)	1:B:702:LEU:C	1:B:703:SER:N	1:B:703:SER:CA	1:B:703:SER:C	2	1.1
(1,68)	1:B:702:LEU:N	1:B:702:LEU:CA	1:B:702:LEU:C	1:B:703:SER:N	4	1.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,61)	1:B:698:VAL:C	1:B:699:PHE:N	1:B:699:PHE:CA	1:B:699:PHE:C	1	1.1
(1,57)	1:B:696:ARG:C	1:B:697:ILE:N	1:B:697:ILE:CA	1:B:697:ILE:C	10	1.1
(1,56)	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	1:B:697:ILE:N	8	1.1
(1,55)	1:B:695:LEU:C	1:B:696:ARG:N	1:B:696:ARG:CA	1:B:696:ARG:C	5	1.1
(1,54)	1:B:695:LEU:N	1:B:695:LEU:CA	1:B:695:LEU:C	1:B:696:ARG:N	15	1.1
(1,50)	1:B:693:ILE:N	1:B:693:ILE:CA	1:B:693:ILE:C	1:B:694:GLY:N	10	1.1
(1,47)	1:B:691:SER:C	1:B:692:LEU:N	1:B:692:LEU:CA	1:B:692:LEU:C	2	1.1
(1,47)	1:B:691:SER:C	1:B:692:LEU:N	1:B:692:LEU:CA	1:B:692:LEU:C	4	1.1
(1,47)	1:B:691:SER:C	1:B:692:LEU:N	1:B:692:LEU:CA	1:B:692:LEU:C	5	1.1
(1,46)	1:B:691:SER:N	1:B:691:SER:CA	1:B:691:SER:C	1:B:692:LEU:N	4	1.1
(1,273)	1:B:837:SER:C	1:B:838:ARG:N	1:B:838:ARG:CA	1:B:838:ARG:C	1	1.1
(1,273)	1:B:837:SER:C	1:B:838:ARG:N	1:B:838:ARG:CA	1:B:838:ARG:C	4	1.1
(1,250)	1:B:826:THR:N	1:B:826:THR:CA	1:B:826:THR:C	1:B:827:ASP:N	9	1.1
(1,248)	1:B:820:ILE:N	1:B:820:ILE:CA	1:B:820:ILE:C	1:B:821:ALA:N	2	1.1
(1,223)	1:B:807:LEU:C	1:B:808:LYS:N	1:B:808:LYS:CA	1:B:808:LYS:C	4	1.1
(1,22)	1:B:677:ASN:N	1:B:677:ASN:CA	1:B:677:ASN:C	1:B:678:TRP:N	2	1.1
(1,22)	1:B:677:ASN:N	1:B:677:ASN:CA	1:B:677:ASN:C	1:B:678:TRP:N	9	1.1
(1,211)	1:B:801:GLN:C	1:B:802:TYR:N	1:B:802:TYR:CA	1:B:802:TYR:C	5	1.1
(1,208)	1:B:800:LEU:N	1:B:800:LEU:CA	1:B:800:LEU:C	1:B:801:GLN:N	11	1.1
(1,20)	1:B:676:THR:N	1:B:676:THR:CA	1:B:676:THR:C	1:B:677:ASN:N	12	1.1
(1,197)	1:B:794:LYS:C	1:B:795:TYR:N	1:B:795:TYR:CA	1:B:795:TYR:C	1	1.1
(1,197)	1:B:794:LYS:C	1:B:795:TYR:N	1:B:795:TYR:CA	1:B:795:TYR:C	9	1.1
(1,194)	1:B:793:LEU:N	1:B:793:LEU:CA	1:B:793:LEU:C	1:B:794:LYS:N	9	1.1
(1,192)	1:B:792:ALA:N	1:B:792:ALA:CA	1:B:792:ALA:C	1:B:793:LEU:N	13	1.1
(1,189)	1:B:790:TRP:C	1:B:791:GLU:N	1:B:791:GLU:CA	1:B:791:GLU:C	14	1.1
(1,189)	1:B:790:TRP:C	1:B:791:GLU:N	1:B:791:GLU:CA	1:B:791:GLU:C	15	1.1
(1,187)	1:B:789:GLY:C	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	11	1.1
(1,187)	1:B:789:GLY:C	1:B:790:TRP:N	1:B:790:TRP:CA	1:B:790:TRP:C	12	1.1
(1,186)	1:B:789:GLY:N	1:B:789:GLY:CA	1:B:789:GLY:C	1:B:790:TRP:N	4	1.1
(1,186)	1:B:789:GLY:N	1:B:789:GLY:CA	1:B:789:GLY:C	1:B:790:TRP:N	12	1.1
(1,185)	1:B:788:ARG:C	1:B:789:GLY:N	1:B:789:GLY:CA	1:B:789:GLY:C	9	1.1
(1,18)	1:B:675:ILE:N	1:B:675:ILE:CA	1:B:675:ILE:C	1:B:676:THR:N	3	1.1
(1,179)	1:B:785:LEU:C	1:B:786:GLY:N	1:B:786:GLY:CA	1:B:786:GLY:C	3	1.1
(1,179)	1:B:785:LEU:C	1:B:786:GLY:N	1:B:786:GLY:CA	1:B:786:GLY:C	10	1.1
(1,174)	1:B:783:GLU:N	1:B:783:GLU:CA	1:B:783:GLU:C	1:B:784:LEU:N	15	1.1
(1,165)	1:B:778:VAL:C	1:B:779:THR:N	1:B:779:THR:CA	1:B:779:THR:C	13	1.1
(1,162)	1:B:777:ILE:N	1:B:777:ILE:CA	1:B:777:ILE:C	1:B:778:VAL:N	6	1.1
(1,162)	1:B:777:ILE:N	1:B:777:ILE:CA	1:B:777:ILE:C	1:B:778:VAL:N	13	1.1
(1,158)	1:B:775:LEU:N	1:B:775:LEU:CA	1:B:775:LEU:C	1:B:776:LEU:N	2	1.1
(1,158)	1:B:775:LEU:N	1:B:775:LEU:CA	1:B:775:LEU:C	1:B:776:LEU:N	3	1.1
(1,156)	1:B:774:LEU:N	1:B:774:LEU:CA	1:B:774:LEU:C	1:B:775:LEU:N	8	1.1
(1,155)	1:B:773:ASP:C	1:B:774:LEU:N	1:B:774:LEU:CA	1:B:774:LEU:C	5	1.1
(1,154)	1:B:773:ASP:N	1:B:773:ASP:CA	1:B:773:ASP:C	1:B:774:LEU:N	1	1.1
(1,153)	1:B:772:ARG:C	1:B:773:ASP:N	1:B:773:ASP:CA	1:B:773:ASP:C	9	1.1
(1,144)	1:B:763:LEU:N	1:B:763:LEU:CA	1:B:763:LEU:C	1:B:764:SER:N	9	1.1
(1,141)	1:B:761:ARG:C	1:B:762:SER:N	1:B:762:SER:CA	1:B:762:SER:C	11	1.1
(1,130)	1:B:756:ILE:N	1:B:756:ILE:CA	1:B:756:ILE:C	1:B:757:TRP:N	2	1.1
(1,127)	1:B:754:ALA:C	1:B:755:LEU:N	1:B:755:LEU:CA	1:B:755:LEU:C	6	1.1
(1,123)	1:B:752:SER:C	1:B:753:LEU:N	1:B:753:LEU:CA	1:B:753:LEU:C	10	1.1
(1,116)	1:B:749:VAL:N	1:B:749:VAL:CA	1:B:749:VAL:C	1:B:750:ASN:N	2	1.1
(1,111)	1:B:746:ILE:C	1:B:747:ARG:N	1:B:747:ARG:CA	1:B:747:ARG:C	6	1.1